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.
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.

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](http://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.

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

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

**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.

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

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**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.

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

<table>
<thead>
<tr>
<th>pg on-column</th>
<th>mass error, ppm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2-formyl thiophene</td>
</tr>
<tr>
<td>1</td>
<td>3.57</td>
</tr>
<tr>
<td>2</td>
<td>4.46</td>
</tr>
<tr>
<td>5</td>
<td>-2.68</td>
</tr>
<tr>
<td>10</td>
<td>-2.68</td>
</tr>
<tr>
<td>20</td>
<td>-2.68</td>
</tr>
<tr>
<td>50</td>
<td>-0.89</td>
</tr>
<tr>
<td>100</td>
<td>0.00</td>
</tr>
<tr>
<td>200</td>
<td>-1.79</td>
</tr>
<tr>
<td>500</td>
<td>2.68</td>
</tr>
<tr>
<td>1000</td>
<td>1.79</td>
</tr>
<tr>
<td>Average</td>
<td>-1.43</td>
</tr>
</tbody>
</table>

**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](http://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
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**
- Squalene
- Lanosterol
- 4,4-dimethyl-5α-cholesta-8,24-dien-3β-ol
- 4α-carboxy-4β-methyl-5α-cholesta-8,24-dien-3β-ol
- Zymosterol
- Ergosterol

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

**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 Wu1, Robert St. Onge2, Sundari Suresh2, Ronald Davis2 and Gary Peltz1
1Department of Anesthesia, School of Medicine, Stanford University
2Biochemistry-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
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.

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.”

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
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

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

<table>
<thead>
<tr>
<th>m/z (experimental)</th>
<th>Formula</th>
<th>Error (ppm)</th>
<th>Score</th>
</tr>
</thead>
<tbody>
<tr>
<td>(M-H)⁺</td>
<td>C₁₆H₁₃O₄</td>
<td>-1.99</td>
<td>80.7</td>
</tr>
<tr>
<td>(M-C₆H₅)⁺</td>
<td>C₁₄H₁₁O₄</td>
<td>-0.18</td>
<td>96.7</td>
</tr>
<tr>
<td>(M-CH=CH-C₆H₅)⁺</td>
<td>C₁₂H₉O₃</td>
<td>-2.9</td>
<td>N/A</td>
</tr>
<tr>
<td>(M-CH₂=CH-C₆H₅)⁺</td>
<td>C₁₀H₇O₂</td>
<td>-0.96</td>
<td>N/A</td>
</tr>
<tr>
<td>-CD</td>
<td>C₉H₆O₂</td>
<td>-0.33</td>
<td>98.1</td>
</tr>
<tr>
<td>-CD</td>
<td>C₈H₅O₂</td>
<td>-3.01</td>
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<tr>
<td>-CH₃</td>
<td>C₇H₄O₂</td>
<td>-0.59</td>
<td>99.5</td>
</tr>
</tbody>
</table>

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

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](http://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](http://www.agilent.com/chem/ultrainert)
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
With the ever-increasing complexity and volume of data generated when analyzing samples such as food, drugs, soil, and water, you need to turn raw data into actionable information. Agilent’s OpenLAB ELN and OpenLAB ECM help you capture, analyze, and share your results, preserving and archiving your intellectual property while facilitating collaboration.

Agilent Value Promise
We guarantee you at least 10 years of instrument use from your date of purchase, or we will credit you with the residual value of the system toward an upgraded model.

Agilent Service Guarantee
If your Agilent instrument requires service while covered by an Agilent service agreement, we guarantee repair or we will replace your instrument for free.

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