

Agilent 5977B GC-MS Single Quadrupole Sole Source Justification.

The Agilent gas chromatograph single quadrupole mass spectrometer (GCMS) is the industry leading benchmark and standard for high performance, reliable and durable GCMS instrumentation. The 5977B GCMS single quadrupole is the current flagship model in a long and proud legacy of GCMS innovations.

Agilent is the market leader in GCMS instruments around the world and has the largest organization of service engineers, applications specialists and research scientists to respond to the needs of our extensive and diverse customer base. This document outlines the various technologies unique to the Agilent 5977B single quadrupole GCMS that gives it superior performance in high sensitivity and long-term durability.

This document was prepared to highlight the proprietary technologies in the Agilent 5977B single quadrupole GCMS hardware and software. Each of the pages provide lock-out specs and the justifications are provided.

Highest Performance, Single Quadrupole GC-MS



Mass range 1.6 to 1,050 m/z
Scan speed up to 20,000 amu/s
Minimum SIM dwell time 1 msec
Maximum SIM ions 60 ions x 100 groups
Proprietary monolithic hyperbolic Au coated quadrupoles
Triple axis- HED/EM detector with up to 10⁶
linear dynamic range
Ships with both MassHunter and Chemstation
Data Analysis software

EI, PCI and NCI

S/N Installation Reference Specifications ^a								
Instrument Configuration	Source	El Scan S/Nb	Sample Concentration (1 µL Injection)	PCI Scan S/N	NCI Scan S/N	High Vacuum System		
Agilent 5977B HES MSD	HES	300:1	0.1 pg/μL OFN			Turbo molecular pump		
Agilent 5977B EI/CI MSD	Extractor for EI, CI source for CI	1,500:1 (EI)	1 pg/μL OFN	1,200:1°	2,000:1 ^d	Turbo molecular pump		
Agilent 5977B Inert Plus El MSD	Extractor	1,500:1	1 pg/μL OFN			Turbo molecular pump		
Agilent 5977B EI MSD	Stainless steel	550:1	1 pg/μL OFN			Turbo molecular pump or diffusion		
Agilent 5977B with 8860 GC	Stainless steel	250:1	1 pg/μL OFN			Turbo molecular pump or diffusion		

- a S/N checkout is only performed if there is no autosampler (which is required for IDL checkout). Helium carrier gas, manual injection using a 30 m × 0.25 mm, 0.25 µm column. When the autosampler is present, these specifications are a reference of the performance. S/N will not be confirmed at installation or familiarization.
- ^b Standard scanning from 50 to 300 u at nominal 272.0 u ion.
- ° 1 µL injection of 100 pg/µL benzophenone (BZP) standard, 80 to 230 u scan at nominal 183 u ion, using methane reagent gas.
- d 2 µL injection of 100 fg/µL OFN standard scanning from 50 to 300 u at nominal 272 u ion, using methane reagent gas.

Agilent 5977B Series GC/MSD System Specifications					
Ionization Mode (Standard)	EI				
Ionization Modes (Optional)	PCI, NCI, EI acquisition with CI source				
El lon Source Type	Four supported sources: stainless steel, inert, extractor, or HES				
Electron Energy	5 to 241.5 eV				
Emission Current	0 to 315 μA				
CI Gases	Dual gas inlet				
Filaments	Dual for EI, single for CI				
Transfer Line Temperature	100 to 350 °C				
Ion Source Temperature	150 to 350 °C				
Quadrupole Temperature	106 to 200 °C				
Mass Filter	Heated monolithic hyperbolic quadrupole				
Ion Source - Mass Filter Interface	Dynamically rampable entrance lens				
Mass Range	1.6 to 1,050 u				
Mass Resolution	Unit mass				
Mass Accuracy	1 μL injection of a 100 pg/μL OFN ^a standard scanning from 50 to 300 u will give its monoisotope at m/z 271.987 ±0.005 ^a				
Spectral Accuracy	1 μL injection of a 100 pg/μL OFN standard scanning from 50 to 300 u will give 99.0 % spectral accuracy⁵				
Mass Axis Stability	Better than 0.10 u/48 hours				
Detector	Series II triple-axis detector with high energy dynode and long life electron multiplier (EM)				
Dynamic Range (Electronic)	106				
Scan Rate ^b	Agilent 5977B Inert Plus (extractor source) and Agilent 5977B HES up to 20,000 u/sec, Agilent 5977B (SS source) up to 12,500 u/sec				
SIM	60 ions × 100 groups				
Pumping System (Helium)	65 L/s diffusion pump and 255 L/s turbo pump with 2.5 m³/hr mechanical pump				
Maximum Recommended Analytical Gas Flow	1.5 mL/min (diffusion pump) 4 mL/min (turbo pump)				
Recommended Maximum Sustained Column Flow to MS ^c	3 mL/min (diffusion pump) 50 mL/min (turbo pump)				
Instrument Control	Agilent MassHunter data system				
Maintenance Accessibility	Source (including filaments, lenses), mass filter ^d , and detector on removable plate for easy access				
Maintenance Scheduling	Early maintenance feedback (EMF) for GC and MSD, user-defined maintenance schedule, with display of current status				
Support Life	Guaranteed 10 years useable life with support for seven years				

^a Only applicable with optional Accurate Mass software package. Scan mode only. Not verified during installation.

^d The heated quadrupole mass filter should not require maintenance, but if maintenance is required, it should be performed by an Agilent service engineer.



^b As scan rate increases, sensitivity will decrease, and resolution may degrade.

^c A high flow rate into a fixed ion source will cause a loss in sensitivity.

Installation checkout specifications

Agilent verifies GC/MSD system performance at the customer site. IDL is a statistically-based metric that more accurately confirms system performance than an S/N measurement. Test specifications are based on splitless injection into an Agilent J&W HP-5ms Ultra Inert 30 m \times 0.25 mm, 0.25 μm column. IDL analyses use lab helium with GC gas filters installed.

See more about the IDL test at http://www.chem.agilent.com/Library/technicaloverviews/Public/5990-8341EN.pdf

Instrument Detection Limit (IDL)

- The industry's most rigorous performance metric
- Based on eight consecutive injections and their statistical analysis of precision (%RSD)
- Measured at an amount near the detection limit
- Accurate assessment of the true detection limit and lower limit of quantification (LLQQ)
- · IDL tested and proved at installation

IDL Installation Checkout Specifications						
Instrument	IDL*	Source				
Agilent 5977B HES MSD	1.5 fg	HES				
Agilent 5977B EI/CI MSD	10 fg (EI)	Extractor for EI, Agilent CI source for CI				
Agilent 5977B Inert Plus El MSD	10 fg	Extractor				
Agilent 5977B EI MSD	24 fg	Stainless steel				
Agilent 5977B with Agilent 8860 GC	40 fg	Stainless steel				

- * IDL statistically derived at 99 % confidence level from the area precision of eight sequential splitless injections of OFN (octafluoronaphthalene)
- HES IDL measured using 10 fg injection, 1 μL injection
- Other IDLs measured using 100 fg, 1 µL injection
- · 30-m column used for IDL checkout
- Helium carrier gas with auto liquid sampler

Agilent GCMS- Designed for use with H₂ carrier gas

Agilent Technologies

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Andrew Delonno Product Safety Engineer Chemical Analysis Solutions

January 25, 2008

Subject: Use of Hydrogen in the 6890 and 7890 Gas Chromatographs

Dear Customer:

I am pleased to respond to your request for information concerning the use of hydrogen as a carrier gas in the 6890 and 7890 Gas Chromatographs produced by Agilent Technologies.

These instruments were designed to use hydrogen as a carrier gas. The Hydrogen Carrier Gas Safety Guide and the operation manuals for the instruments contain safety instructions, but it is recommended that anyone working with flammable or explosive gases take a lab safety course covering proper gas handling and use.

Some laboratory precautions that are recommended for controlling hydrogen build up include directing vent lines into a fume hood and leak-testing the gas connections, lines, and valves before operating the instrument. Because hydrogen leaks frequently originate in tubing and connections external to the gas chromatograph (e.g., at the tank), hydrogen leak-testing

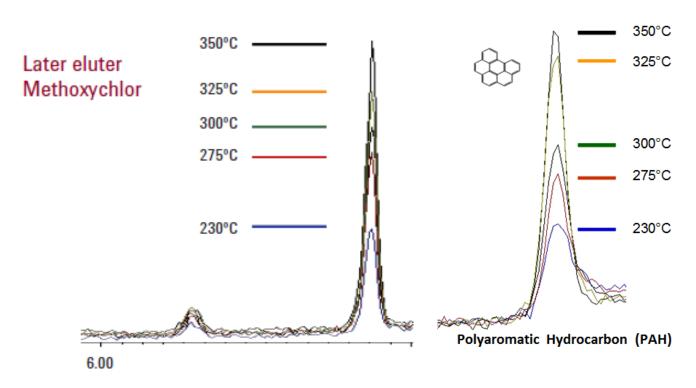
Agilent 8890 gas chromatographs and 5977B mass spectrometers are designed to use hydrogen as a carrier gas. Numerous safety features are built into the instruments to prevent accumulation and potential explosions inside the GC and MS; however, in the rare case an explosion occurs, these instruments have been designed <u>and explosion</u> tested to ensure maximum safety.

Safety Features of the Agilent 8890GC with H₂

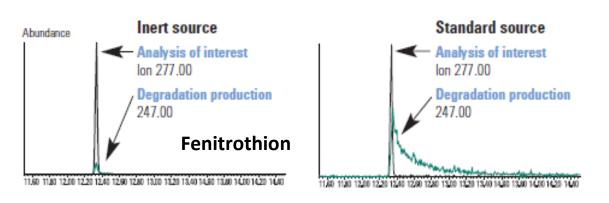
- Pressure and flow set-points are continuously monitored. If set-points are not met (ex. broken column) then the electronic pneumatic control (EPC) shuts off
- The EPC have flow limiting frits to prevent large flow of H₂ in the case of EPC malfunction. In a two fault
 condition, such as a missing column and a valve seating fault, the frit will mechanically limit the H₂ flow
 to a level that has been experimentally shown to pose no increased risk due to the hydrogen leakage
- The GC vents the oven cavity prior to initiating the heating sequence on the heater coils
- The oven heater hardware control has a controlling triac and a double pole controlling relay to prevent the oven heater from faulting into an "on" position when the control or user has turned the oven heater off
- The oven is not sealed shut with respect to H₂ and does not contain areas where air will not circulate (dead volumes). This allows for very light small molecular gases, such as H₂, to easily diffuse out of the oven cavity; furthermore, the rear oven flaps are automatically opened half way when the oven is placed into an "off" state
- If there is an explosion in the oven for any reason, the oven door is designed to buckle under the explosion pressure and assist in safely releasing the oven pressure from the oven cavity
- The 8890 has an optional H2 sensor module that checks for uncombusted free hydrogen in the GC Column Oven.

High Temperature Non-coated Ultra-Inert Ion Source

The ionization source on the 5977B is made with a non-coated, ultra inert material. The ultra-inert source is produced from a patented inorganic vapor deposition process and is programmable to 350°C. The ultra-inert material cannot be damaged or removed from multiple cleanings because it is not a coating. The ultra-inert material provides very robust operations for samples in complex matrices; better response for compounds that typically stick (adhere to hot metal surfaces) and sharper peaks for high boilers (late eluters).

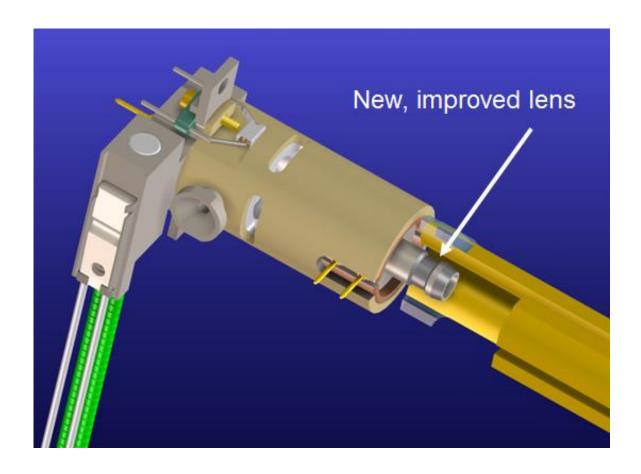


Enhanced response at higher temperatures on the ultra-inert source



Unique Entrance Lens Eliminates Need for Pre-filters

Non uniform electrical fields at the entrance and exit of quadrupoles- also known as fringe fields- can greatly affect ion transmission and thus the sensitivity of the system. Agilent overcomes the limitations of fringe field effects by directly injecting the ions from the source into the first quadrupole by the entrance lens. Voltage on this lens is dynamically ramped synchronously with analyzer voltage to focus maximum ion signal for every m/z into the center of the quadrupole field (the quadrupole sweet spot). This ensures maximum transmission of ions from the source into the mass analyzer.

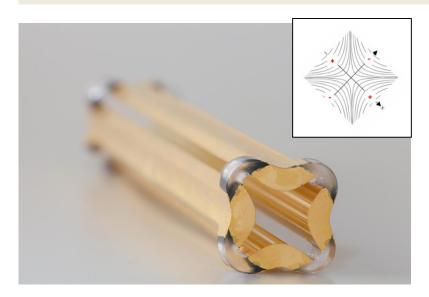


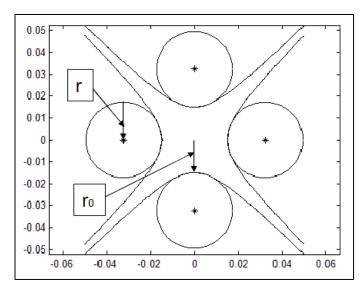
Quadrupole Mass Analyzer- Agilent quadrupoles have hyperbolic geometry

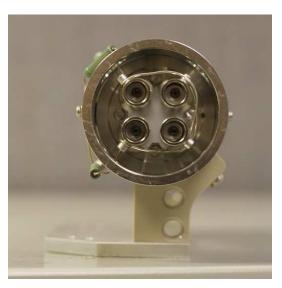
Ideally rods with hyperbolic geometries should be used in a quadrupole for best ion transmission and resolution.

In practice it is <u>extremely</u> difficult and expensive to make a perfect (end to end) hyperbolic geometry so round rods are often used to approximate a quadrupole field.

Hyperbolic surfaces yield the greatest mass resolution for the least amount of power







Round rods will create electrical field distortions which ultimately limits ion transmission (and performance) of the quadrupole system

Agilent Quadrupoles are Hyperbolic, Gold-coated, Quartz and Proprietary!



Quartz has the lowest coefficient of linear expansion (expansivity; α)

$$\delta L = \alpha L_0 \delta t$$

[t = °C; δL = change in length (m); L_0 = length at 0 °C]

α varies greatly for different materials

Stainless steel = 17.3 Inconel (Ni alloy) = 12.6 Glass pyrex = 4.0 Quartz, fused = 0.59



Low thermal expansion means dimensions and alignments do not change with heat. After maintenance, the quartz quads can be baked at 200 °C. Under operation, the quartz quads can be run at 150 or even 200 °C

Heated quadrupoles result in more stable tunes and methods over a longer period of time in real world sample environments. Heated quadrupoles also allow for the instrument to thermally equilibrate, stabilize and be operational within hours of pump down after vent.

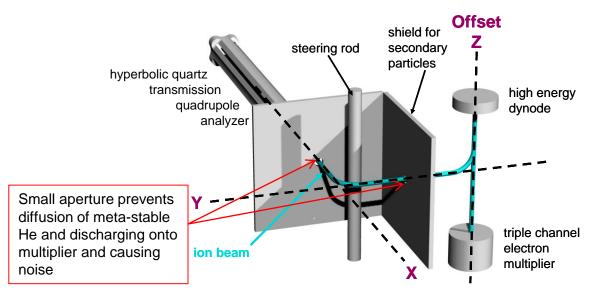
No metal quads can be heated!

Stainless steel and nickel have large coefficients of expansion relative to quartz. Slightest imperfection in r_0 (1 in $10^4 \sim 0.5~m$ m for 5mm r_0) can cause field distortions and render quadrupoles ineffective

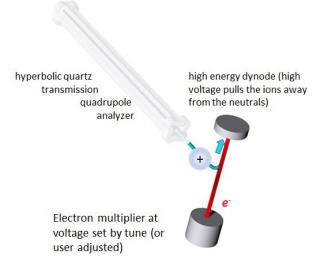
Heat is the "friend" of GC/MS methods – true for the source and analyzer! Why? Compounds that elute at hot temperatures can condense on cold surfaces. Condensation will result in contamination and reduced robustness of the method.

High Performance Triple-Axis Detector

The detector in the Agilent 5977A single quadrupole is placed in a triple off-axis configuration from the EI source to further reduce noise. Conventional off-axis designs places the detector off-axis from the noisy source; however, the detector will still be exposed to neutral noise from the metastable helium. Minimizing the noise allows for greater instrument detection limits and a greater linear dynamic range (6 orders) of operations.



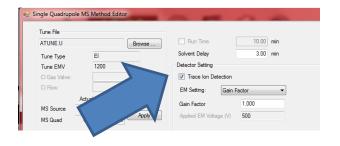
Agilent Triple Off-Axis detector



Conventional off-axis design

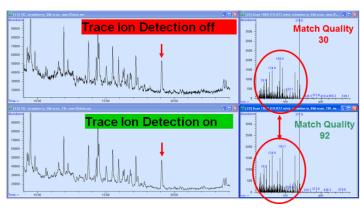
A significant source of noise for single quadrupole instruments using the conventional off-axis detector design is meta-stable helium generated in an electron impact source. Meta-stable helium is not charged and is therefore unfiltered by the quadrupole mass analyzer. The highly energetic meta-stable helium discharge on the detector results in elevated chromatographic baseline (noise). The triple off-axis detector gives the Agilent 5977A unparalleled sensitivity by minimizing both the chemical and neutral noise and long operational life.

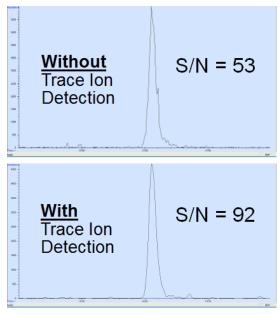
Trace Ion Detection- Improve detection of trace level analytes



The advanced electronics in the 5977A mass spectrometer allow for the ability to process the raw acquired data. Trace Ion Detection (TID) dramatically reduces baseline noise and improves peak shape and spectral fidelity. This feature produces better library matches at trace levels.

Combined with Agilent's unique Deconvolution capabilities in MassHunter Unknowns Analysis and Chemstation Deconvolution Reporting Software (DRS), compounds can be detected even when they coelute and much of the tedium and uncertainties are removed from complex analyses.





Summary of features of TID

- Better peak shapes and therefore better and more consistent integrations
- Better spectral matches in complicated samples
- Improved signal-to-noise ratio for better detection limits
- Better ion area (and peak height) reproducibilities for enhanced detection limits

Agilent Gas Chromatographs- Precise, reliable pneumatic control

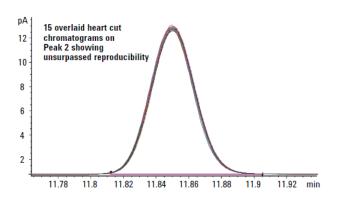
The Agilent GC electronic pneumatic controls (EPCs) are extremely precise and can control pressure to ± 0.001 psi. Agilent EPCs correct for temperature with a specified temperature coefficient of 0.001 psi/°C.

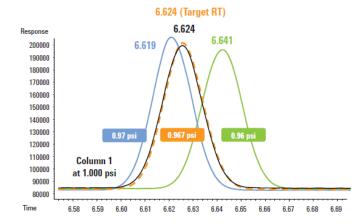


Pneumatic manifolds reduce the need for parts and seals, improving gas flow precision and stability. Integrated electronics and advanced mechanical design further enhance dependability and versatility

Run	Peak 1*	Peak 2*
1	9.0839 min	11.8492 min
2	9.0835	11.8492
3	9.0841	11.8494
4	9.0846	11.8496
5	9.0851	11.8507
6	9.0849	11.8502
7	9.0845	11.8504
8	9.0849	11.8500
9	9.0847	11.8504
10	9.0853	11.8502
11	9.0852	11.8502
12	9.0851	11.8508
13	9.0847	11.8503
14	9.0848	11.8507
15	9.0853	11.8506
Average	9.0847 min	11.8501 min
Standard Deviation	0.000527	0.000535

*Heart-cut from column 1.





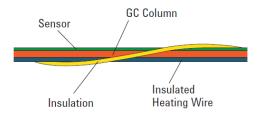
Agilent Retention Time Lock (RTL)

technology is included in all Agilent GCs. RT Locked methods provide constant retention times for all peaks regardless of inlet, detector, operator, time or location.

RTL methods from Agilent enhance productivity and capabilities immediately

Agilent Gas Chromatographs- Low Thermal Mass Columns

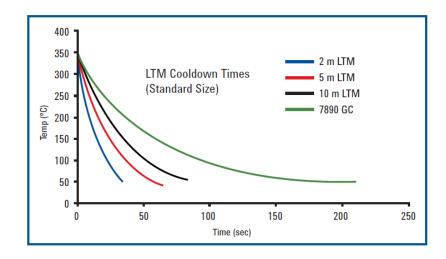
Agilent proprietary Low Thermal Mass (LTM) column technology provides for independent heating and cooling capabilities of up to 4 capillary columns on one GC. LTM equipped GCs can allow for simultaneous independent analyses with two separate detectors. LTM equipped GCs can allow for multidimensional separation techniques.



LTM columns

LTM columns are conductively heated by the insulated heating wire wrapped around the capillary GC column. Real-time error fluctuations between temperature setpoint and column temperature are less than 1°C over the entire temperature range at a program rate of 120 °C/min.

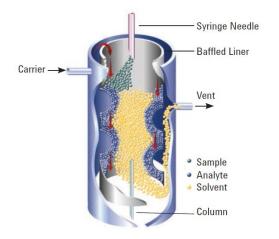




LTM maximum heat rate is 1800 °C/min LTM cool rate is faster than a conventional oven

Agilent Gas Chromatographs- MultiMode Inlet

Agilent proprietary MultiMode Inlet (MMI) provides the flexibility of a standard Agilent split/splitless inlet, combined with programmable temperature vaporizing (PTV) capabilities which allow for large volume injection. Cool injections are also possible for improved signal response. The MMI uses the same glass liner and septa as the Agilent Split/Splitless inlet reducing cost and consumable inventory in a lab.



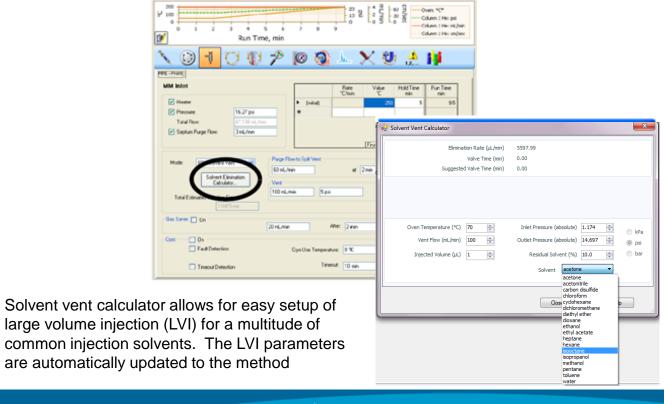
Temperature range of -160°C to 450 °C

Temperature programming of up to 10 ramps at up to 900 °C/min

Maximum temperature 450°C

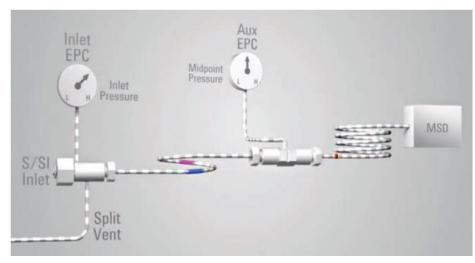
Injection Modes: Hot S/SL, Cold S/SL, all in pulsed mode, solvent vent mode, residue removal mode

EPC pressure range 0 to 100 psig



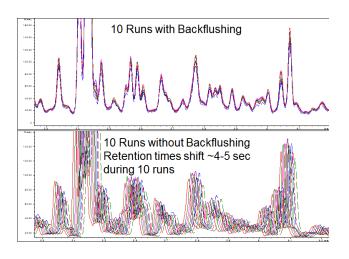
Agilent Gas Chromatographs- Capillary Flow Technology

Agilent proprietary Capillary Flow Technology (CFT) are ultra-inert, low thermal mass, low dead volume devices to make secure leak-free capillary connections that can withstand the temperature extremes and cycles of a GC oven and precisely divert carrier gas flow. Capillary flow techniques such as backflush dramatically saves time, consumables costs and improves method performance





CFT Backflush works by reversing the carrier gas flow at a point designated in the method. The reversed carrier gas through column 1 ensures all heavy matrix components are flushed out the hot inlet and split vent. This eliminates the need for long high temperature bake out after the analytes have eluted from the column. Agilent CFT backflush can be placed in a variety of configurations: pre-column, mid-column and post-column. Backflush calculators provided in MassHunter software allows for easy setup

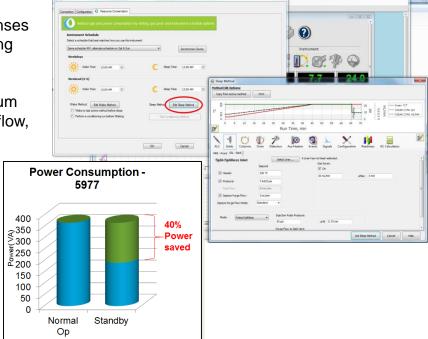


Reduce Operating Expenses- Environmentally Friendly Green Features

Reduce operating expenses with built-in energy saving features. Customizable sleep time and method allows for saving of helium carrier gas by reducing flow, lowering temperature of

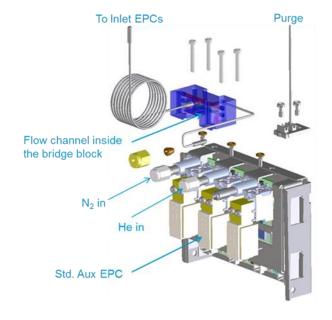
heated zones and reducing power consumption of foreline rotary pump[±] when instrument is not in use.

Set instrument wake time and method so instrument is properly conditioned and ready for use.



[±]pump power savings available only on instruments with turbo molecular pump and DS42i rotary pump

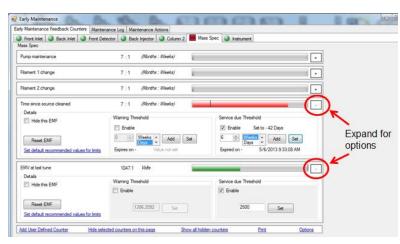
Save money on expensive carrier gas by plumbing nitrogen gas into the electronic pneumatic control (EPC) to allow for purging of the GCMS with N₂ gas while on standby to conserve precious helium carrier. The wake method will switch to helium carrier gas and the instrument can be operational after one conditioning run.



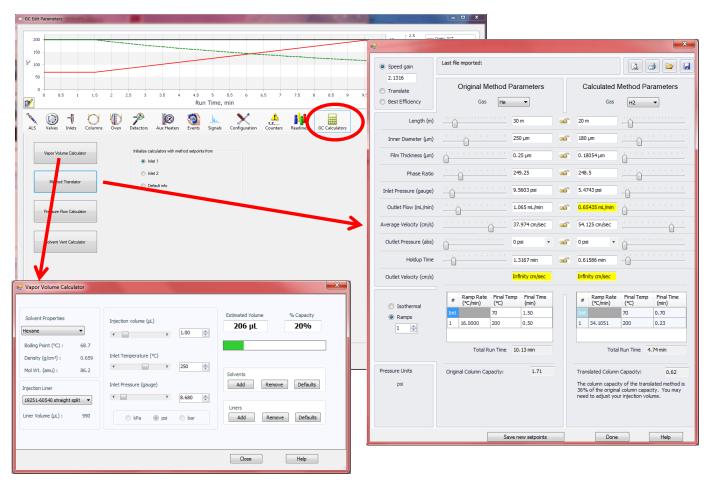
User Friendly Software- Integrated calculators and monitors to enhance productivity and capabilities

Powerful built-in programs help users easily calculate important method parameters such as vapour volume; solvent vent for large volume injections; method translation from one column or carrier gas to a different one and pressure/flow for capillary flow technologies (ex. backflushing)

Users can customize their Early
Maintenance Feedback to monitor



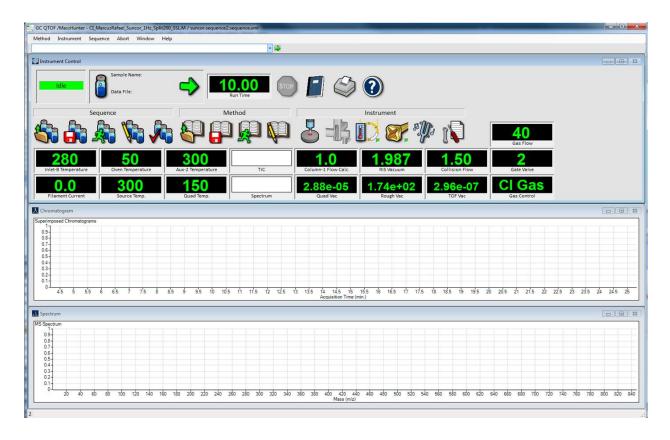
every region of their GCMS without relying on manually updated logbooks



MassHunter Software

MassHunter can be used to process all Chemstation data files

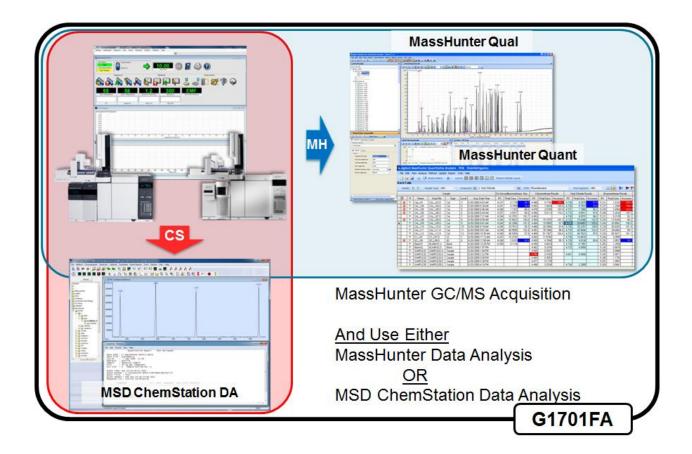
MassHunter Data Analysis software can process all legacy Chemstation data files and Varian ion trap data files. MassHunter can also import Chemstation quantitation databases so legacy Chemstation data files can continue to be quantitated and processed easily and immediately in MassHunter.



MassHunter acquisition is very similar to the Chemstation interface

MassHunter is the common platform for Agilent LC-MS/MS, ICP-MS and GC-MS/MS technologies. The software is extremely powerful and the 64-bit architecture takes full advantage of 64-bit operating systems so that even the largest and complex data files are processed efficiently.

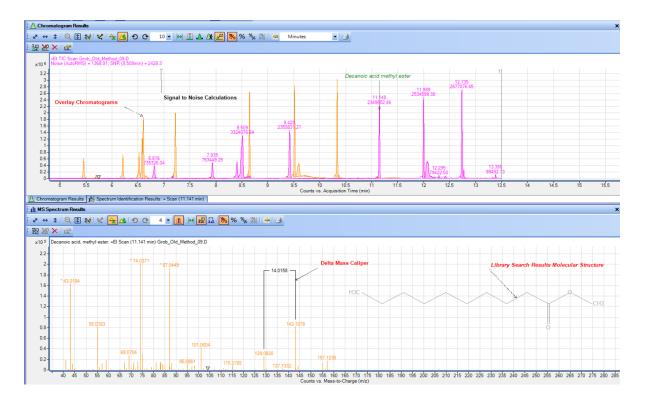
5977A GCMS ships with both MassHunter and Chemstation Data Analysis software



The G1701FA MassHunter software comes with both licensed copies of MassHunter and Chemstation Data Analysis software. Chemstation users can continue their workflow uninterrupted but can also use MassHunter which is installed and co-resident with Chemstation Data Analysis. All user generated custom libraries are fully compatible with and interchangeable between MassHunter and Chemstation.

G1701FA MassHunter operates under Windows 7-64 bit operating system.

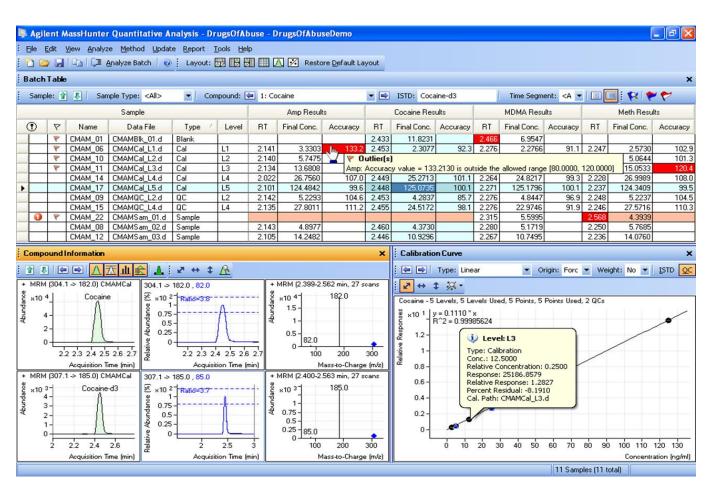
MassHunter Software- Qualitative Analysis



MassHunter Qualtitative Analysis is ideal for method development and R&D investigations. It allows the user to do typical qualitative operations such as Overlay Chromatograms, Calculate S/N, Annotating Features, Mass Caliper, Library Searching from various libraries (NIST, Wiley, Custom Library), Mass Calculator, Formula Calculator, EIC.

The attractive and intuitive Graphic User Interface (GUI) enables the user to access tools with the click of a button. The MassHunter can be customized without the need for any Macros to fit your needs and workflow.

MassHunter Software- Quantitative Analysis



MassHunter Quantitative Analysis is extremely powerful and versatile for quantitative applications. MassHunter Quantitative Analysis is based on a batch model so multiple samples are analyzed at once. The batch table window shows multiple compounds with compound information such as the quantitation, qualifier ions and calibration curve. High outliers are shown in red and low outliers shown in blue for immediate identification.

The parameter-less MS/MS integrator as the name implies does not have any parameters. It quickly and accurately integrates peaks and distinguishes them from noise spikes over five orders of magnitude. The parameter-less integrator virtually eliminates the need for manual integration.

MassHunter Software- Fully Capable of Processing Legacy Chemstation *.D and Varian Ion trap .SMS files

All legacy Chemstation *.D and Varian ion trap *.SMS files can be translated and processed with MassHunter through a quick and easy process. MSD translator and MSWS data translators are included with all copies of MassHunter.

The *in-place* translation option writes a MassHunter readable file in the Chemstation data folder; the *out-of-place* translation writes a MassHunter translated file in a separate directory so the original data file is not touched to meet the requirements of regulated environments.

ChemStation (.D)

Data

MassHunter Quant

MassHunter Quant

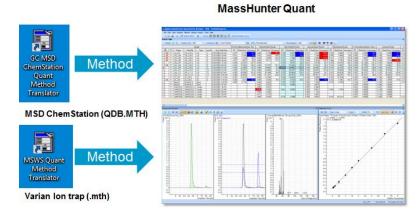
MassHunter Qual

MassHunter Qual

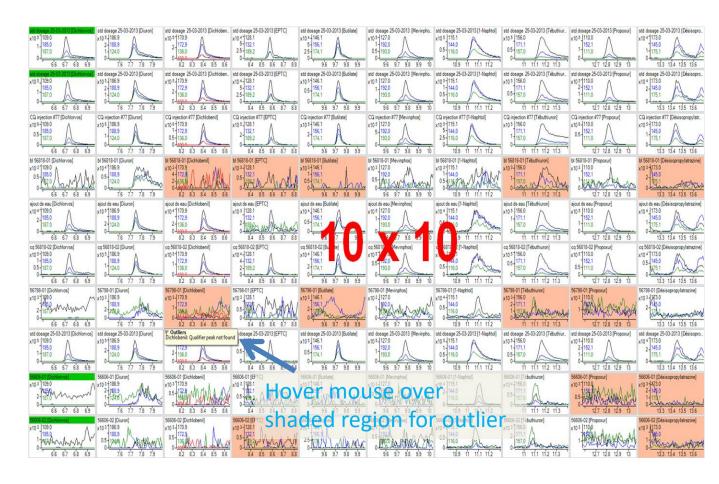
MassHunter Qual

MassHunter Qual

There is no need to reconstruct quantitative calibration databases with the Quant Method Translators. Seamlessly transition to MassHunter Quant by translating old Chemstation or Varian MSWS quantitative databases accurately, quickly and easily.



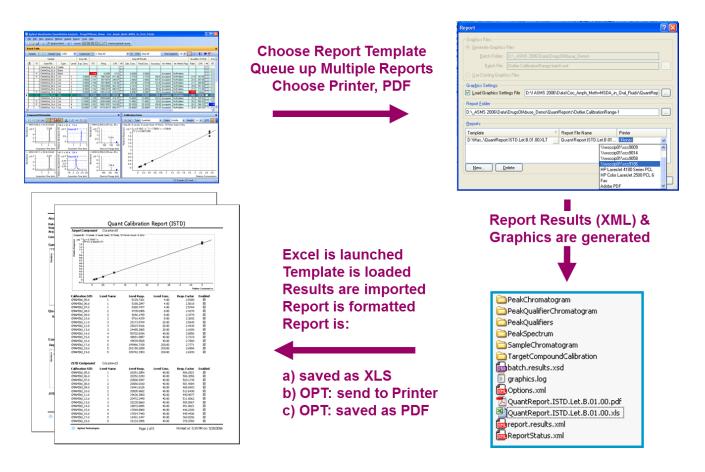
MassHunter Software- Quantitative Analysis Batch at a Glance



The Batch at a Glance feature in MassHunter Quantitative Analysis is an extremely powerful and efficient way of identifying outliers or peaks that have interferences or are improperly integrated. The Batch at a Glance window can be sized by the user from 2x2 up to a maximum of 10x10. This view can also be scrolled to see all the peaks (if there are more than 100) in the batch analysis. This greatly eliminates manually opening multiple data files and tediously checking each peak for proper integration or outliers.

The outlier detection in MassHunter Quant uses up to 20 different criteria that can be set by the user to identify outliers. Outliers can be flagged and filtered and a separate outlier report can be generated. Outliers in the matrix view will show up as a shaded window.

MassHunter Software- Quantitative Analysis Reporting



The reporting feature in MassHunter Quantitative Analysis is based on Microsoft Excel 2003 (or higher) and XML. There are a multitude of report templates for multiple applications. Customizable report templates can also be easily created using familiar Excel functions and tools.

Agilent GC-MS Single Quadrupole Summary

Maximum Signal

- Inert MSD source with novel entrance lens
- Highly efficiency, quartz, hyperbolic quadrupole analyzers
- Increase ion transmission through to the HED-EM

Minimum Noise

- Neutral noise eliminated with Triple-Axis Detector configuration
- Trace Ion Detection from advanced high speed electronics

Maximum Reliability

Proven MSD inert source and hot quartz quadrupole

The Agilent Value Promise— 10 years of guaranteed value.

In addition to continually evolving products, we offer something else unique to the industry—our 10-year value guarantee.

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

The Agilent Service Guarantee



Should your Agilent instrument require service while covered by an Agilent service agreement, we guarantee repair or we will replace your instrument for free.

Only Agilent offers a comprehensive industry first 10-year value guarantee. The unique technologies mentioned in this document not only ensures superior performance but robust and reliable use for 10 years of continuous operations. You can buy with the peace of mind that your investment will give you high quality returns for the next decade