

Gas Chromatograph Mass Spectrometer

GCMS-QP2020

UFMS
ULTRA FAST MASS SPECTROMETRY



Gas Chromatograph Mass Spectrometer **GCMS-QP2020**



The importance of high-performance analytical instruments for monitoring microscopic quantities of compounds related to environmental pollution and human health, and for developing and evaluating new, highly functional materials and chemical products continues to grow. The GCMS-QP2020 has been designed to meet these needs. Featuring enhanced instrument functionality, analysis software, databases, and a sample introduction system, the GCMS-QP2020 will help maximize the capabilities of your laboratory.



Ultra High Speed GC-MS That Offers a Dramatic Leap in Sensitivity and Productivity

Provides Higher Sensitivity and Reduced Operation Costs

The vacuum system adopts a new differential exhaust turbomolecular pump and achieves maximum sensitivity under all conditions for GC analysis. In addition to helium, the system can operate with hydrogen or nitrogen as the carrier gas, which enables operation cost reduction. In addition, the high-sensitivity, high-speed analysis capability shortens analysis times and maximizes laboratory productivity.

Dramatic Improvement in the Efficiency of Multicomponent Simultaneous Analysis

The GCMS Insight software package dramatically improves the sensitivity and efficiency of multicomponent simultaneous analysis. The Smart SIM method creation program creates methods that provide higher sensitivity in multicomponent analyses. Furthermore, LabSolutions Insight, which significantly shortens data analysis times, dramatically heightens the efficiency of data analysis procedures.

Databases with Retention Indices to Support Analysis

Databases are available to match various requirements, including environmental analysis, food analysis, off-flavor analysis, and forensic analysis. All the databases include retention indices, so you can start analysis even without standard samples. The retention indices can also be used to easily create methods for a variety of more accurate qualitative and quantitative analyses.

Configure Optimal Analysis Systems to Meet Your Needs

With a sample injection system that matches the sample form and the concentrations of the components being measured, as well as a 2D chromatography system that makes full use of the high-speed scan capability, you can configure optimal analysis systems to suit a variety of your analytical needs. And since all these analysis systems are supported by Shimadzu you can put your mind at ease when using them.

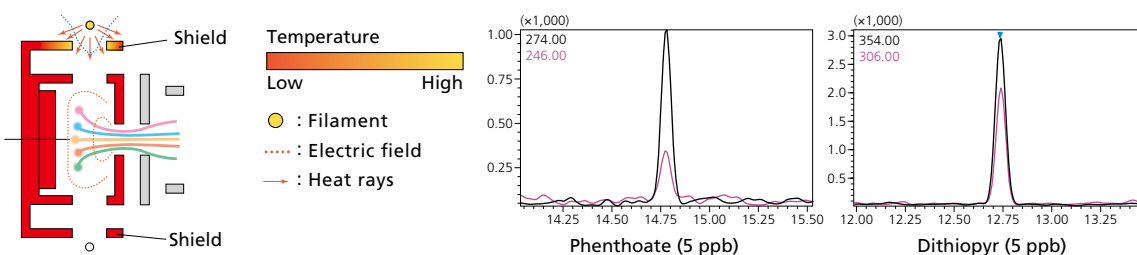
Provides Higher Sensitivity and Reduced Operation Costs

High-Performance Ion Source

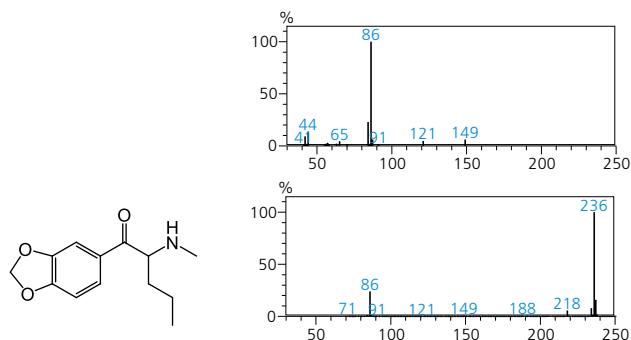
High sensitivity, stable analysis is achieved by incorporating patented technology for the ion source. In addition, the system is equipped with a **Quick-Cl** function that enables checking molecular ions in CI mode without stopping the MS. This demonstrates its capabilities in both quantitative and qualitative analyses.

* Limited to the NCI model.

Using patented technology, the shield plate suppresses the accelerating voltage and thermal radiation from the filament to achieve a space inside the ion source that is stable, with few active sites.



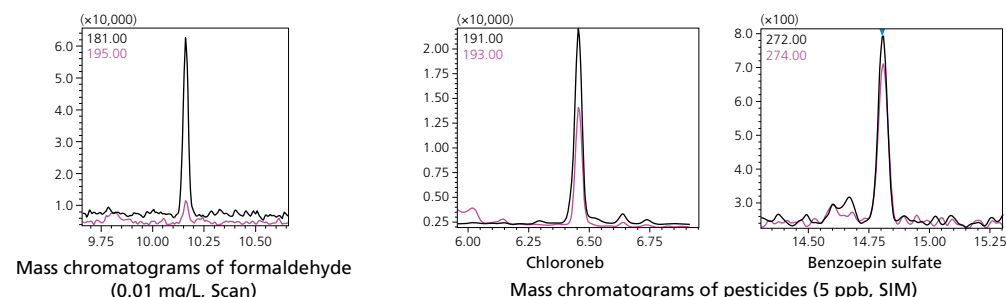
Even though confirmation of molecular related ions is difficult with the EI method, data can be acquired by Quick-Cl immediately without stopping the MS.



EI Mass Spectrum (Top) and CI Mass Spectrum (Bottom) for Pentylone, a Type of Cathinone

Adopts a New Large-Capacity Pump

A new turbomolecular pump with improved exhaust efficiency has been adopted. This significantly improves performance when not only helium but also hydrogen or nitrogen is used as the carrier gas. In addition, the differential exhaust system evacuates the ion source and quadrupole separately, thereby achieving the optimal MS state under all carrier gas conditions.



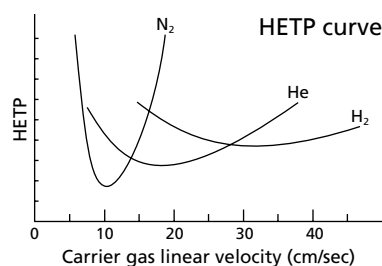
Analysis Results with Hydrogen Carrier Gas

High-Performance Gas Chromatograph

Long-term stability is achieved for retention times thanks to AFC (advanced flow control) with built-in compensating technology for room temperature fluctuations. In addition, the constant linear velocity control mode keeps the linear velocity of the carrier gas constant even if the column oven temperature changes, so the best GC separation is always achieved.

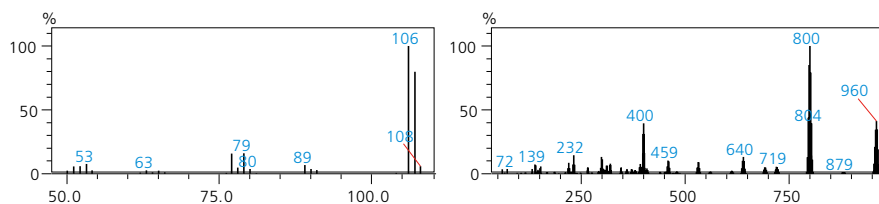


Advanced Flow Controller (AFC)



High-Accuracy MS Filter with Pre-Rod

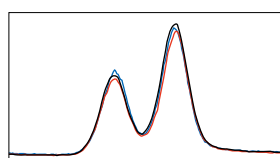
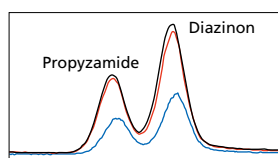
The MS filter incorporates a metal rod to prevent contamination of the quadrupole. This results in stable MS performance directly after startup. The system covers a wide practical mass range region, from m/z 1.5 to 1090.



Mass Scan Spectrum of o-Toluidine (Left) and of Decabromodiphenyl (Right)
Enables highly accurate analysis from high molecular to low molecular compounds.

High-Speed Scan Control Technology Advanced Scanning Speed Protocol (ASSP™)

The rod bias voltage is automatically optimized during high-speed data acquisition, which minimizes sensitivity deterioration during high-speed scans of 10,000 u/sec or faster. The sensitivity obtained is at least five times better than with conventional systems. This is effective for scan data sensitivity improvements and favorable mass spectrum acquisition, particularly in high-speed analysis with Fast-GC/MS, simultaneous Scan/SIM, FASST analysis, and applications using GC × GC-MS. (Patent: US6610979)



Black: 1,111 u/sec
Red: 5,000 u/sec
Blue: 10,000 u/sec

Chromatogram Intensities at Different Scan Speeds

At scan speeds of 10,000 u/sec and faster, the ions are accelerated at the optimal voltage using the ASSP function, thereby suppressing signal speed reductions across a wide m/z range.

Dramatic Improvement in the Efficiency of Multicomponent Simultaneous Analysis

GCMS Insight Software Package

The new software which packages automatic method creation function and multi data processing program dramatically improves the efficiency of daily analysis procedure.



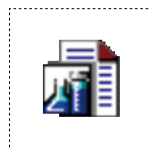
More Convenient Multicomponent Analysis

The Smart SIM automatic method creation function automatically configures the SIM program to suit the retention times. Even in cases where there are a number of compounds and they are apportioned to multiple methods, the methods can be integrated while maintaining the sensitivity as is. This significantly reduces the number of analysis cycles and the measurement time, improving productivity.



Smart SIM

The optimal MS table is automatically created



SIM method file

- 41 : Chlorpropham
- 42 : Ethalfuralin
- 43 : Dichlofamid metabolite
- 44 : Naled
- 45 : Flusilazole metabolite
- 46 : Dicrotophos
- 47 : Trifluralin
- 48 : 2,6-Dichlorobenzamide
- 49 : Bendiocarb
- 50 : Disubenzofos
- 51 : Benfluralin
- 52 : Monocrotophos
- 53 : Sulfotep
- 54 : Cadusafos
- 55 : Di-allate-1
- 56 : Phorate
- 57 : alpha-HCH
- 58 : Di-allate-2
- 59 : Desmedipham deg
- 60 : Thionet
- 61 : Hexachlorobenzene
- 62 : Dicloran
- 63 : Dimethoate
- 64 : Simazine
- 65 : Fenitrothion
- 66 : Carbofuran
- 67 : Chlorobutyl
- 68 : Atrazine

For the databases used with Smart SIM, Shimadzu GCMS methods currently in use can be used as is.

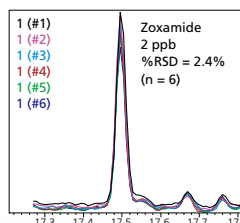
Input		m/z for SIM or Scan											
Scan#	Type	Acq. Mass	Method No.	Compound name (s)	Type	m/z	Rel. I.	Type	m/z	Rel. I.	Type	m/z	Rel. I.
1	Target	SIM	1	Acetaminophen	T	111.0	100.00	Ref. 1	111.0	100.00	T	111.0	100.00
2	Target	SIM	1	Acetaminophen	T	129.0	100.00	Ref. 1	129.0	100.00	T	129.0	100.00
3	Target	SIM	1	Acetaminophen	T	151.0	100.00	Ref. 1	151.0	100.00	T	151.0	100.00
4	Target	SIM	1	Acetaminophen	T	173.0	100.00	Ref. 1	173.0	100.00	T	173.0	100.00
5	Target	SIM	1	Acetaminophen	T	195.0	100.00	Ref. 1	195.0	100.00	T	195.0	100.00
6	Target	SIM	1	Acetaminophen	T	217.0	100.00	Ref. 1	217.0	100.00	T	217.0	100.00
7	Target	SIM	1	Acetaminophen	T	239.0	100.00	Ref. 1	239.0	100.00	T	239.0	100.00
8	Target	SIM	1	Acetaminophen	T	261.0	100.00	Ref. 1	261.0	100.00	T	261.0	100.00
9	Target	SIM	1	Acetaminophen	T	283.0	100.00	Ref. 1	283.0	100.00	T	283.0	100.00
10	Target	SIM	1	Acetaminophen	T	305.0	100.00	Ref. 1	305.0	100.00	T	305.0	100.00
11	Target	SIM	1	Acetaminophen	T	327.0	100.00	Ref. 1	327.0	100.00	T	327.0	100.00
12	Target	SIM	1	Acetaminophen	T	349.0	100.00	Ref. 1	349.0	100.00	T	349.0	100.00
13	Target	SIM	1	Acetaminophen	T	371.0	100.00	Ref. 1	371.0	100.00	T	371.0	100.00
14	Target	SIM	1	Acetaminophen	T	393.0	100.00	Ref. 1	393.0	100.00	T	393.0	100.00



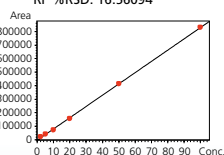
High-sensitivity, high-accuracy analysis is enabled in comparison to the group measurement method. In a batch analysis of 434 components, favorable repeatability and calibration curves were obtained, even down to the trace-quantity region, improving quantitative performance.



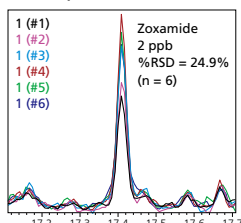
Smart SIM



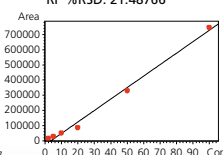
Y = 8320.518X - 2899.459
R² = 0.999566
R = 0.999783
Average RF: 8604.262
RF SD: 1,424.947
RF %RSD: 16.56094



Conventional Method (Group Measurement)



Y = 7547.102X - 26544.7
R² = 0.9921897
R = 0.9960872
Average RF: 6020.259
RF SD: 1,293.612
RF %RSD: 21.48766



Smart Analysis of Hundreds of Data Files LabSolutions Insight

Multi-analyte Data Review

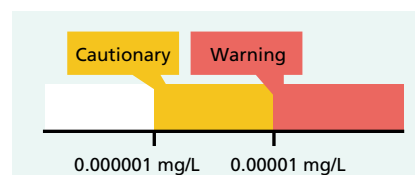
With LabSolutions Insight software, quantitative results for a complete series of data files can be displayed side-by-side for comparison and QC review. All of the chromatograms for a selected target compound can be displayed simultaneously, making it easy to review the detected peaks and confirm the quantitative results. Color-coded QA/QC flags quickly identify any outliers that require further examination.

Color-coded QA/QC Flags

In LabSolutions Insight, quantitative results can be compared to established criteria, and any outliers are color-coded for easy identification and further review. Five color-coded criteria levels can be defined, making it easy to determine which data points are outliers, and which specific QC criteria were not met. Any changes made to calibration curves or manual peak integration are immediately reflected in the color-coded flags.

Example of Using Flags for Quantitative Review

The following example illustrates how an orange flag was set to identify moldy odor compound concentrations that exceeded a defined cautionary limit of 1.0 ppt (part-per-trillion), and a red flag was used as a warning to identify those which had exceeded 10 ppt. In the figure below, quantitative results are tabulated at the top of the screen, while the bottom of the screen simultaneously displays peak identification and integration. Both views include the color-coded flags.



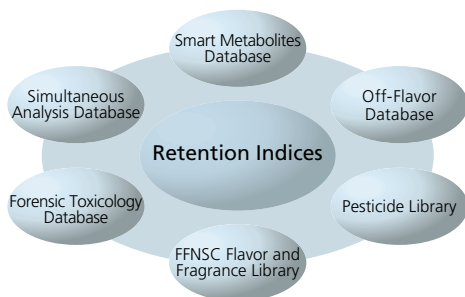
System Configurations Using Multiple Client Computers

Data acquired from multiple analytes can be reviewed or confirmed using client computers connected via a LAN or other network. If multiple systems are used, data obtained from each system can be reviewed from any client computer. Even in the case of multiple analysts using the same system, the ability to separate analytical work from measurement work improves work efficiency.

Databases with Retention Indices to Support Analysis

Databases Using Retention Indices

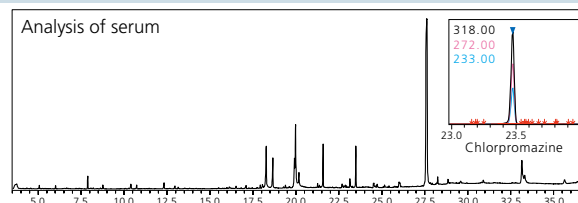
There are databases for environmental analysis, food analysis, and biological sample analysis. Retention indices can be used effectively for the identification of components and the adjustment of retention times.



Other Mass Spectra Libraries

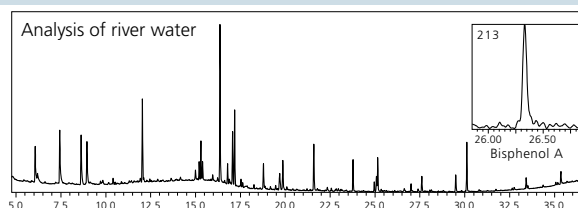
- NIST Mass Spectral Library
Registered with 276,248 spectra.
- WILEY Mass Spectral Library
Registered with 719,000 spectra.
- GC/MS MPW DRUG Library
Drugs, toxicants, pesticides, environmental pollutants (8,650 compounds)

GC/MS Forensic Toxicological Database



It is pre-registered with more than 1400 mass spectra including free-, TMS- and TFA-body types for compounds that are required in forensic toxicological analysis of drugs of abuse, drugs for psychiatric and neurological disease, and other medicines and pesticides.

Compound Composer Database Software for Simultaneous Analysis (Environmental Analysis)



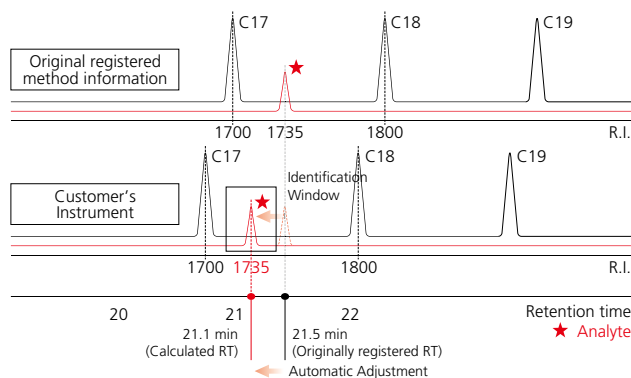
Simultaneous GC/MS analysis supporting identification and quantification of 942 environmental pollutants can be performed. The retention times and calibration curve information of environmentally hazardous chemical substances are registered, so approximate concentrations can be obtained, even when it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

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*.

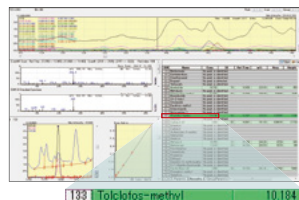
* Requires alkane mix which is sold separately.



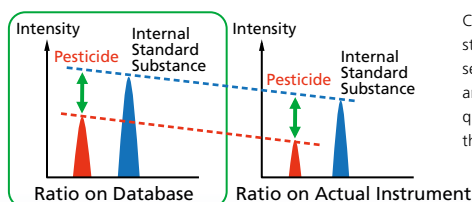
Quantitation Analysis Without Using Standard Samples

Quick-DB GC/MS Residual Pesticides Database is preregistered with calibration curves created utilizing pesticide surrogates, enabling quantitative analysis without the trouble of creating methods using standards. A total of 478 components are contained in the database, enabling the comprehensive quantitative analysis of pesticides.

(Compound Composer Database Software and GC/MS Forensic Toxicological Database also contain this function.)



Example of Analysis of Pesticides in an Actual Sample
(Orange extract, spiked with 10 ng/mL of Each Pesticide)

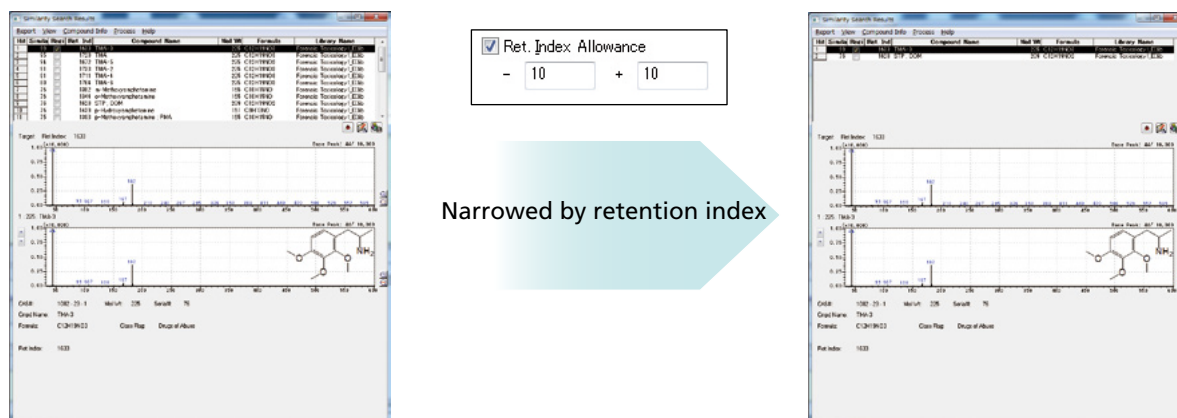


Calibration curves of the relative ratio of internal standard substances are preregistered. A semi-quantitative value is acquired only by adding an internal standard to a sample. If accurate quantitative values are required, be sure to quantify them using a conventional method.

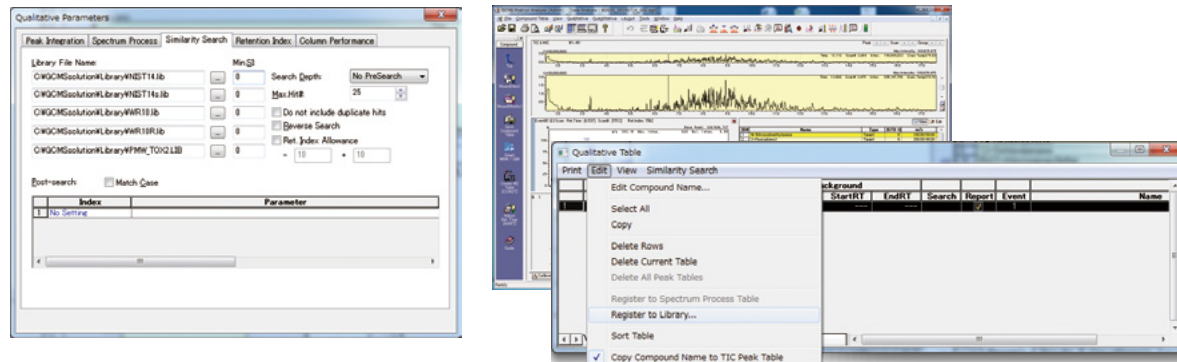
Comprehensive Qualitative Functions

With GCMSsolution, multiple retention index groups can be selected, and searches can be narrowed using a variety of conditions. Accurate qualitative analysis can be performed even for isomers with similar mass spectra.

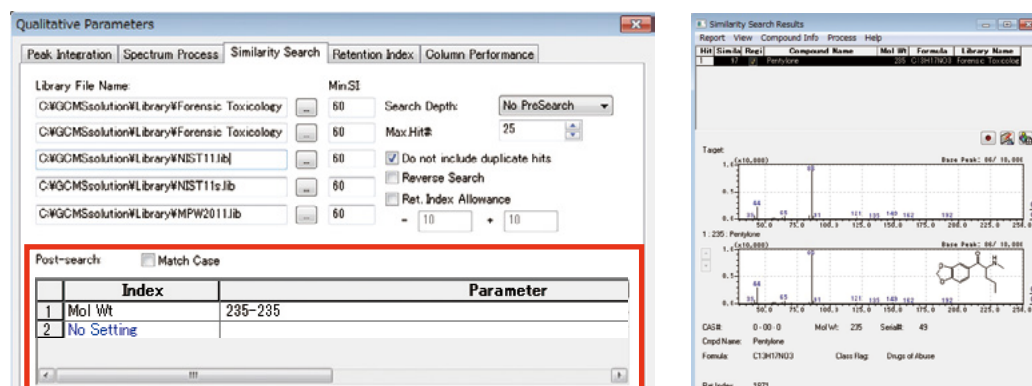
(These functions can be used with the pesticide library and the toxicological database.)



Up to 10 library files can be configured. In addition to the public NIST and Wiley libraries, a variety of library files can be configured. A function to create private libraries is provided, so these are easy to create.



More accurate qualitative analysis is possible by assessing molecular weights from the CI mass spectrum when searching for unknown compounds, and by preregistering molecular weights in a post search index when performing EI mass spectral searches.



Configure Optimal Analysis Systems to Meet Your Needs

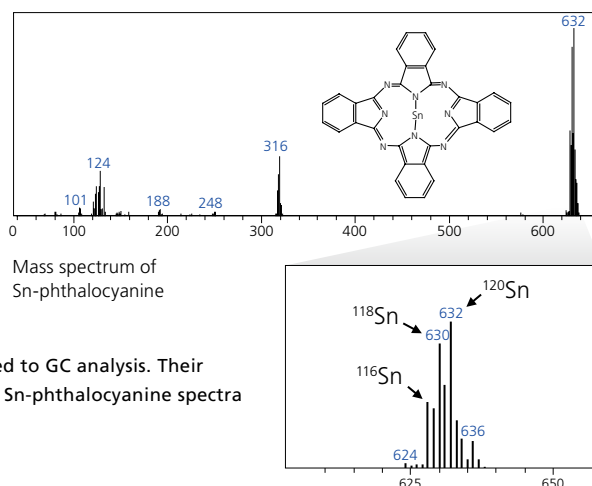
Various System Configurations

For GC-MS analysis, different system configurations may be required depending on the application and sample-introduction needs. The GCMS-QP2020 offers a wide variety of system configurations and sample-introduction devices to enable an expanded range of applications.



DI-2010 Direct Sample Inlet Device

The DI probe allows a sample to be introduced directly into the ion source without passing 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.

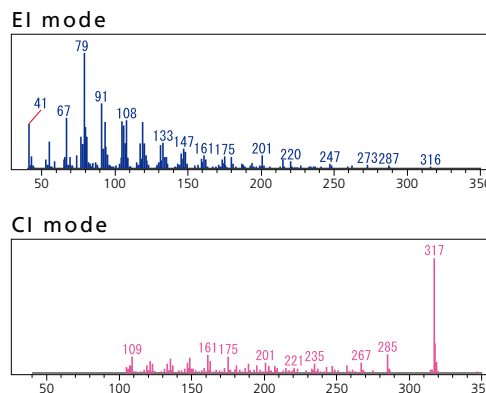


Components that are thermally degradable or difficult to vaporize are not suited to GC analysis. Their mass spectra can be obtained easily using the DI probe. Above is an example of Sn-phthalocyanine spectra obtained using the DI probe.

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 EI and CI. In cases where the identification of molecular ions is difficult by EI, it is easily accomplished by CI.

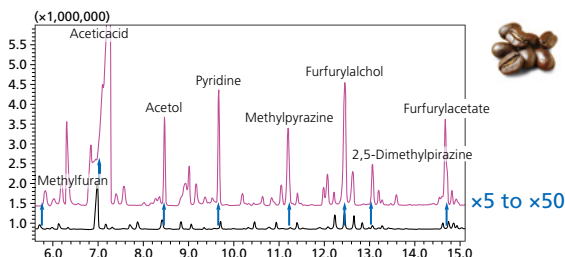
Headspace Analysis System



The HS-20 series of headspace samplers provides strong support for all volatile component analyses, for everything from research to quality control.

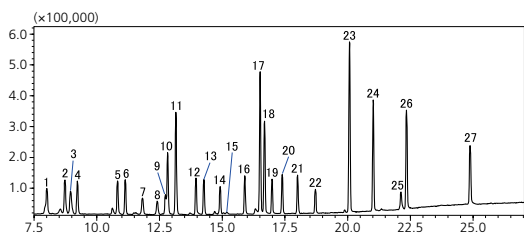
There is a loop model capable of static headspace analysis, and a trap model capable of trap headspace analysis.

High-Sensitivity Analysis of Fragrant Components in Coffee



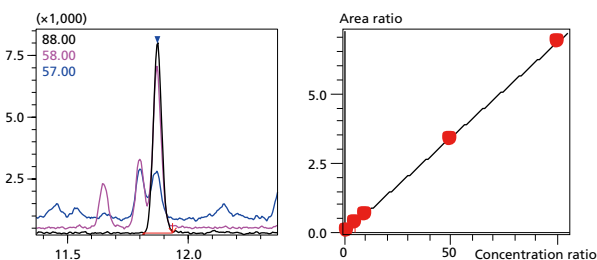
Trace quantities of fragrant components undetectable with conventional headspace samplers can be qualified and quantified by combining the high-sensitivity, electronically cooled trap with GCMS.

Aqueous VOC Analysis



1. 1,1-dichloroethylene, 2. dichloromethane, 3. MTBE, 4. *trans*-1,2-dichloroethylene, 5. *cis*-1,2-dichloroethylene, 6. chloroform, 7. 1,1,1-trichloroethane, 8. carbon tetrachloride, 9. 1,2-dichloroethane, 10. benzene, 11. fluorobenzene (IS), 12. trichloroethylene, 13. 1,2-dichloropropene, 14. bromodichloromethane, 15. 1,4-dioxane-d8 (IS), 16. 1,4-dioxane, 17. *cis*-1,3-dichloropropene, 18. toluene, 19. *trans*-1,3-dichloropropene, 20. 1,1,2-trichloroethane, 21. tetrachloroethylene, 22. dibromochloromethane, 23. *m,p*-xylene, 24. *o*-xylene, 25. bromoform, 26. *p*-bromofluorobenzene (IS), 27. 1,4-dichlorobenzene

Analysis of a trace amount of volatile organic compounds can be performed with the loop mode.



SIM Chromatogram (5 µg/L) and Calibration Curve (1–100 µg/L) of 1,4-Dioxane

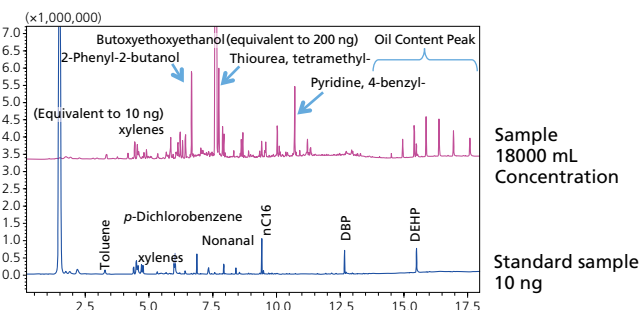
Thermal Desorption Analysis System



The thermal desorption system heats the sample tube, focuses the gas released, and introduces it into the GC-MS. It is used for measurements of VOCs (volatile organic compounds) in air, and for measurements of trace components released from resins and other samples.

With the TD-20, an electronic cooler is adopted to cool the focusing unit; therefore, liquid nitrogen and other coolants are not required.

Analysis of Gas Generated from Electrical Parts

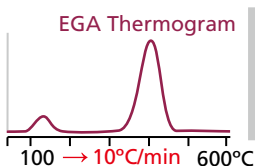
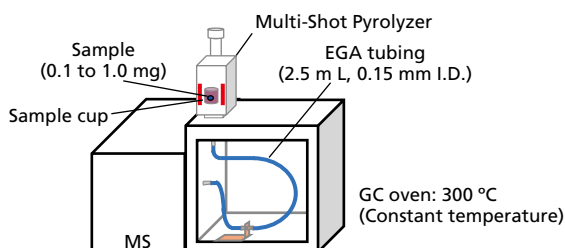


Components Detected with 18 L Outgas (Concentrated) from Electronic Parts Maintained at 70 °C

Pyrolysis System



EGA-MS

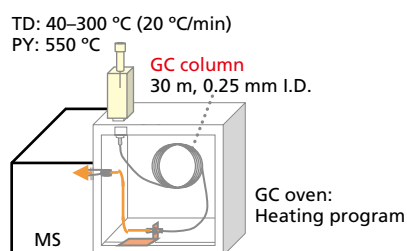


Analysis of thermogram corresponding to temperature

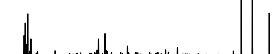
Qualitative analysis using the MS spectrum

High molecular compounds are subjected to pyrolysis at temperatures of 500 °C or higher, and the obtained pyrolytic products are analyzed with GC and GC-MS. These pyrolytic products reflect the structure of the original high molecular compounds. Accordingly, they enable the identification and higher order structural analysis of the polymers. In addition, search software utilizing a pyrolysis library assists in the identification.

Single-Shot (Thermal Desorption, TD) Double Shot (Pyrolysis, PY)-GC/MS



Cycle 1: Thermal desorption (TD-GC/MS) - Analysis of additives



Cycle 2: Pyrolysis (Py-GC/MS) - Analysis of resin



GC×GC-MS System

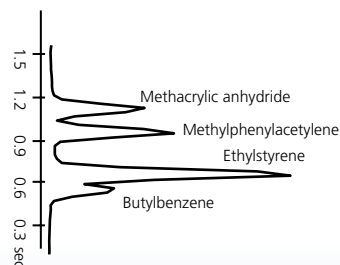
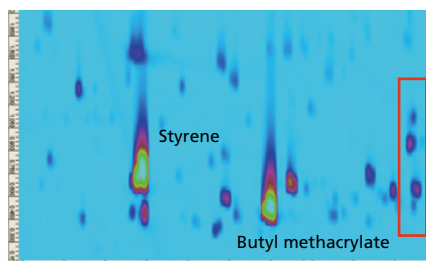


With comprehensive 2D chromatography (GC×GC), chromatographic separation of complex samples is achieved via 2D separation. The Py-GC/MS chromatogram is very complex, but GC×GC separation enables a higher degree of separation and qualitative confirmation.

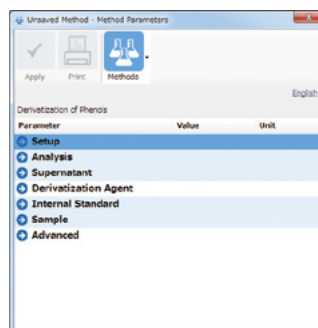
Analysis of Styrene-Butyl Methacrylate by Py-GC×GC-MS



ChromSquare Analysis Software



AOC-6000 Autosampler

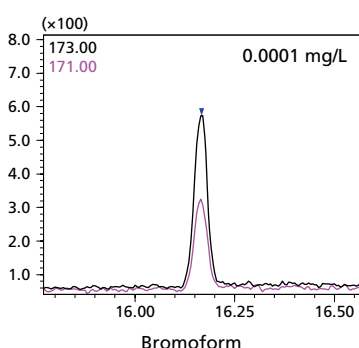
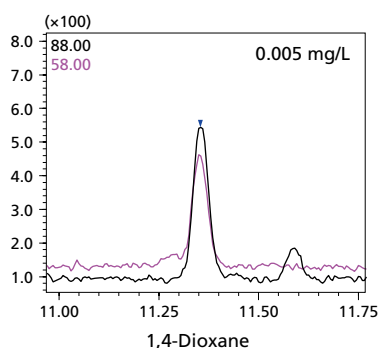


AOC-6000 Control Software

This is compatible with three sample introduction methods: liquid injection, HS (headspace) injection, and SPME (solid-phase microextraction) injection. It can be controlled with GCMsolution software.

The overlap function, which improves the efficiency of continuous analysis, can also be used. Automatic syringe replacement (10 μ L to 1000 μ L) and a stirring function enable sample dilution, the automatic addition of internal standard substances, and the automatic creation of calibration curve samples.

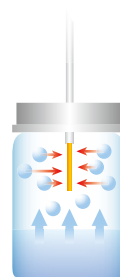
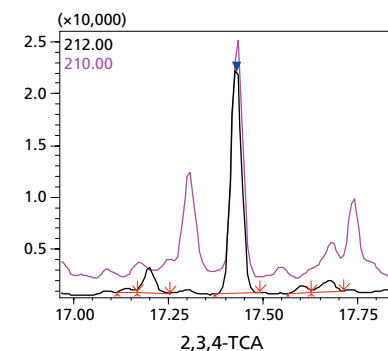
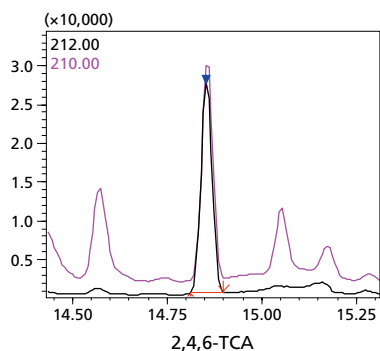
Aqueous VOC Analysis with Headspace Mode



Headspace Mode

Analysis of a trace amount of VOC can be performed with the headspace mode using a syringe.

Analysis of Trichloroanisole in Wine with SPME Mode



SPME Mode

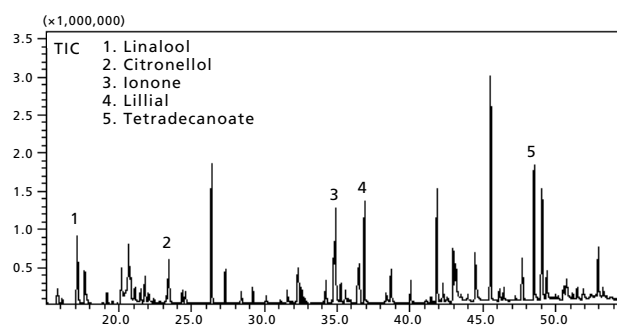
A trace amount of odor compounds was detected by concentration effect with SPME mode at high sensitivity. (5 ng/L)

OPTIC-4 Multimode Sample Inlet

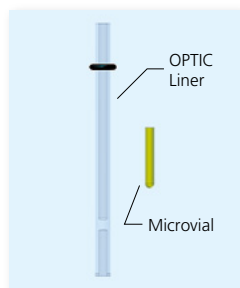


The OPTIC-4 multimode sample inlet is a GC injection port that enables a variety of sample injection modes for GC-MS, including large-quantity injection, inlet derivatization, thermal desorption, and DMI (difficult matrix introduction). Combining this with an autosampler enables automatic replacement of inserts, improving productivity in multisample analyses.

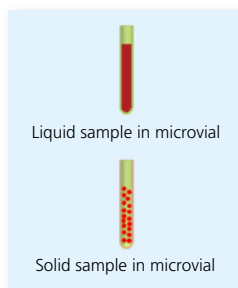
DMI (Difficult Matrix Introduction) Mode Simplifies Pretreatment



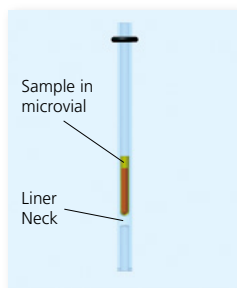
An undiluted shampoo solution was placed directly in a microvial and measured in DMI mode, enabling the selective analysis of volatile components.



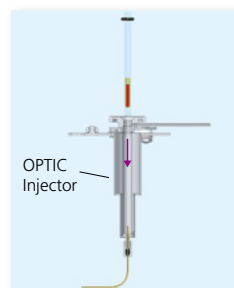
Liner and microvial



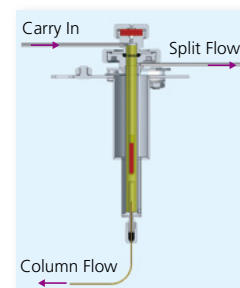
Liquid or solid samples are placed in the microvial.



The microvial containing the sample is placed in the liner.

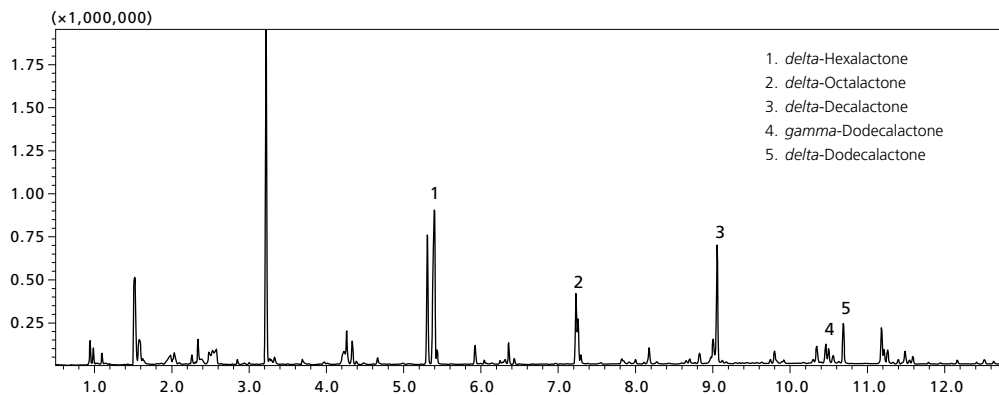


The liner is inserted in the inlet. (Automatic liner replacement is possible as an option.)



The liner is heated, and volatile and semivolatile compounds are introduced to the separation column. Nonvolatile compounds remain in the microvial.

Thermal Desorption Analysis Enables Detection of a Trace Amount of Volatile Compounds



A piece of butter was placed in a vial, headspace gas was collected by an adsorptive agent at ambient temperature, and then a thermal desorption analysis was performed. Various types of volatile components in butter were detected.

GC/MS Off-Flavor Analyzer



Information Registered in Database

Compound Name (E)	Ret. Index	Quadrant	Quadrant	Quadrant	Comment (E)	Threshold
Benzophenone	2470	0.08 (11)	0.48 (11)	0.0000	Burnt, Burnt sugar	10
2,4,6-Tribromophenol	1801	0.0000	0.1492	0.0004	Odorous	100
1-Trichloroaniline	2188	0.11 (11)	0.1471	0.0000	Odorous	1000
2,4,6-Trichlorophenol	2182	0.00 (11)	0.1471	0.0000	Odorous	1
2,4,6-Trichlorophenol	2182	0.00 (11)	0.1471	0.0000	Odorous	1

Primary odor components

GC/MS analytical conditions

Retention time information

MS and calibration curve information

Sensory information of odor components

Odor characteristics

Odor threshold value

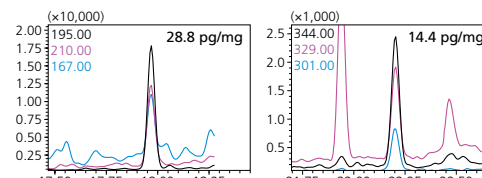
This system combines GC-MS with a database of major odor-causing substances and sensory information (types of smells and odor thresholds). It provides the total solution required for off-flavor analysis.

This product was developed in cooperation with Daiwa Can Company.

Check of the Quality of a Smell

Name	Conc	Unit	Threshold	Description
Benzophenone	2.543	pg/mg	10.000	Almond, Burnt sugar
2,4,6-Tribromophenol	2241.933	pg/mg	100.000	Lodoform

Disinfectant odor



Mass chromatogram of 2,4,6-Trichloroanisole (Left) and 2,4,6-Tribromoanisole (Right) in Food Packaging

Py-Screener Phthalate Ester Screening System



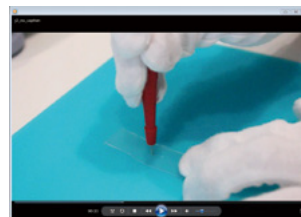
The use of phthalate esters is restricted in toys and food packaging, and they are expected to be classified as restricted substances in the RoHS(II) directives. This system is simple to operate, even for novices. It consists of special software to support a series of procedures from sample preparation to data acquisition, data analysis and maintenance, as well as special standard samples and a sampling toolkit.

Sample Preparation Does Not Require Organic Solvents

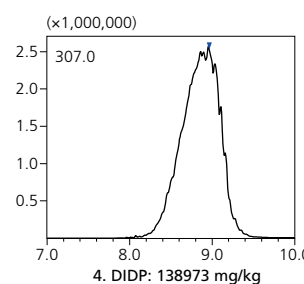
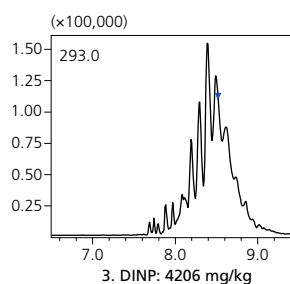
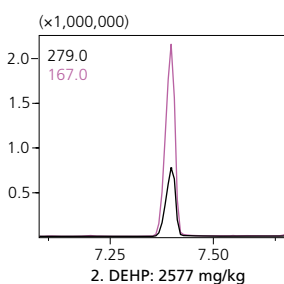
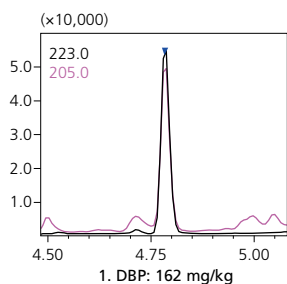
Standard samples and test samples can be prepared without using organic solvents.



Standard Samples Containing Phthalate Ester for Py-GC/MS



Preparation of Resin Standard Samples



Mass Chromatogram of Compounds Detected When Measuring a PVC Cable

Speed Beyond Comparison

UFMS

ULTRA FAST MASS SPECTROMETRY



GCMS-QP2020
GCMS-QP2010 SE



GCMS-TQ8040



LCMS-8030



LCMS-8040



LCMS-8050



LCMS-8060



LCMS-2020



LCMS-IT-TOF



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