









Taking GC-MS to the Limit





High-Speed Performance – PP. 6–7

- Achieves a maximum scan speed of 20,000 u/sec
- ASSP[™] technology provides greater sensitivity
- Ultra-fast data acquisition rates ideal for comprehensive GC×GC and Fast-GC



Increased Productivity — PP. 8–9

- Analysis cycle time cut in half*
- Significantly reduced maintenance downtime*
- · Easy exchange of columns for improved productivity*



Eco Friendly P. 16

- 36% reduction in power consumption in analysis standby mode*
- 30% reduction in CO₂ factory emissions**

There is increasing public interest in the analysis of trace compounds that contribute to environmental pollution, affect human health and in research related to novel compounds. Reducing running costs and lessening the impact on the environment by increasing analytical efficiency and decreasing power consumption are universal goals. The GCMS-QP2010 Ultra was developed by engineers who accepted the challenge to meet these needs.

* Based on our specified conditions

** Compared with previous model

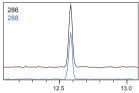
Superior Mass Spectrometry Technology

Superior Technology That Achieves High Sensitivity and Stability

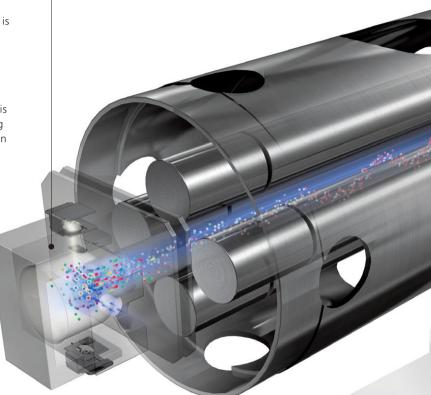
High-Efficiency Ion Source

Provides the foundation of an ion generation and transmission system which efficiently creates, then delivers, ions to the dectector, resulting in a GC-MS with the highest sensitivity specification in its class.

The effect of filament potential on the ion source is reduced by placing more distance between the filament and ion source box along with the addition of a shield plate. The result is that a higher percentage of the generated ions are transported to the optical system and detector. Another benefit of this design is that the ion box is maintained at an uniform temperature, eliminating hot and cold zones. The result is that condensation and thermal breakdown can be managed. (Patent pending)



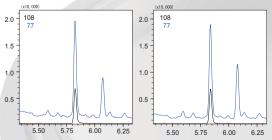
High-sensitivity analysis of chlorpyrifos-methly (5 ppb)



High-Capacity Differential Vacuum System

A high-capacity dual-inlet turbomolecular pump with a differential vacuum system maintains dual zone vaccum and enables the column flow rate to be set to a maximum of 15 mL/min.

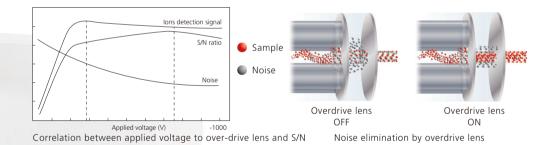
Twin Line column system allows two capillary columns to be simultaneously installed into the mass analyzer without loss of sensitivity.



Chromatogram of chloroacetic acid methyl ester (25 ppb) Left: Twin Line MS analysis Right: Single column analysis The rod bias voltage is automatically optimized during ultrahigh-speed data acquisition, thereby minimizing the drop in sensitivity that would otherwise occur above 10,000 u/sec. The GCMS-QP2010 Ultra achieves a level of sensitivity better than five times that of older instruments, and is particularly effective for scan measurement in applications related to fast-GC/MS and Comprehensive GC/MS (GC×GC/MS). (Patent: US6610979)

Overdrive Lens (Noise Elimination Technology)

The addition of an overdrive lens, positioned in front of the electron multiplier, serves to reduce the random noise that occurs with ion transmission, improving the S/N ratio. When applied, this lens acts as a filter designed to remove low mass ions that would otherwise interfere with the spectral scan. (Patent: US6737644)

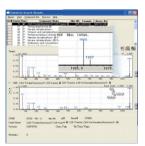


High-Performance Quadrupole Mass Filter

Combining a quadrupole mass filter designed for high precision with Shimadzu's patented technology for mass scanning produces ideal mass filter characteristics (Patent: US5227629).

This system includes a removable and easily cleaned pre-rod lens that reduces contamination of the rod assembly which would otherwise occur with long-time use.

The GCMS-QP2010 Ultra can perform manual mass calibration by using fragment ion m/z 1066 of Tris(perfluorononyl)-S-triazine (molecular weight 1485) as well as mass calibration by auto-tuning. This feature makes it possible to obtain accurate mass assignment across the entire mass range.



Confirmation of mass spectrum of Tris(perfluorononyl)-S-triazine



Ultra Fast

Equipped with High-Speed Data Acquisition and Processing Via the Newly Developed ASSP™ Function

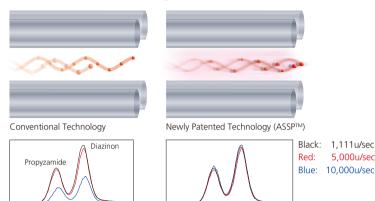
The relatively slow scan speeds of older GC-MS systems have proven to be a limiting factor when adapting the techniques of "Fast GC" or comprehensive GC×GC to the guadrupole GC-MS platform. Data acquisition speeds of 30 Hz or less and 10,000 u/sec are marginal at providing enough points across an ultra sharp, fast GC or a GC×GC peak for reliable quantitation.

A new technology has been developed which allows us to increase the scan speed of our GC-MS system. This technology, Advanced Scanning Speed Protocol (ASSPTM), is the key to faster data acquisition.

Incorporated in the new GCMS-QP2010 Ultra, it is a firmware protocol that optimizes the ion transmission hardware parameters combined with a highly efficient data collection algorithm allowing acquisition speeds of 20,000 u/sec and 100 Hz. ASSPTM provides the added benefit of maintaining system sensitivity at elevated scan speeds and virtually eliminates mass pattern skewing.(patent: US6610979)

1,111u/sec

5,000u/sec





Variation of chromatogram intensity at each scan speed ASSP™ optimizes the ion transmission optics to maintain ion signal intensity across the entire mass range as the scan speed of the system increases.

High Sensitivity and High Speed Scanning

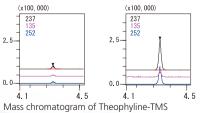
Fast GC/MS analysis is performed using ultra narrow-bore capillary columns. The resulting peaks are very sharp and elute very guickly. To fully define these peaks, between10 to 20 points are needed. In most cases, data collection at the conventional rate of between 10 and 30 Hz is inadequate. The GCMS-QP2010 Ultra provides the solution with 20,000 u/sec scan rate and 100 Hz collection and processing speed.

Improved Sensitivity

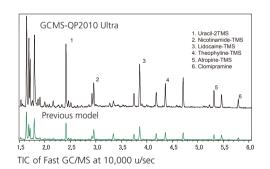
During high-speed scan analysis, a decrease in ion signal strength is observed in older GC-MS systems. ASSP™ acts to minimize these drops which result in a higher signal to noise ratio and thus, overall greater sensitivity

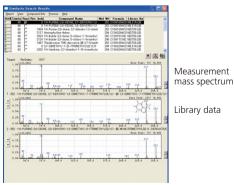


The ASSP™ function makes it possible to reduce the drop in sensitivity that may occur in the high mass region of a spectral scan. This means that high quality results can be obtained in library-based similarity searches.



Left: Previous model Right: GCMS-QP2010 Ultra

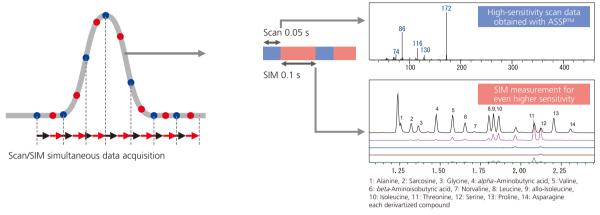




Similarity search of mass spectrum obtained at 10,000 u/sec

Scan/SIM Analysis Improved using ASSP™

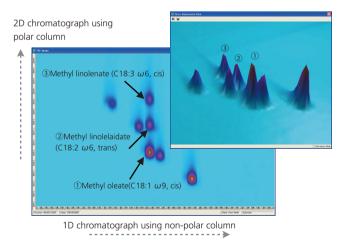
FASST (Fast Automated Scan/SIM Type) is a data acquisition technique that allows the user to collect scan data and SIM data in a single analysis. It is used in the dual role of collecting qualitative Scan data and quantitative SIM data. Applying ASSP™ technology allows the user to collect more channels of SIM data in a SIM/scan cycle by allowing the SIM dwell times to be shortened by as much as 5 times over the previous model.



Amino acid analysis in simultaneous Scan/SIM data acquisition

Comprehensive 2 Dimensional Gas Chromatography (GC×GC)

Comprehensive (GC×GC) chromatography is a powerful technique that combines two capillary columns of complementary, orthogonal stationary phases, using a mid-point modulating device. The resulting peaks are very narrow and fast eluting, requiring very fast data collection rates to properly measure.



Separation of the trans and cis forms of a fatty acid methyl ester

GCMS-QP2010 Ultra delivers the high-speed scanning that the GC×GC technique demands. ASSP[™] facilitates data collection and processing without compromising sensitivity or spectral integrity.



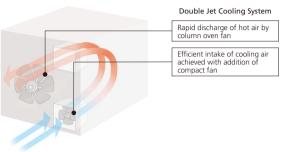
Enhanced Throughput

Variety of Functions for Enhanced Productivity in the Laboratory

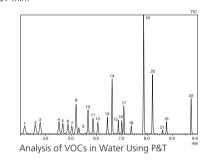
Reduction of analysis time, shortening of maintenance time and quick column exchange are productivity enhancing measures desired by every busy lab. The GCMS-QP2010 Ultra is equipped with a variety of functions that fulfill these requirements.

High-Speed Oven Cooling for Shorter Analysis Cycle

The GC is able to cool from 350°C to 50°C in approximately 2.7 minutes, an improvement of 2.6 minutes from the previous model. This was accomplished thru the development of a "double jet cooling system". Imagine your VOC analysis cycle time being cut in half. The GCMS-QP2010 Ultra makes this a reality by combining Fast GC technology with rapid oven cooling, effectively increasing sample throughput in your lab!



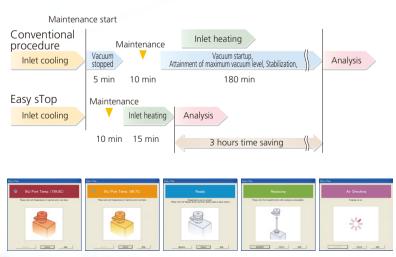




The combination of a high-speed GC/MS method and a fast oven cooling rate dramatically reduces the analysis cycle. This VOC analysis is reduced by more than half.

Easy sTop for Major Reduction of Maintenance Time

Many applications require that the injection port undergoes maintenance on a frequent basis. With the GCMS-QP2010 Ultra, maintenance is possible without venting the MS so downtime is minimized.





The Easy sTop navigator assists in taking the appropriate steps.

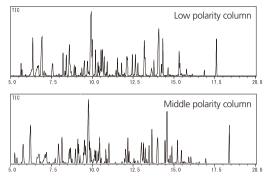
Twin Line MS System Eliminates the Need to Swap Columns

The GCMS-QP2010 Ultra is capable of accepting installation of two narrow-bore capillary columns into the MS simultaneously. This allows you to switch applications without physically modifying the column installation. Simply decide which column is best for your analysis and choose the associated injection port.



Installing two columns in one MS is possible with the GCMS-QP2010 Ultra because of its high-capacity dual-inlet turbomolecular pump.

* The Twin Line MS System requires an optional installation kit and is limited to certain column dimensions.



Analysis of flavor and fragrance components using complementary column phases

Sensitivity Comparison Table

Compound	Single Column	Double Column	
Methamidophos	1149179	1132498	
DDVP (Dichlorvos)	392962	388569	
EPTC	632087	641883	
Butylate	455472	442888	
Acephate	1803821	1903527	
MIPC (Isoprocarb)	1029203	1052476	
BPMC (Fenobucarb)	1527113	1544812	

Column flow rate Column total flow rate 1.7 mL/min 3.4 mL/min

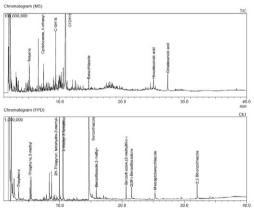
Simultaneous Data Acquisition with Two Detectors Improves Efficiency of Data Comparison Work

By splitting the flow at the end of the analytical column and sending the eluted components to multiple detectors, the chromatographer is able to acquire multiple chromatograms simultaneously. This technique is useful for various applications. One example is a single injection into an analytical column, where the effluent is split to an FPD and MS, providing positive identification and allowing for selective GC detection with quantitation in the same run.

Advanced Flow Technology



Sample loss is reduced with a deactivated splitting device.



Simultaneous detection using MS and FPD of a pyrolyzed rubber sample

Sulfur compounds are selectively detected by the FPD and qualitative analysis is performed using the mass spectrometer simultaneously.





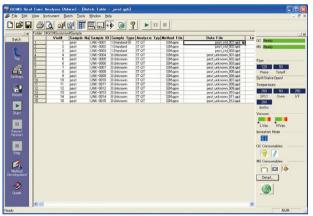
Workstation Software Combines Ease of Use and Versatile Functionality **GCMSsolution**

GC/MS analyses require optimization of many operating parameters. Data analysis may require many calibrations to be performed, and many unknowns to be quantified with results reported. GCMSsolution workstation software combines ease of use with versatile functionality to effectively perform these tasks.

GCMS Analysis Program

This program performs the batch processing settings required for the GC-MS instrument configuration, MS tuning, analytical condition settings, and continuous analysis. Indication of the usage frequency of consumable items provides a convenient guide for maintenance. There is also an "MSNAVIGATOR," which provides detailed assistance for maintenance with photos. In addition, GCMSsolution is newly equipped with an "Ecology mode" function used to save power and carrier gas consumption.

In order to maintain the integrity of sample information, files used to manage sample names and ID numbers are loaded directly to GCMSsolution software, registered in the acquired data, and output to reports. This helps improve the reliability of data information.



Analysis Program Window

By selecting the Ecology mode, consumption of electric power in standby mode and carrier gas usage can be reduced. Ecology mode can be entered automatically at the end of a batch or series of batch runs.



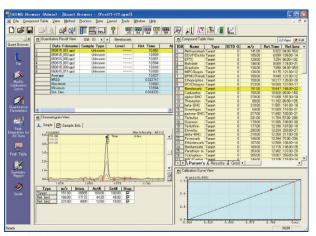
GCMS Browser Program

Quantitation Browser

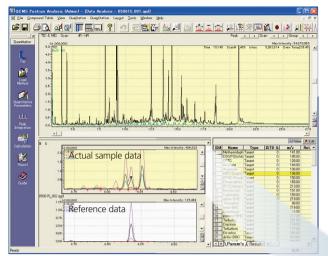
Browser is an off-line program allowing the user to perform statistical analyses and monitor quality control from batch runs or on multiple data files. Apply modified method post-run processing parameters to previously run data very quickly and instantly see the new results.

Data Browser

This function is used to compare chromatograms or mass spectra of multiple data files.



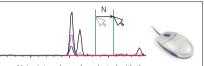
Quantitative Browser Program Window



Post-Run Program Window

GCMS Post-Run Analysis Program

This program performs various tasks related to qualitative and quantitative analysis and post-run reporting. Analyses of detection limit target analytes with significant matrix interference can be challenging. GCMS post run offers tools to help successfully perform your analysis. Overlay your unknowns with low standard runs. Re-plot your chromatograms with just a single ion or a list of multiple ions. Compare the MS data with selective GC detectors such as FPD or ECD for positive confirmation. Up to three channels of data can be viewed simultaneously. Determine the single-to-noise ratio for any peak with the click of your mouse. These are just a few of the many features.



Noise intervals can be selected with the mouse.

The report format can be edited simply by using the mouse to paste the items to

Highly Flexible Report Customization

be output into a blank report window in the desired positions and with the desired sizes. Build your own custom report by choosing from a wide variety of items including chromatograms, spectra, spectrum search results, and quantitative analysis results. Or choose from a selection of template files for quantitative and qualitative analysis, and once a format has been determined, reports of the same format can be created simply by specifying the report file name.



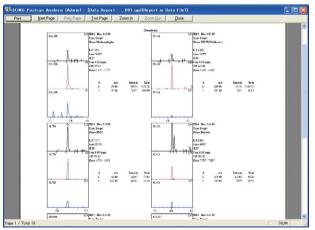
Macro setting for reporting items

Macros for Reports

Macro functions that facilitate the display of required information on reports make it possible to produce a more diverse range of information. They can be used simply by pasting variables for items of information displayed in the help window into the property dialog boxes of report items.

(Macro examples)

Sample names, sample IDs, vial numbers, data files, S/N values, start-up and finish time of S/N noise, and comments, etc.

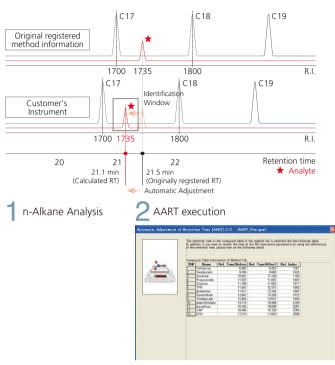


Report Preview Window



Functions Using Retention Indices

Automatic Adjustment of Compound Retention Time (AART)



The AART (Automatic Adjustment of Retention Time) function can estimate the retention times of target components from retention indices and the retention times of an alkane standard mix*. * Requires alkane mix which is sold separately.

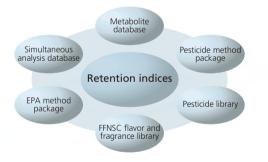
Adjustment of retention time

Compound Name	Predicted RT	Measured RT	RT Error
Mono-BDE (BDE-001)	1.561	1.564	-0.003
Mono-BDE (BDE-002)	1.745	1.746	-0.001
Mono-BDE (BDE-003)	1.968	1.960	0.008
Di-BDE (BDE-010)	5.192	5.174	0.018
Di-BDE (BDE-007)	6.292	6.267	0.025
Di-BDE (BDE-008&BDE011)	6.782	6.761	0.021
Di-BDE (BDE-012)	7.098	7.075	0.023
Di-BDE (BDE-013)	7.157	7.132	0.025
Di-BDE (BDE-015)	7.542	7.517	0.025
Tri-BDE (BDE-030)	9.588	9.554	0.034
Tri-BDE (BDE-032)	10.857	10.822	0.035
Tri-BDE (BDE-017)	11.299	11.263	0.036
Tri-BDE (BDE-025)	11.379	11.344	0.035
13C Tri-BDE (BDE-028L)	11.884	11.851	0.033
Tri-BDE (BDE-028&033)	11.884	11.863	0.021

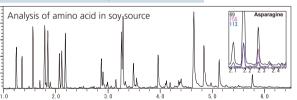
Adjustment can cover many points, from low boiling points to high boiling points, so accurate adjustment is possible over a wide retention time range.

Databases Using Retention Indices

There are databases for environmental analysis, food analysis, and clinical analysis. Retention indices can be used effectively for the identification of components, as well as the adjustment of retention times.

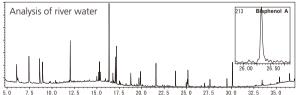


GC/MS Metabolites Spectral Database



This database consists of a mass spectra library (with retention indices) for amino acids, fatty acids, and organic acids and method files in which analytical conditions and data analysis conditions for the analysis of amino acids, fatty acids, and organic acids are set.

Compound Composer Database Software for Simultaneous Analysis (Environmental Analysis)



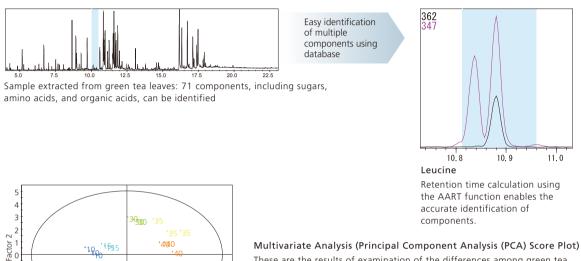
Simultaneous GC/MS analysis supporting identification and quantification of 942 environmental pollutants can be performed. The retention times and calibration curve information of environmentally hazardous chemical substances are registered, so approximate concentrations can be obtained with compounds even when it is difficult to obtain standards.

Applied Data Analysis

Metabolome Profiling Analysis

Metabolome analysis (Metabolomics) can be used for the comprehensive analysis of metabolites in a wide variety of fields. For example, it is used in the field of medicine for diagnostic marker discovery and pathogenic analysis, in the field of pharmaceuticals for the discovery of biomarkers that express drug efficacy and toxicity, and in the field of food products for quality control and prediction.

GC/MS offers high-resolution chromatographic data and produces mass spectra that are unique to each compound, and is therefore suited to the separation and detection of large numbers of metabolites. The database includes retention indexed spectra for positive identification of specific metabolites.



These are the results of examination of the differences among green tea leaves of different rankings. The numerals in the figure indicate the rankings assigned in a tea competition. With respect to principle component 1, the higher ranked tea leaves and the lower ranked tea leaves are positioned separately to the right and left sides of the graph, clearly indicating their quality differences.

Data File Conversion Function

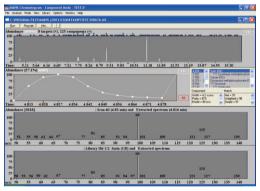
-10-9 -8 -7 -6 -5 -4 -3 -2 -1 0 1 2 3 4 5 6 7 8 9 10 Factor 1

5

-3

GC-MS measurement data can be converted to AIA, JCAMP, ASCII, mzData, or mzXML format for output. Private libraries can also be converted to JCAMP format. This bolsters support for combined use with the AMDIS program provided by NIST. The AMDIS program allows the identification of target components and the discovery of unknown components using a mass spectrum deconvolution function. (The NIST Library must be purchased separately.)

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Deconvolution analysis using AMDIS program



A Comprehensive Range of Accessories

AOC-20i/s Automatic Liquid Sample Injection System

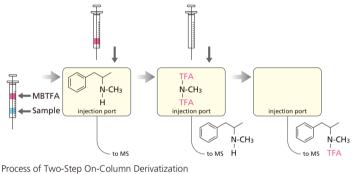


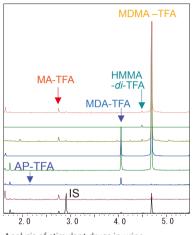
The AOC-20i autoinjector is capable of holding up to a maximum of 15 vials (150 vials if the AOC-20s sampler is installed). The selection of microsyringes consists of a standard 10 μ L type, small-capacity 0.5 μ L and 5 μ L types, and large-capacity 50 μ L and 250 μ L types.

The solvent flush method, where solvents and standard samples are held in the syringe together with samples obtained from the vials before injection, can also be used. Using two AOC-20i units simultaneously makes it possible to introduce the same sample into two injection ports and implement two lines of analysis using MS and GC detectors. The Twin Line MS System allows analysis to be performed alternately between two columns of different phase chemistries.

Two-Step On-Column Derivatization

On-column derivatization, where the sample is derivatized inside the column, is now possible. This is effective for the analysis of stimulant drugs, such as amphetamine, methamphetamine, and MDMA, in urine. Until now, the derivatization procedure required manual preparation that took 30 minutes. Now, this procedure can be completely automated and performed in only 4 seconds using the optional package.





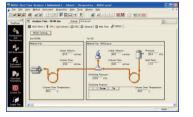
Analysis of stimulant drugs in urine

Advanced Flow Technology

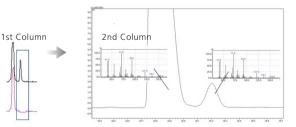
Shimadzu Advanced Flow Technology series includes the following:

- Multidimensional system for high-resolution chromatography
- · Heart-cut system for high-resolution chromatography at a lower cost
- Backflushing kit to reduce the analysis time
- · Detector-splitting kit to enhance identification capability
- · Detector-switching system to introduce target components into the appropriate detector

Specialized software is available for each technique, providing powerful support for the determination of complex analytical conditions.



Parameters setting by MDGCsolution Compounds which cannot be separated in the 1st column are introduced to the 2nd column with different phase chemistries.



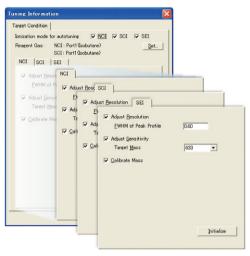
Analysis of Optical Isomers of Linalool in Lavender Oil using Multidimensional System

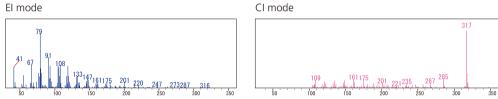
Chemical Ionizations

In addition to commonly-used electron ionization (EI), both chemical ionization (CI) and negative chemical ionization (NCI) are available. CI is suited for confirmation of ionized molecular weight. NCI can be used to detect functional groups having a large electron affinity such as halogens. Tuning is fully automated for any ionization method: EI, CI, or NCI. Any of three types of reagent gases (methane, isobutane, or ammonia) can be used.

The ion source for NCI can be used with either EI or CI, making it possible to switch between ionization methods without having to replace the ion source.

If high-sensitivity measurement is required, use a specialized ion source.



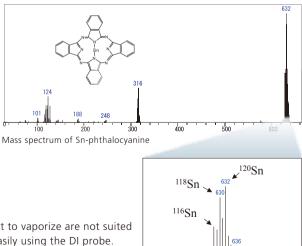


Mass spectrum of cis-5,8,11,14,17-Eicosapentaenoic Acid Methyl Ester (C20:5n3) in El and Cl In cases where the identification of molecular ions is difficult by El, it is easily accomplished by Cl.

Direct Injection System DI-2010

The DI Probe allows a sample to be introduced directly into the ion source without being passed through a GC column. It is an effective technique for obtaining mass spectra of synthetic compounds that do not chromatograph well. A DI system can be incorporated into a standard GC-MS configuration without making any changes to the GC. It is then possible to switch between conventional GC column chromatography and DI analysis without making any hardware changes.





624

625

Components that are thermally degradable or difficult to vaporize are not suited to GC analysis. Their mass spectra can be obtained easily using the DI probe. Above is an example of Sn-phthalocyanine spectra obtained using the DI Probe.



650

Eco Friendly

Eco-Friendly Design for Lower Running Costs in the Laboratory

There is increasing public interest in reducing running costs and environmental stress. Reducing power consumption is a common concern not only for the reduction in a laboratory's energy cost, but also as a way to reduce CO₂ emission. In addition, helium carrier gas is a non-renewable, valuable natural resource. The GCMS-QP2010 Ultra has eco-friendly features for saving power and carrier gas.

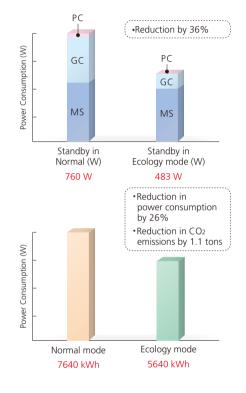


Saving Power Consumption with an "Ecology mode" for Reduced Instrument Running Costs

Equipping the instrument with "Ecology mode" reduces the power consumed in analysis standby mode by 36%, compared with the previous model. In nighttime GC-MS operation Ecology mode can be set automatically, which makes it possible to reduce unnecessary power consumption.

Reduction of Power Consumption in Analysis Standby Mode

When Ecology mode is entered, unnecessary power consumption by the GC, MS, and PC is automatically eliminated. The consumption of carrier gas is also automatically reduced. Furthermore, Ecology mode can be entered automatically after continuous analysis, so power and carrier gas can be saved automatically after the completion of nighttime analysis.



Reduction of Annual Power Consumption

If Ecology mode is used over one year of operation*, power consumption can be reduced by 26% and CO₂ emissions can be reduced by approx. 1.1 tons.

*) This is based on 6 hours of use per day for 260 days over the course of a year under our standard analytical conditions.

Consideration of Global Warming

Using a setup in which Ecology mode is incorporated into the GC-MS production line reduces CO₂ emissions discharged by 30%. At Japanese production plants, we have incorporated photovoltaic power facilities. The maximum power generated is 25 kW, and we expect an annual power generation effect of 22,000 kWh, which corresponds to an annual reduction in CO₂ emissions of 8.3 tons.

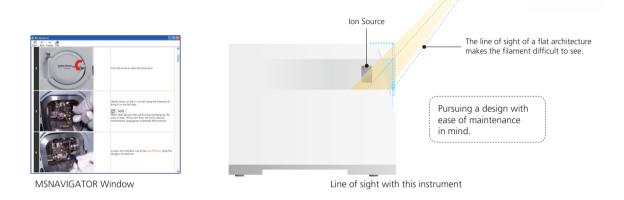




User Friendly

Design Offers the Ultimate in Ease of Use

When changing the ionization method or performing maintenance of the area around the ion source, parts inside the evacuation system must be handled. The GCMS-QP2010 Ultra uses a front-opening chamber in a design that is both visually pleasing and practical, allowing maintenance to be performed with ease from the front of the instrument. "MSNAVIGATOR," which supports maintenance, has been improved to help the user perform instrument maintenance.



Comprehensive Selection of Documents and Packages of Tools and Consumable Items Facilitate Ease of Use

We have prepared a "Quick Navigation" to allow even first-time operators to use GC-MS with ease and an "Operation Guide" that explains operations as they are encountered in the flow of analysis. We have also prepared packages with photos that allow easy recognition of the types and part numbers of tools and consumable items, and thereby support operation and maintenance of the instrument.





Versatile System Configurations

The GCMS-QP2010 Ultra can be configured in multiple ways to meet an expanded range of applications.

Headspace Analysis (Environmental, Food and Chemical Analysis)

The headspace sampling technique is used in a variety of industries, including foods and flavors, environmental and pharmaceutical. Any volatile target analyte that can be driven out of solution with heat and agitation into the headspace above a liquid is suitable for analysis by this technique. The GCMS-QP2010 Ultra is the perfect platform for headspace analyses.

Purge & Trap Analysis (Volatile Organic Compounds Analysis in Water)

The Purge and Trap sampling technique is used for concentrating volatile organic compounds from environmental matrices and then introducing the concentrated sample into the GC-MS for analysis. With its sensitivity and ruggedness, the GCMS-QP2010 Ultra is an outstanding choice for environmental analyses.



AOC-5000 is a GC sample introduction system that combines liquid, large volume and head-space injection as well as solid-phase microextraction (SPME) in one single instrument. This unique capability allows quick switching from one application to another on the same GC workstation.



Thermal Desorption is a technique for air sample concentration. It utilizes a small tube filled with the appropriate sorbent material. Samples are collected in the field and transported.



A multi-dimensional GC/GCMS system performs separation using two columns of orthogonal phases. The system employs a pressure switching heart-cut device (Multi-Deans Switch) to direct the effluent of the first column on to a second column. The Multi-Deans Switch assembly has been designed to install directly into a GC-2010 Plus and be combined with a GCMS-QP2010 Ultra. This system provides the ultimate in chromatographic performance.



Pyrolysis is performed on plastics, rubbers and resins. The resulting pyrolysates are analyzed by GC-MS, and the chromatograms reflect the original structure of the polymer. Identification of monomers as well as information related to sophisticated structural analysis of the polymer is possible. The GCMS-QP2010 Ultra is well-suited for this application.



The Comprehensive GC/MS (GC×GCMSq) technique employs a modulator to link two capillary columns of complementary orthogonal phases. The technique requires a GC-MS system capable of very fast data collection to fully capture the very narrow, fast eluting compounds. Sensitivity is also an important requirement for many Comprehensive GC×GC applications. The GCMS-QP2010 Ultra was developed with this multi-dimensional technique in mind. Its best-in-class data collection speeds and superior sensitivity make it the top choice for Comprehensive Chromatography.

Optional Software

AOC-5000 Control Software

Allows management of AOC-5000 parameters in GCMSsolution, and works with GCMSsolution to perform batch analysis.

EPA Optional Software

Supports analysis according to US EPA regulations. Specialized reports and quality assurance functions are available.

Compound Composer Database Software 2nd Edition for Simultaneous Analysis

The retention times, mass spectra and calibration curves for 942 hazardous chemicals are registered in the database. In combination with the prediction of retention times using n-alkanes (retention index), the database supports highly reliable compound identification. In addition, approximate quantitative results for hazardous chemicals can be confirmed without using calibration standards.

Mass Spectral Libraries

NIST Library

The main library contains spectra for 191436 general compounds, and 219743 of these spectra are registered in a sub-library. More than 99.9% of these spectra are accompanied by structural information. In this library, retention indices are given for about 90% of the compounds.

Wiley Library

This library contains spectra for about 592000 general compounds and 662000 of these spectra.

Pesticide Library 3rd edition

This is a library containing mass spectra for 578 compounds measured using the electron ionization (EI) method and 383 compounds measured using the negative chemical ionization (NCI) method. Highly reliable identification is possible using the mass spectra of the EI and NCI modes together. The library also includes a method for analyzing pesticide residues in food and tap water.

FFNSC (Flavor and Fragrance Natural and Synthetic Compounds) Library

This is a library for 1830 fragrance-related compounds. The library contains mass spectra as well as retention indices, allowing retention-indexed searches.

Drug Library

This library contains spectra for 7840 compounds, including drugs, poisons, pesticides and environmental pollutants.

GC/MS Metabolite Mass Spectral Database

This database contains mass spectral library and method files that specify analytical conditions and data analysis parameters for amino acids, fatty acids, and organic acids.





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