Agilent 7200 Q-TOF for GC/MS

ACHIEVE MAXIMUM QUALITATIVE AND QUANTITATIVE POWER FOR CHALLENGING APPLICATIONS

The Measure of Confidence

Agilent Technologies

Maximize detection selectivity and confidently analyze both targets and unknowns

Complex matrices and trace-level analyses demand your best qualitative and quantitative data. Now, a new technology helps you find the answers you seek.

Agilent 7200 Q-TOF for GC/MS: Achieve high resolution, accurate mass, full-spectrum sensitivity, and MS/MS selectivity for your toughest analysis

Agilent's 7200 Q-TOF for GC/MS is the world's first Q-TOF designed specifically for gas chromatography. It redraws the boundaries of GC/MS technology by combining the separation power of Agilent's 7890 Series GC with application-tested MS components from our 7000 Triple Quadrupole GC/MS and 6500 LC/Q-TOF systems. The results: robust GC/MS operation, outstanding selectivity, full spectrum acquisition with high sensitivity, fast data rates, and accurate mass information to simplify molecular characterization and structural confirmation.

The world's first Q-TOF for GC/MS combines the proven separation power of Agilent's 7890 GC with the high detection selectivity and accurate mass information of a TOF analyzer.

Your first choice for exceptional qualitative *and* quantitative analysis

The Agilent 7200 Q-TOF for GC/MS combines the sought-after features of our flagship GC/MS systems with the following advanced capabilities:

High resolution and mass accuracy

Low-ppm mass accuracy – combined with 15x to 50x greater resolution than a single quadrupole MS – gives you the power to analyze target, non-target, and unknown compounds with much greater reliability.

Low detection limits and excellent linearity

A full-spectrum with sensitivity greater than that of quadrupole MS lets you capture accurate mass spectra at low pg on-column for most compounds. Dual gain mode expands this range to 10^5.

Unparalleled MS/MS selectivity

The detection selectivity of high-resolution MS/MS dramatically surpasses other MS/MS analyzers. Moreover, accurate mass product ion spectra help confirm targets and non-targets as well as elucidate unknown compounds.

Simplify your analysis of accurate mass MS and MS/MS files

Agilent MassHunter software provides valuable tools for identification, quantitation, and confirmation.

- Find compounds in complex samples by applying deconvolution optimized for EI or CI data.
- The combination of library search results and calculated formulas for molecular and fragment ions simplifies compound identification.
- Perform multivariate statistical analysis on several data files using Mass Profiler Professional – a mass spectrometry-centric program.

Accurate mass information lets you qualitatively and quantitatively recognize compounds with maximum confidence.

Time-tested design with leading-edge enhancements

Full 7890 GC capabilities

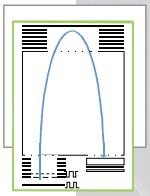
Includes multimode inlet, high-performance backflush, and fast, low-thermal mass column technology.

High-sensitivity extractor ion source

Programmable up to 350 °C for robust compatibility with complex matrices.

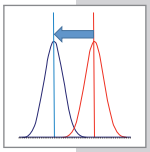
Hot quartz monolithic hyperbolic quadrupole

Can be heated to 200 °C – without resolution or sensitivity loss – to eliminate contamination from high-temperature GC peaks.



Stable, high-performance TOF technology

Agilent's orthogonal TOF technologies deliver consistent performance for thousands of LC/TOF and LC/Q-TOF systems.



Internal reference mass (IRM) correction

When necessary, an IRM compound can be introduced into the source for maximum mass accuracy.

Removable ion source

Computer control of both the transfer line and vacuum interlock position ensure trouble-free ion source replacement in about 30 minutes.

To learn more about the capabilities of the Agilent 7200 Q-TOF for GC/MS, visit **www.agilent.com/chem/GCMS_QTOF**

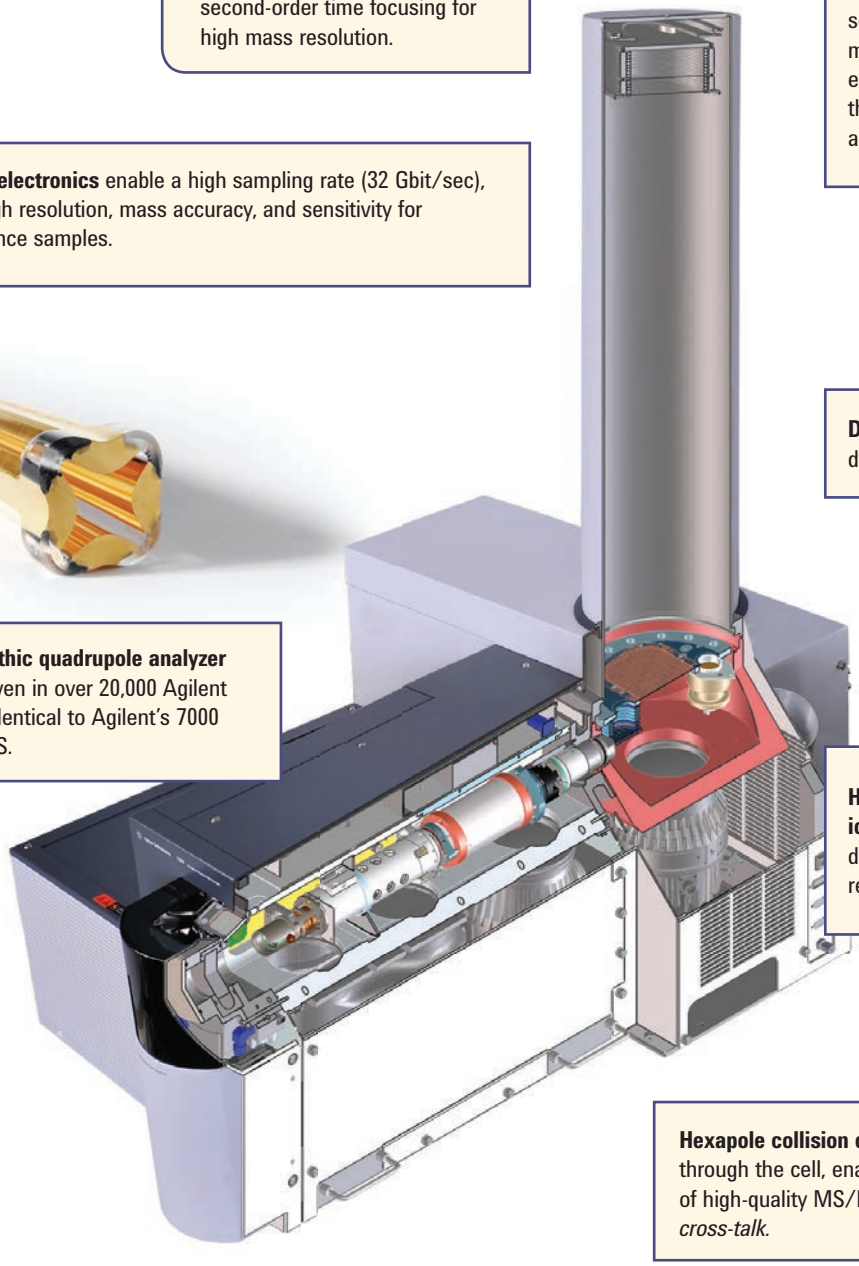
Agilent's 7200 Q-TOF for GC/MS system combines proven technologies with new – and unique – features

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

Proprietary INVAR flight tube, sealed in a vacuum-insulated shell, maintains 24/7 mass accuracy by eliminating temperature-related thermal mass drift. Its longer length also improves mass resolution.

4 GHz ADC electronics enable a high sampling rate (32 Gbit/sec), ensuring high resolution, mass accuracy, and sensitivity for low-abundance samples.

Dual gain amplifiers expand the dynamic range up to 10^5.



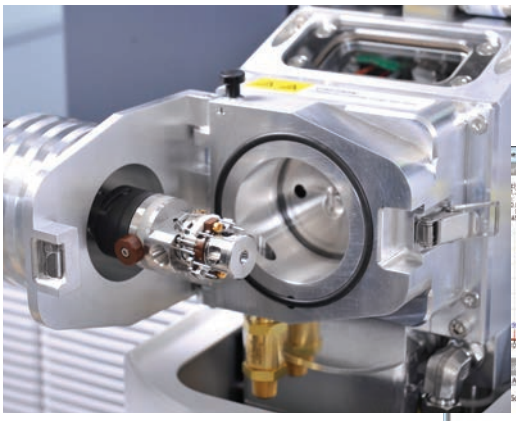
Hot, quartz, monolithic quadrupole analyzer is performance-proven in over 20,000 Agilent MS systems, and identical to Agilent's 7000 Quadrupole MS/MS.

Hybrid channel plate photomultiplier ion detector delivers single ion detection sensitivity, excellent time resolution, and a large linear range.

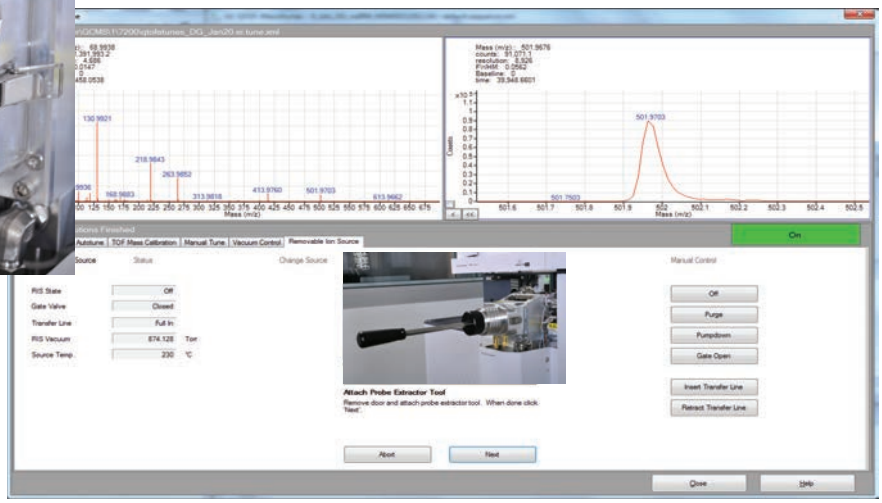
Hexapole collision cell accelerates ions through the cell, enabling faster generation of high-quality MS/MS spectra *without cross-talk.*

Three turbomolecular pumps, including two single-stage pumps and one split-flow pump for the source and quadrupole analyzer, create an optimal vacuum for every region of the analyzer assembly.

Excellent linearity and mass accuracy enable analysis of targets, non-targets, and unknowns



NEW removable ion source (RIS) *lets you change the complete ion source – including repeller, ion volume, extraction lens, and dual filaments – in about 30 minutes without venting.*

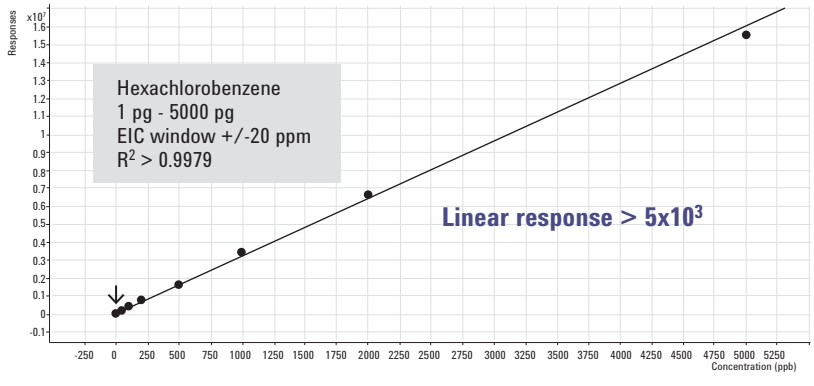


User-friendly videos and software *guide you through all the necessary steps for source removal and installation – making the process safe and error free.*

pg on-column	mass error, ppm	
	2-formyl thiophene	2-acetyl thiazole
1	-3.57	-0.79
2	-4.46	-0.79
5	-2.68	-0.79
10	-2.68	0.79
20	-2.68	0.00
50	-0.89	1.57
100	0.00	1.57
200	-1.79	1.57
500	2.68	1.57
1000	1.79	-1.57
Average	-1.43	0.31

New Internal Reference Mass (IRM) *is a proprietary system that locks the mass axis for each scan to a calibrant compound. IRM ensures low-ppm mass accuracy under the most complex chromatographic conditions.*

Analog-to-digital (ADC) Detector: *The 4 GHz sampling rate of ADC electronics enables exceptional linearity in high-resolution mode. For an even wider linear range, dual-gain amplifiers simultaneously process detector signals through both low-gain and high-gain channels, extending the dynamic range up to 10^5.*



To learn more about the capabilities of the Agilent 7200 Q-TOF for GC/MS, visit **www.agilent.com/chem/GCMS_QTOF**

Results *prove* how GC/Q-TOF technology makes exceptional qualitative and quantitative analysis *real* – and *easy*

With its low-ppm mass accuracy and high resolving power, Agilent's 7200 Q-TOF for GC/MS can help you reduce uncertainty, minimize false positives, confirm database search results, and generate molecular formulas for unknowns.

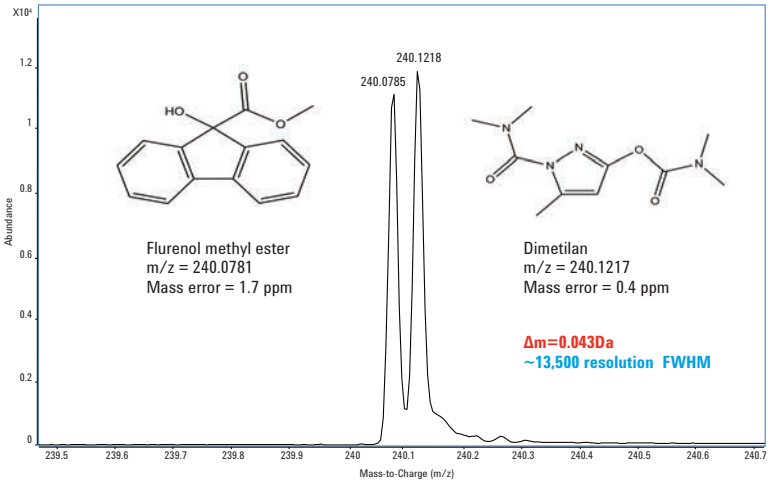
Fast, trouble-free setup

Our automated acquisition software guides you through each step of the tuning and mass calibration process for precise high resolution and accurate mass operation.

Superior resolving power is essential for confident analyte identification

Resolution of 13,500 (FWHM) easily resolves two compounds with nominal masses of 240 Da, whose exact masses differ by only 0.0436 Da.

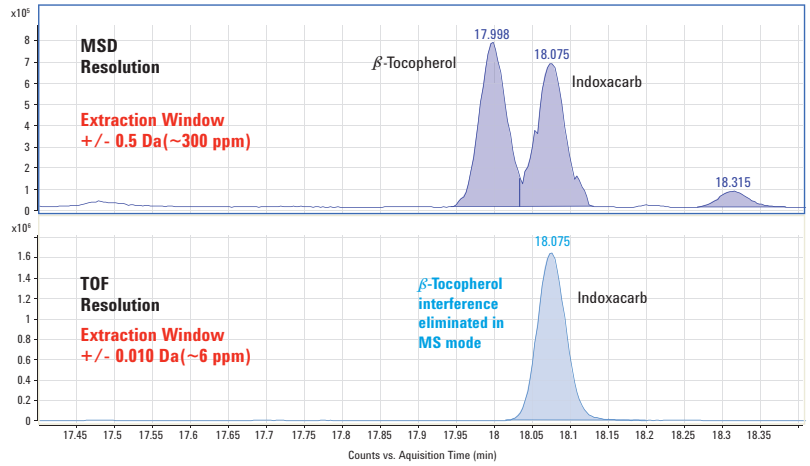
Superior resolving power is indispensable in confidently identifying analytes in complex matrices.



Accurate mass allows for efficient elimination of matrix interferences

Using an extraction window of 0.010 Da, the fragment ion of the target analyte, Indoxacarb (150.01195 Da), can easily be separated from the matrix interference ion of β-Tocopherol (150.06839 Da). This facilitates reliable quantitative analysis.

When more selectivity is needed, MS/MS with accurate mass can help separate target analytes and matrix interferences further.

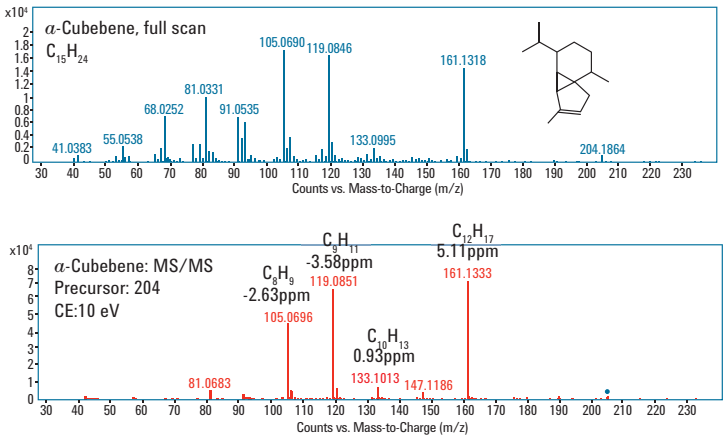


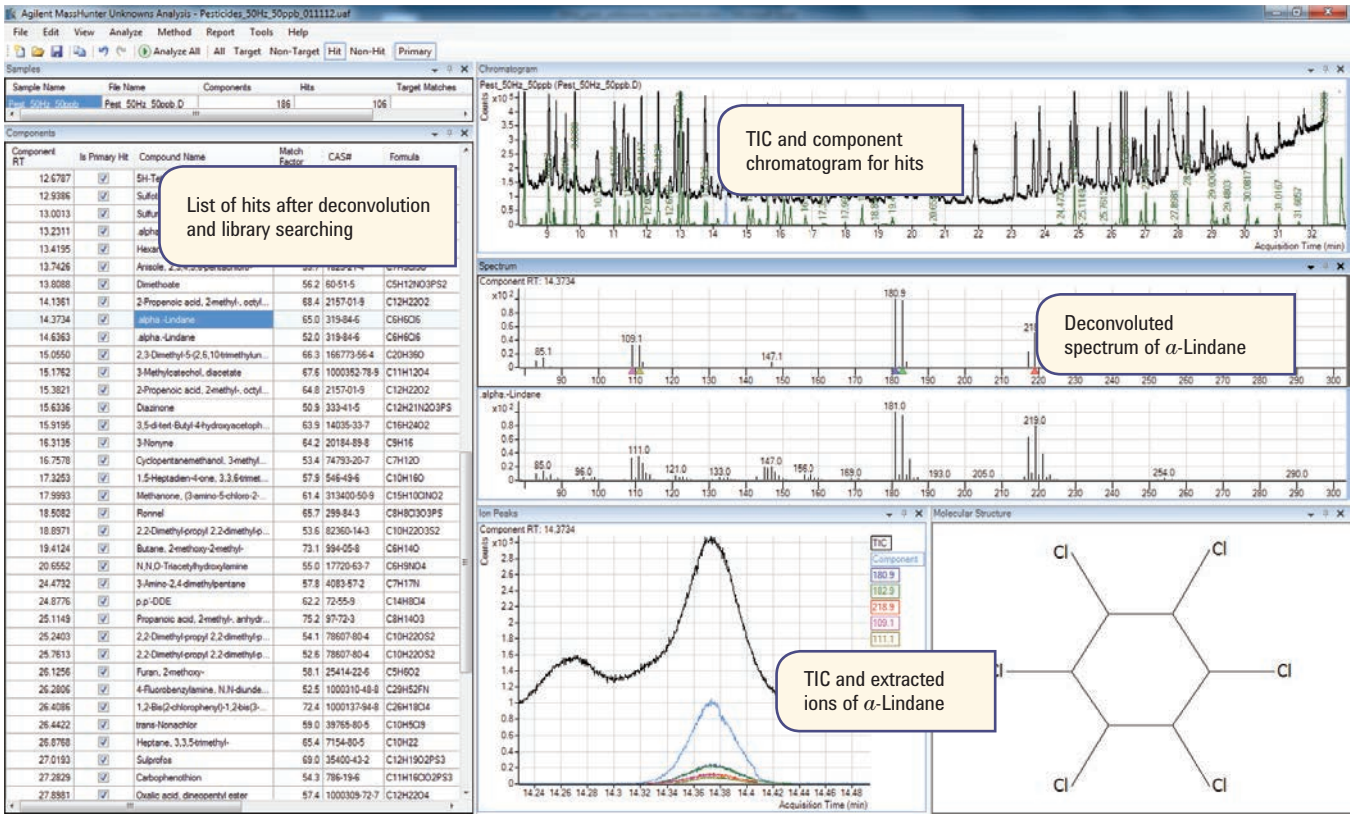
Unambiguous structural clarification and target confirmation

The identity of target and unknown compounds can be confirmed using a variety of techniques.

- Conducting an EI spectra library search
- Determining the PCI molecular ion
- Performing MS/MS dissociation of multiple precursor ions to document fragmentation pathways – *an Agilent exclusive*
- Calculating molecular formulas for all ions from accurate mass data

For very complex separations, such as the α-Cubebene example at right, MS/MS selectivity also generates a simplified spectrum to facilitate structure elucidation.





High-speed spectral acquisition is another fundamental advantage of TOF MS. *Rates as fast as 50 Hz allow you to efficiently resolve a substantial number of components by chromatographic deconvolution with MassHunter's Unknowns Analysis tool.*

To learn more about the capabilities of the Agilent 7200 Q-TOF for GC/MS, visit **www.agilent.com/chem/GCMS_QTOF**

Analyze and visualize changes in cellular function

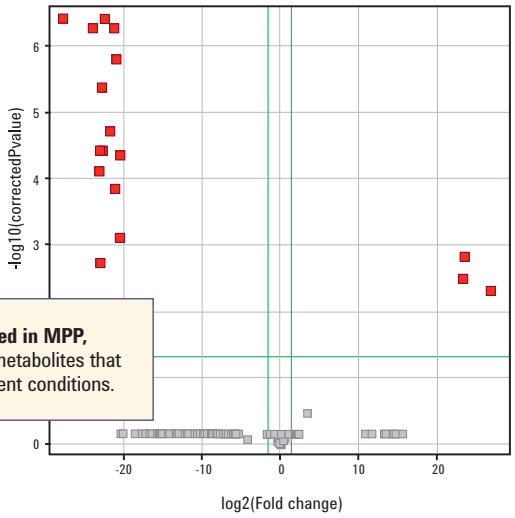
Metabolomics is a powerful tool in understanding metabolic changes under distinct conditions. Complex metabolomic studies will take advantage of high full spectrum sensitivity and mass accuracy of GC/Q-TOF, as well as its MS/MS capability to assist in structural elucidation of unknown metabolites. The extended dynamic range of the 7200 GC/Q-TOF will allow for accurate and simultaneous quantification of a broad range of metabolites present in a cell.

In one simple experiment, Agilent's 7200 Q-TOF for GC/MS provided the accurate mass information, excellent sensitivity in full scan mode, and dynamic range essential for identifying and quantifying all pathway intermediates of interest, thus unambiguously revealing the step in the biochemical pathway affected in a treated sample.

Mass Profiler Professional (MPP) was used for statistical data evaluation. The analysis included data filtering, baseline correction, and significance testing. The software's visualization tools were also indispensable for data interpretation.

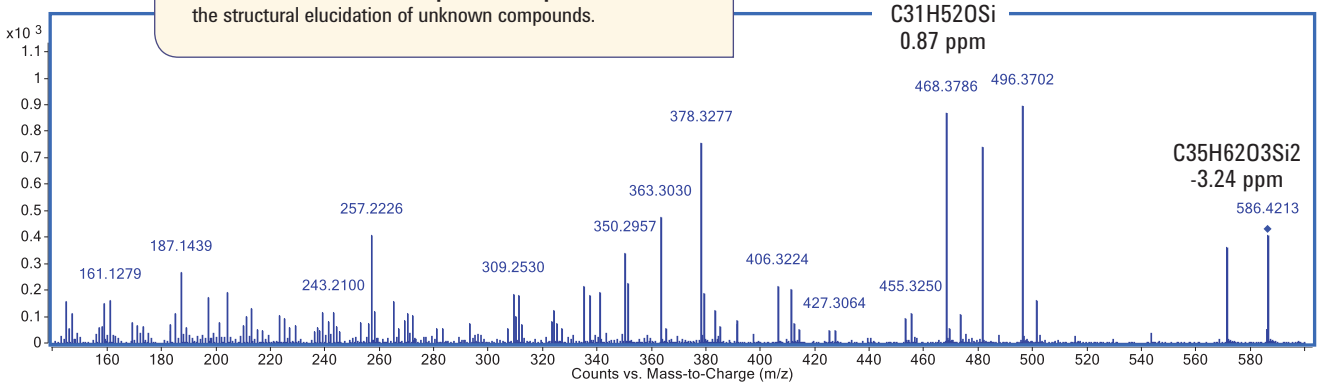
Metabolites significantly changed in treated sample	Fold change in treated sample
Squalene	2.5 (down)
Lanosterol	1.7 (up)
4,4-dimethyl-5α-cholesta-8,24-dien-3β-ol	1.4 (up)
4α-carboxy-4β-methyl-5α-cholesta-8,24-dien-3β-ol	**360.8 (up)**
Zymosterol	2.9 (down)
Ergosterol	1.3 (down)

Ergosterol biosynthesis pathway



Significance analysis, performed in MPP, facilitates the identification of metabolites that change their levels under different conditions.

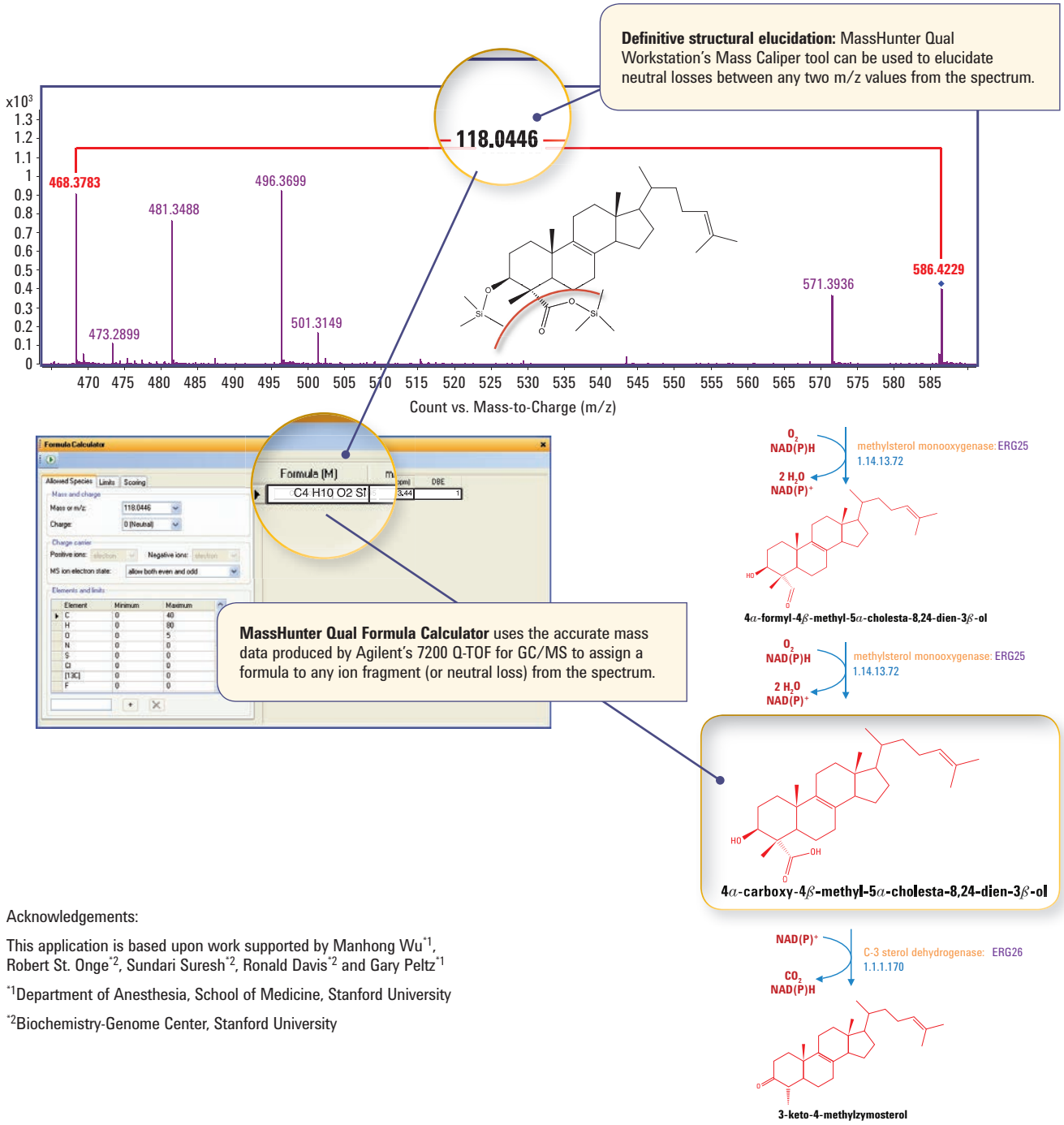
MS/MS with accurate mass product ion spectrum facilitates the structural elucidation of unknown compounds.



Confirm the proposed structure of a metabolite based on accurate mass product ion spectrum

Metabolomic studies often recognize a significant number of non-targets and unknown metabolites as potentially playing a critical role in biological interpretation of the data. Therefore, the structure of these important metabolites has to be confirmed or elucidated.

The pairing of Agilent's 7200 Q-TOF for GC/MS with MassHunter Workstation software is ideal for this type of study.



Acknowledgements:

This application is based upon work supported by Manhong Wu[*1], Robert St. Onge[*2], Sundari Suresh[*2], Ronald Davis[*2] and Gary Peltz[*1]

[*1]Department of Anesthesia, School of Medicine, Stanford University

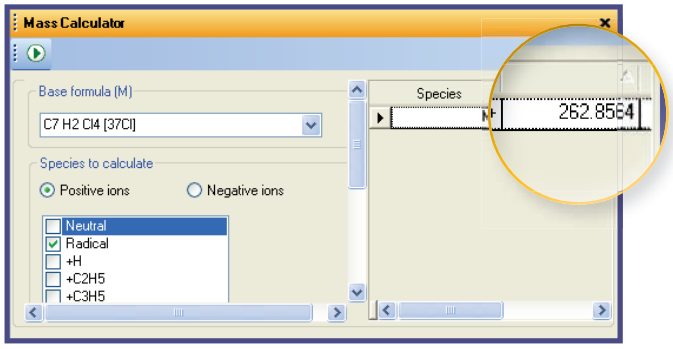
[*2]Biochemistry-Genome Center, Stanford University

To learn more about the capabilities of the Agilent 7200 Q-TOF for GC/MS, visit **www.agilent.com/chem/GCMS_QTOF**

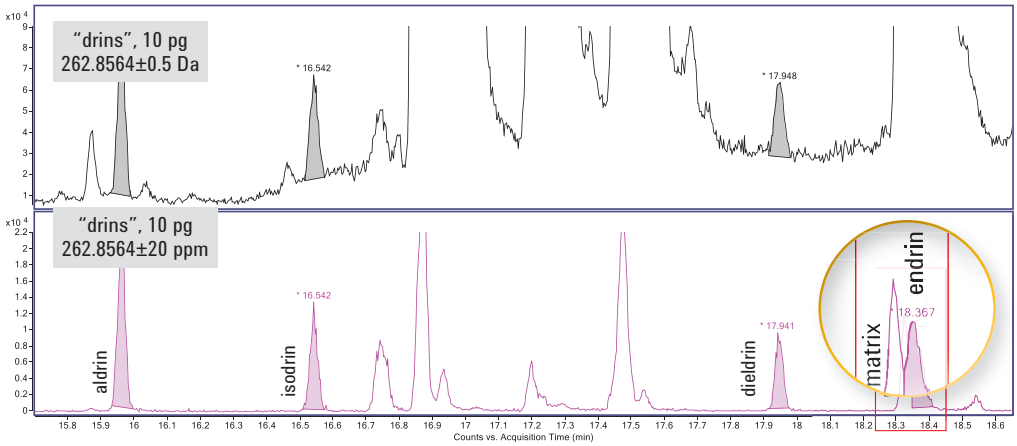
Perform confident screening and identification of contaminants in challenging matrices

Comprehensive food safety screening involves both the quantitative analysis of frequently occurring contaminants and the qualitative analysis of non-target compounds and unknowns.

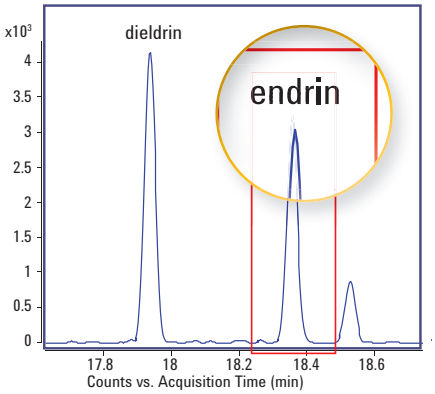
Success often depends upon high sensitivity in full scan mode as well as accurate mass information for target confirmation or unknowns analysis.



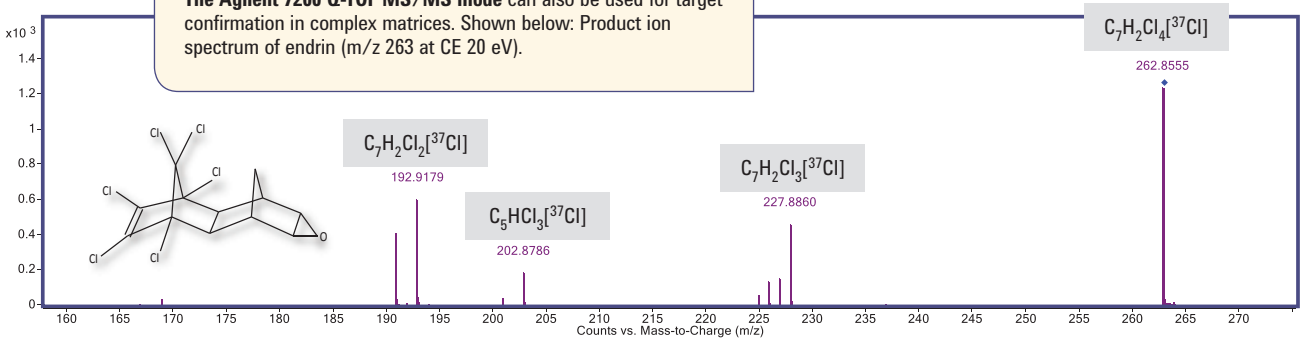
MassHunter Qual Mass Calculator is used to obtain the theoretical masses of the target compounds in both EI and CI modes. Theoretical mass can be used for further qualitative evaluation and quantitative analysis.



Ultimate selectivity in MS/MS mode: Agilent 7200 Q-TOF for GC/MS easily resolves targets from coeluting matrix interferences when high resolution/accurate mass alone is not enough.



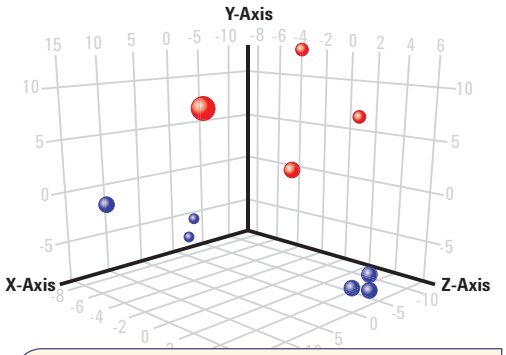
The Agilent 7200 Q-TOF MS/MS mode can also be used for target confirmation in complex matrices. Shown below: Product ion spectrum of endrin (m/z 263 at CE 20 eV).



Evaluation of extra virgin olive oil

To construct a GC/Q-TOF data-based model that could predict whether an olive oil would pass the extra virgin sensory test, Mass Profiler Professional (MPP) software was used. The model utilized five specific compounds to predict the sensory test's outcome.

In addition to the EI spectral data, positive CI accurate mass spectra were necessary to confirm a molecular ion for the compounds used in the model.

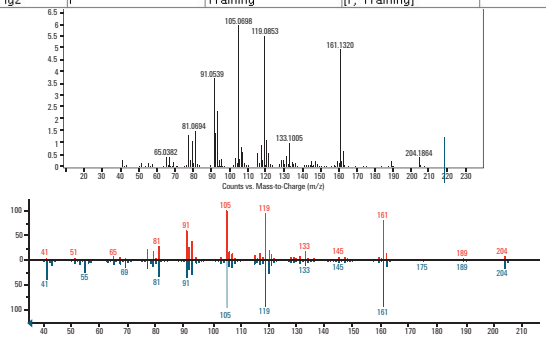


Principal Component Analysis (PCA) in MPP, shows how the data clusters. The blue samples passed the sensory test, while the red samples failed.

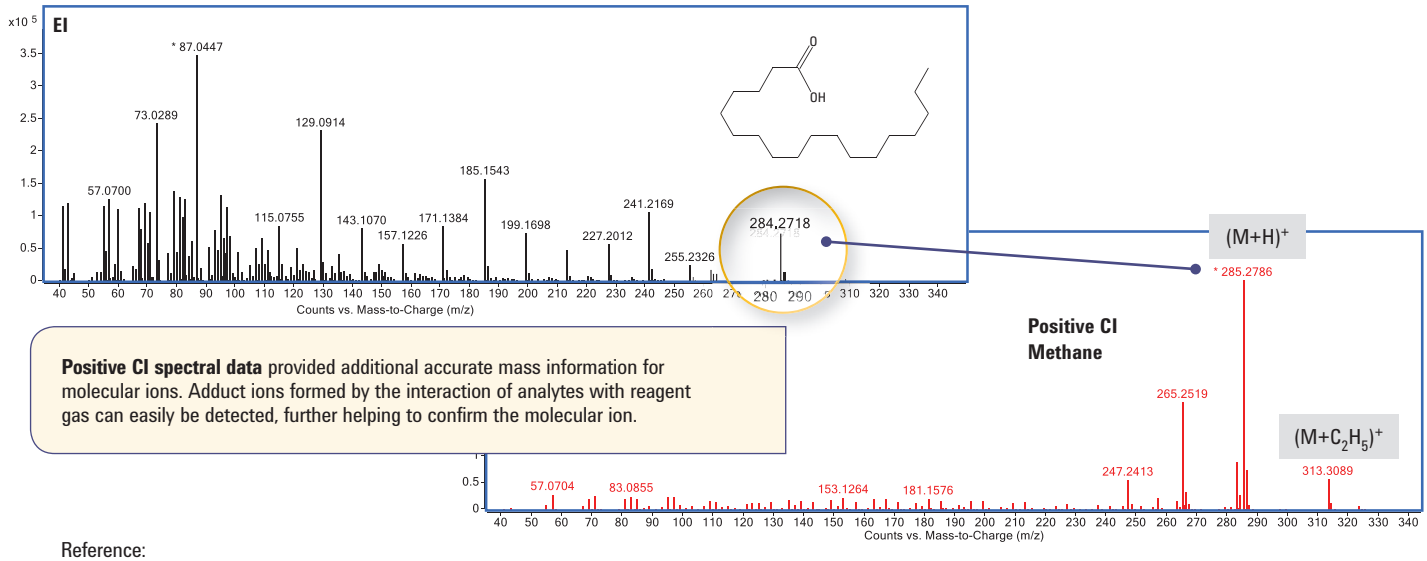
The MPP Prediction Model correctly predicted the pass/fail status of all samples. The samples not used for building the prediction model are listed with the training variable set as "None."

Prediction Results

Identifier	Grade	Training	Predicted(Class Pre...	Confidence
PAC1-EI-1: Ig2	F	None	[F, Training]	1.000
ESC2-EI-1: Ig2	P	Training	[P, Training]	1.000
ESC1-EI-1: Ig2	P	Training	[P, Training]	1.000
SAC1-EI-1: Ig2	F	None	[F, Training]	1.000
RFC2-EI-1: Ig2	P	None	[P, Training]	1.000
RSA2-EI-1: Ig2	P	None	[P, Training]	1.000
CSC1-EI-1: Ig2	F	Training	[F, Training]	1.000
RSA1-EI-1: Ig2	P	Training	[P, Training]	1.000
EFC1-EI-1: Ig2	P	None	[P, Training]	1.000
FSW2-EI-1: Ig2	F	Training	[F, Training]	1.000



The Agilent 7200 Q-TOF for GC/MS generates spectra that can be searched against the commercially available nominal mass EI spectral libraries.



Positive CI spectral data provided additional accurate mass information for molecular ions. Adduct ions formed by the interaction of analytes with reagent gas can easily be detected, further helping to confirm the molecular ion.

Reference:

Analysis of Medium Volatility Sulfur Compounds in Coffee Using Agilent GC/Q-TOF: Pub. No. 5990-9076EN

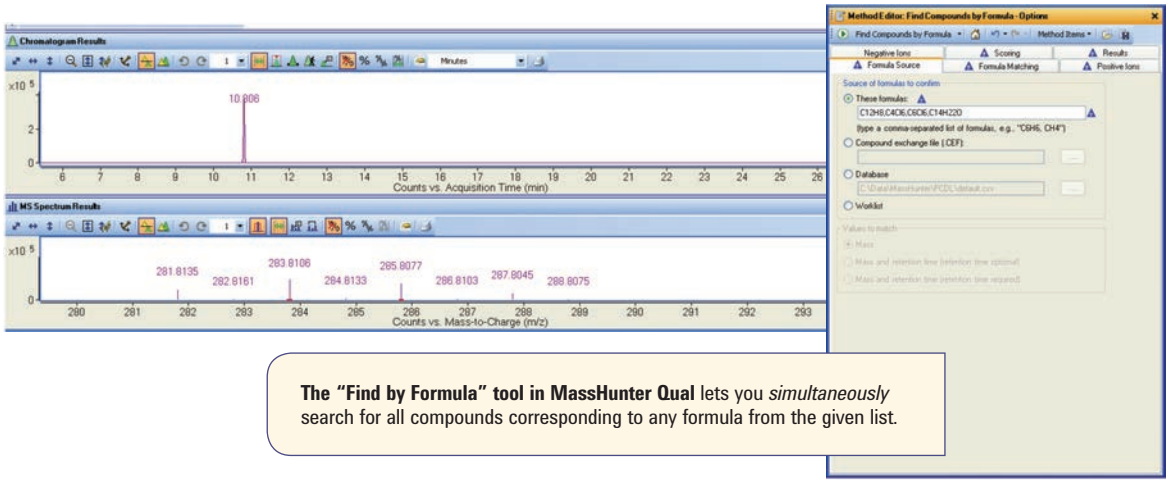
Olive Oil Characterization using Agilent GC/Q-TOF MS and Mass Profiler Professional Software: Pub No. 5991-0106EN

To learn more about the capabilities of the Agilent 7200 Q-TOF for GC/MS, visit **www.agilent.com/chem/GCMS_QTOF**

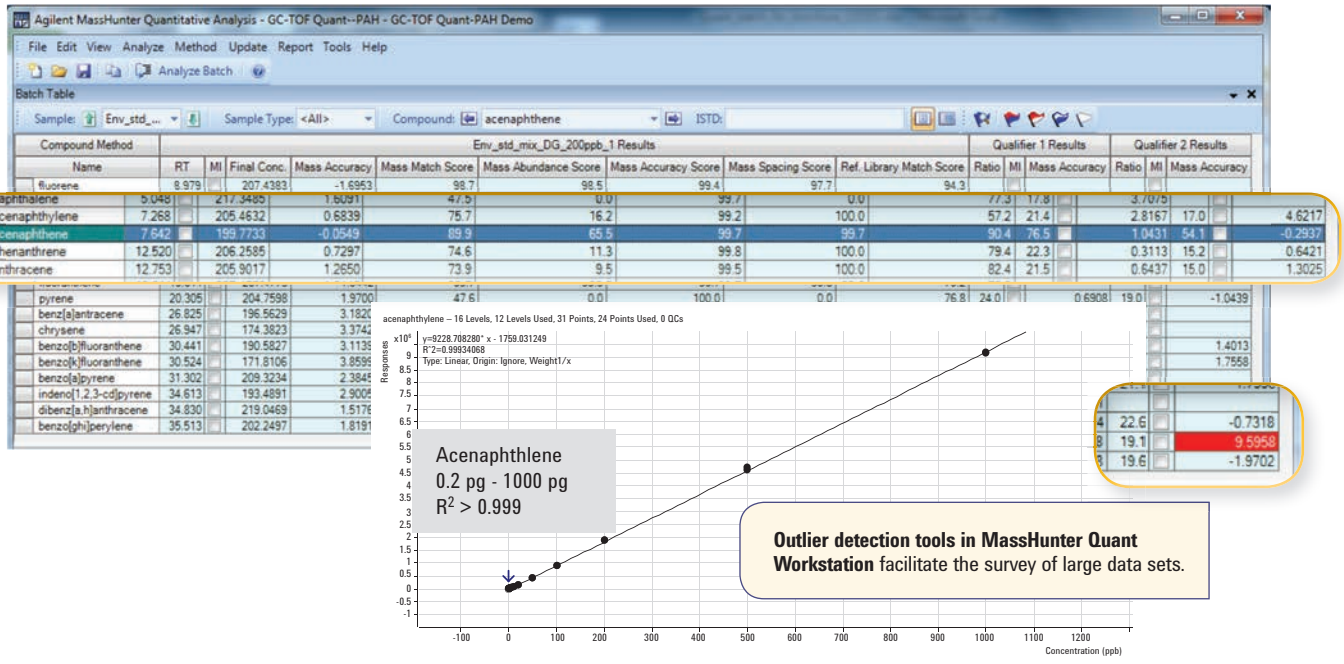
Carry out reliable screening for target compounds, and identify unknowns

One of the greatest environmental analysis challenges lies in identifying and quantitating large numbers of compounds, many of which are present at trace levels in complex matrices. For this type of application, the following features are essential:

- Highly sensitive accurate mass full spectral acquisition
- A wide dynamic range
- Easily automated qualitative analysis
- Batch processing for target compounds



The "Find by Formula" tool in MassHunter Qual lets you *simultaneously* search for all compounds corresponding to any formula from the given list.



Outlier detection tools in MassHunter Quant Workstation facilitate the survey of large data sets.

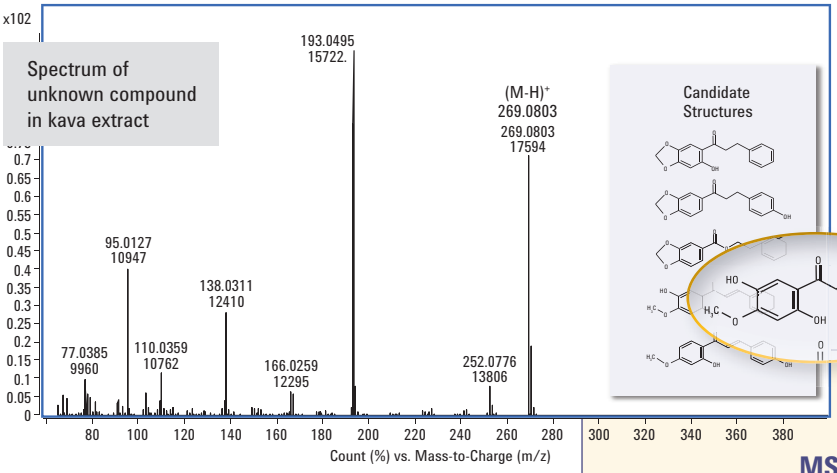
Reference:

Analysis of Biomarkers in Crude Oil Using Agilent 7200 Q-TOF for GC/MS:
Pub. No. 5990-9477EN

Combine accurate mass and product ion spectra to elucidate the structure of unknown compounds

Herbal extracts contain a large number of compounds that need to be identified; however, commercial EI spectral libraries do not always contain mass spectral data for compounds of interest. In these instances, the accurate mass product ion spectra generated by the Agilent 7200 Q-TOF for GC/MS can be invaluable for establishing relationships between fragment ions, thus assisting structure correlation.

Identification of unknowns in kava extract



Of the 5 candidate structures, only one fits the losses identified by MS/MS experiments on multiple precursor ions.

MS/MS experimental measurements

	m/z (experimental)	Formula	Error (ppm)	Score
(**M**-H)$^+$	269.0803	$C_{16}H_{13}O_4$	-1.99	80.7
(**M**-C_6H_5)$^+$	193.0494	$C_{10}H_9O_4$	-0.18	96.7
(**M**-CH=CH-C_6H_5)$^+$	167.0334	$C_8H_7O_4$	-2.9	N/A
(**M**-CH_2=CH-C_6H_5)$^+$	166.0259	$C_8H_6O_4$	-0.96	N/A
-CO	138.0311	$C_7H_6O_3$	-0.33	98.1
-CO	110.0359	$C_6H_6O_2$	-3.01	N/A
-CH_3	95.0127	$C_5H_3O_2$	-0.59	99.5

Accurate mass information of the product ion spectrum helps eliminate any ambiguity between different neutral losses that have the same nominal mass.

Reliable peak identification and compositional data capabilities make the Agilent 7200 Q-TOF for GC/MS ideal for these additional applications

Food Testing and Flavors
- Natural products

Energy/Chemicals
- Quality control
- Detecting trace analytes in petroleum products

Forensic/Toxicology
- Doping control
- Post-mortem screening, discovery and confirmation

To learn more about the capabilities of the Agilent 7200 Q-TOF for GC/MS, visit **www.agilent.com/chem/GCMS_QTOF**

Dependable, consistent analysis from the industry's best GC and GC/MS systems

Agilent 7890 Series GC: better separations, better MS performance

- **Unparalleled reliability:** 5th-generation electronic pneumatics control and digital electronics raise the bar on precise retention time locking
- **Higher productivity:** Faster oven ramp-up/cool down and advanced automation features shorten analysis cycles, reduce ion source maintenance, and let you get more done in less time
- **Robust backflush** promotes retention time stability and faster cycling

Agilent 5975C Series GC/MSD

- Advanced separation capabilities
- Powerful productivity enhancements
- Real-time self-monitoring instrument intelligence

Agilent 240 Ion Trap GC/MS

- Broadest range of ionization and scanning techniques – EI, CI, MS/MS, MS^n
- Highest EI and CI full scan sensitivity
- Robust operation and extended uptime

Agilent 7000 Series Triple Quadrupole GC/MS

- The only Triple Quadrupole GC/MS with a proprietary heated quartz quadrupole analyzer specifically for GC analysis
- Routine femtogram-level sensitivity and superior selectivity
- Up to 500 MRM transitions per second

Agilent GC and GC/MS Analyzers

- Ready-to-use packaged workflow solutions for over 60 major applications
- Pre-configured and factory tested with application-specific method and standards checkout mixture

A lifetime of peak performance for your instrument – plus maximum productivity for your lab

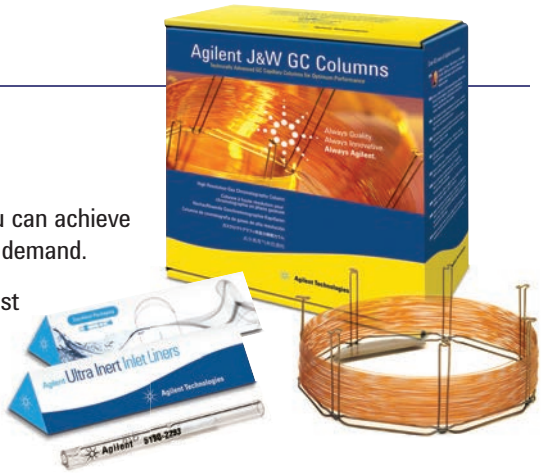
As the world's chromatography leader, Agilent is uniquely positioned to bring you innovative sample prep products, GC columns, and supplies to help you meet your toughest analytical challenges.

Achieve accurate, reproducible results with fewer repeated samples

Only Agilent offers a complete line of sample prep products to suit your analyses and instrumentation.

- **Agilent Bond Elut polymeric SPE products** provide the cleanest extracts and selectively remove interferences from complex matrices. Choose from over 40 phase functionalities in more than 30 formats – the widest variety on the market today.
- **Agilent's industry-leading QuEChERS kits** are a cost-effective way to make sample preparation faster, easier, and more reliable.

To learn more, visit **www.agilent.com/chem/sampleprep**



Perform trace-level analysis with confidence

Agilent Ultra Inert GC solutions work together to create an inert flow path, so you can achieve the parts-per-billion – or parts-per-trillion – detection levels that today's analyses demand.

- **Agilent J&W Ultra Inert GC columns** are tested with the industry's toughest test probe mixture to ensure consistent column inertness and exceptionally low column bleed.
- **Agilent Ultra Inert liners** provide a robust, reproducible, and reliable inert flow path – with or without glass wool.

For more information about ensuring an inert GC flow path, visit **www.agilent.com/chem/ultrainert**

Agilent stands behind your lab's every effort with unmatched expertise, services, and informatics

Compliance

With over 100,000 qualification deliveries, plus decades of quality testing experience, Agilent is a trusted source for the system qualification and proof of calibration you need to comply with regulations.

Real-time support and reporting

The "systems intelligence" built into each Agilent instrument can help you pre-empt instrument problems and reach the highest levels of uptime and productivity.

Agilent OpenLAB

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