


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.



Delivering Smart Solutions

Provides Higher Sensitivity and Reduces Operational Costs

The vacuum exhaust system, which features a new differential exhaust turbomolecular pump, achieves the highest sensitivity under all GCMS conditions. In addition to helium, it can be operated with confidence using hydrogen or nitrogen as the carrier gas, which helps reduce operational costs. In addition, analysis times can be shortened while retaining high speed and high sensitivity, which contributes to the optimization of laboratory productivity.

Easily Obtains All the Information Required for Qualitative Analysis

In addition to conventionally used mass spectra, qualitative analysis is supported by three types of valuable information: retention indices, molecular weight information from CI, and accurate mass*. Even higher level qualitative analysis can be performed by combining this information with mass spectra.

Dramatically Improves the Efficiency of Multicomponent Batch Analysis

The GCMS Insight software package dramatically improves the sensitivity and efficiency of multicomponent batch analysis. The Smart SIM method creation program creates methods to improve the sensitivity in multicomponent analysis. Further, LabSolutions Insight dramatically improves the efficiency of the data processing.

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 analytical needs. And since all these analysis systems are supported by Shimadzu you can put your mind at ease when using them.

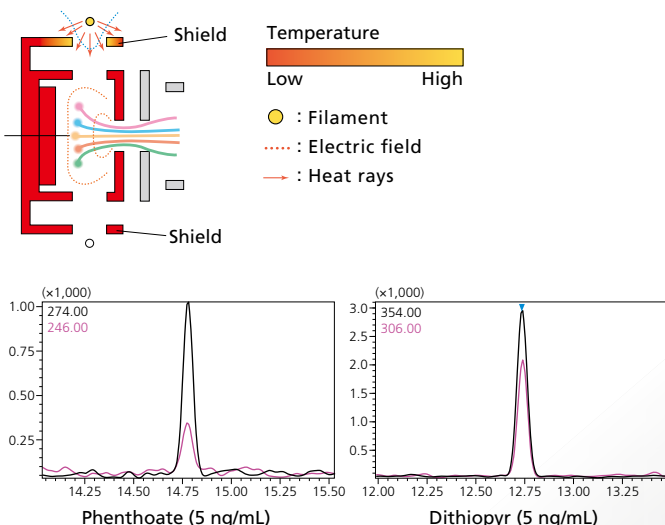
*Accurate mass refers to the accurate mass calculated mathematically by MassWorks™. MassWorks is a trademark of Cerno Bioscience.

Provides Higher Sensitivity and Reduces Operational Costs

Technology Achieves High Sensitivity

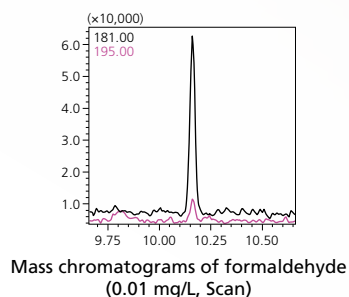
High-Performance Ion Source

The high-performance ion source achieves stable, high-sensitivity analysis. It features a shield plate with patented technology (patent: US7939810) that suppresses the accelerating voltage and thermal radiation from the filament. In addition, the Quick-CI function demonstrates its effectiveness in qualitative analysis. This function can perform measurements by switching between EI and CI modes, with the same ion source and without stopping the MS.

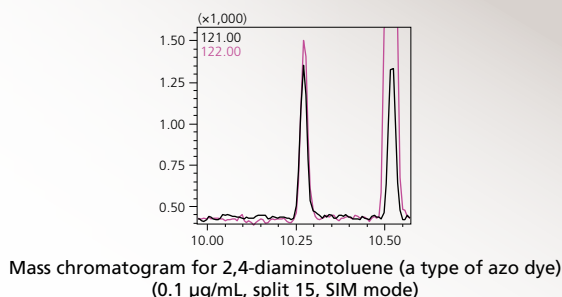


A New Large-Capacity Pump

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 Utilizing Hydrogen as the Carrier Gas



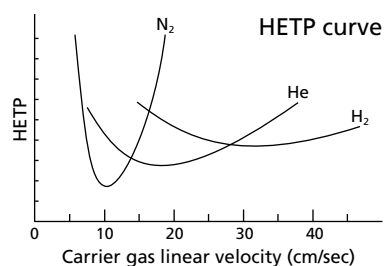
Analysis Results Utilizing Nitrogen as the Carrier Gas

High-Performance Gas Chromatograph

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

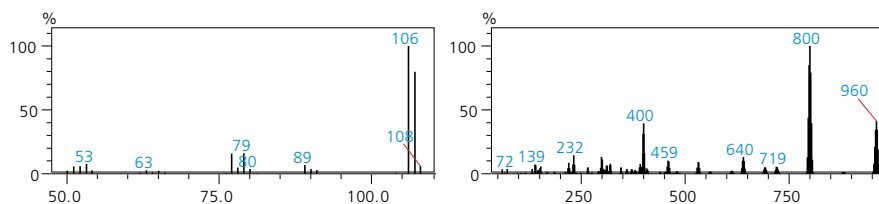


Advanced Flow Controller (AFC)



High-Accuracy MS Filter with Pre-Rod

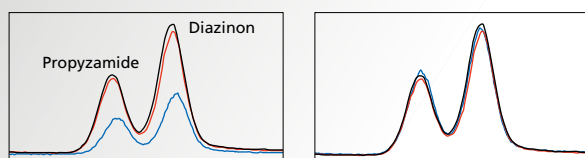
The MS filter incorporates a metal rod to prevent contamination of the quadrupole. This results in stable MS performance directly after startup. The system covers a wide practical mass range region, from m/z 1.5 to 1090.



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.

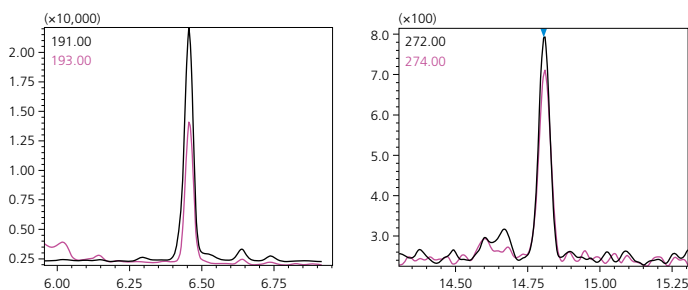
Provides Higher Sensitivity and Reduces Operational Costs

Reduced Operation Costs Using Alternative Carrier Gases

Hydrogen and nitrogen are less expensive than helium and are readily available, so they are attracting attention as alternative carrier gases. The high-performance Advanced Flow Controller (AFC) provides accurate control even with hydrogen and nitrogen. In addition, the new large-capacity differential exhaust system enhances the vacuum performance when hydrogen or nitrogen is used as the carrier gas, so the optimal MS state is achieved under all carrier gas conditions.

Example of Application Using Hydrogen as the Carrier Gas

Hydrogen and nitrogen provide less sensitivity than helium. However, chromatogram patterns equivalent to when helium is used can be obtained by using a short column with a narrow internal diameter. EZGC™ Method Translator*¹, a method conversion program provided by Restek, can convert the analysis conditions when helium is used to the optimal analysis conditions for the alternative carrier gas.



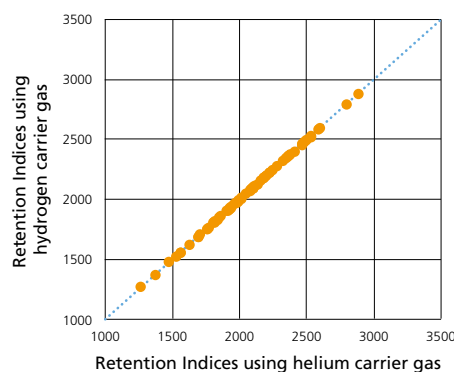
Mass chromatograms of pesticides (5 ng/mL, SIM)



| Carrier Gas | Original | Translation |
|--|-----------|-----------------|
| Carrier Gas | Helium | Hydrogen |
| Column | | |
| Length | 30.00 | 20.00 m |
| Inner Diameter | 0.25 | 0.18 mm |
| Film Thickness | 0.25 | 0.36 µm |
| Phase Ratio | 250 | 125 |
| Control Parameters | | |
| Column Flow | 1.42 | 1.28 mL/min |
| Average Velocity | 43.92 | 76.14 cm/sec |
| Holdup Time | 1.14 | 0.44 min |
| Inlet Pressure | 99.80 | 101.02 kPa |
| Outlet Pressure (abs) | 0.00 | 0.00 kPa |
| Oven Program | | |
| <input type="radio"/> Isothermal <input checked="" type="radio"/> Ramps | | |
| Ramp Rate (°C/min) | Temp (°C) | Hold Time (min) |
| 20 | 180 | 0 |
| 5 | 280 | 3 |
| <input type="radio"/> Isothermal <input checked="" type="radio"/> Ramps | | |
| Ramp Rate (°C/min) | Temp (°C) | Hold Time (min) |
| 30.7 | 180 | 0 |
| 7.1 | 280 | 2.1 |
| Control Method | | |
| Constant Pressure | | |
| Results | | |
| Solve for: <input checked="" type="radio"/> Efficiency <input checked="" type="radio"/> Speed <input type="radio"/> Translate <input type="radio"/> Custom | | |
| Run Time | 30.00 | 20.59 min |
| Speed | | 1.46 x |

EZGC Method Translator

The retention indices are essentially unchanged even when the conventionally used analysis conditions are converted for using hydrogen as the carrier gas. Mass spectral libraries containing retention indices and databases provided by Shimadzu should be used.

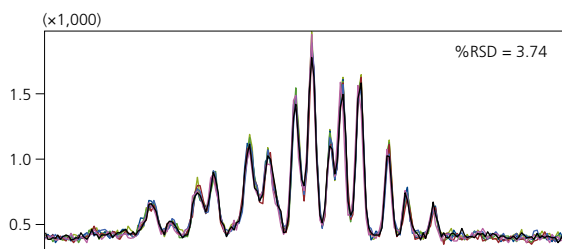
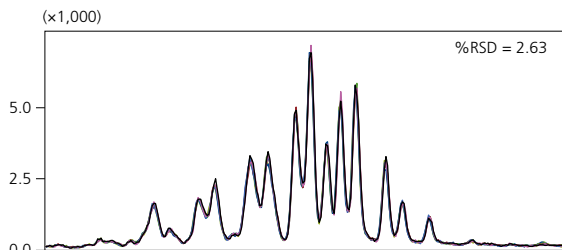
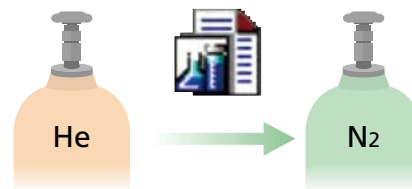


Correlation Between Retention Times with Hydrogen and Helium as the Carrier Gases for 70 Pesticides Translation to Analysis Conditions for Hydrogen as the Carrier Gas Utilizing EZGC Method Translator

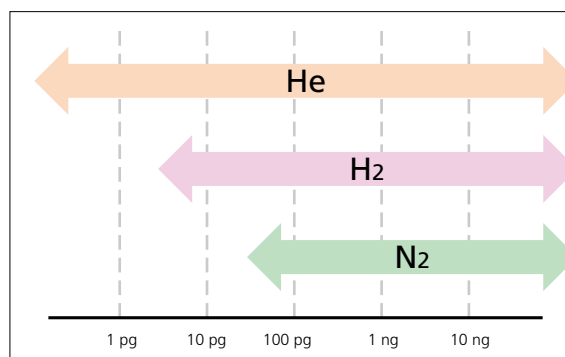
*1 EZGC is a trademark of Restek Corporation. For details, refer to the Restek Corporation website. <http://www.restek.com/ezgc-mtfc>

Example of Application Using Nitrogen as the Carrier Gas

The use of helium as the carrier gas is a major contributor to instrument operating costs. Nitrogen is approximately 10 times less expensive than helium gas, so significant reductions in operating costs can be expected by utilizing nitrogen as the carrier gas.

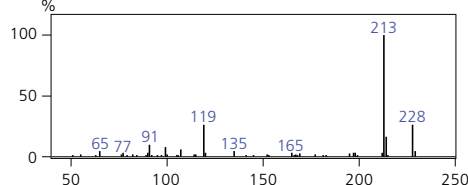
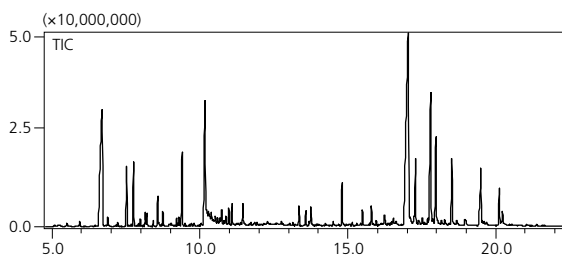
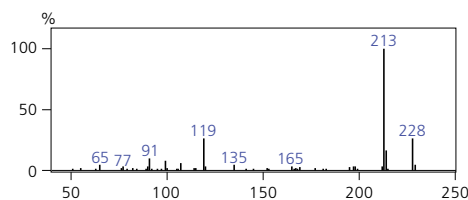
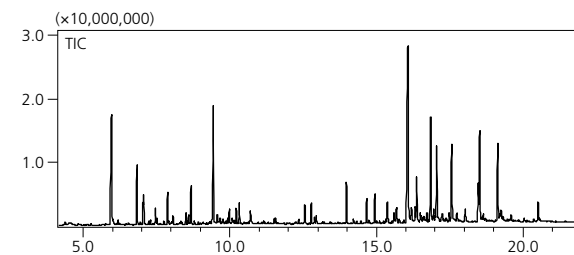


SIM Mass Chromatogram for DINP (0.5 µg/mL, overlay at 7 replicates)
 Top: Helium Carrier Gas (99.99%, with gas purification filter)
 Bottom: Nitrogen Carrier Gas (99.99%, with gas purification filter)



Indication of Measurement Range for Each Carrier Gas (On-Column Amount)
 These measurement ranges are at best only guidelines, and may be unsuitable depending on the target compound sensitivities and the compound characteristics.

Equivalent chromatogram patterns and mass spectra were obtained even though the analysis conditions used with helium as the carrier gas were converted for using nitrogen as the carrier gas. This can be applied for purposes of qualitative analysis including the analysis of evolved gases from polymeric materials.

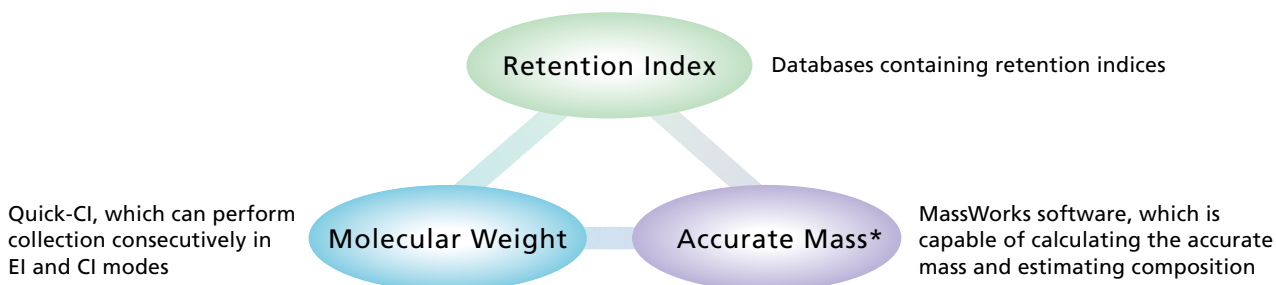


Sample Analysis of the Instantaneous Thermal Decomposition of an Electronic Board Utilizing Py-GC/MS (mass spectrum for bisphenol A)
 Top: Helium Carrier Gas (99.99%, with gas purification filter)
 Bottom: Nitrogen Carrier Gas (99.99%, with gas purification filter)

Easily Obtains All the Information Required for Qualitative Analysis

Three Types of Valuable Information Support High-Accuracy Qualitative Analysis

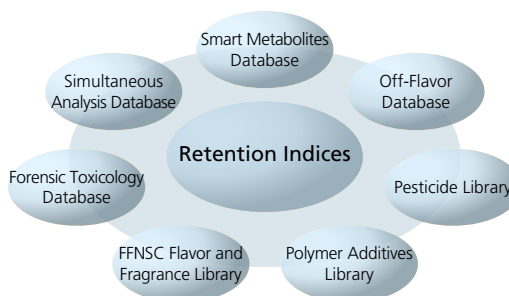
With GC/MS, which has significant qualitative capabilities, a wealth of fragment information is obtained, so it is used as a means of identifying unknown compounds. A mass spectral library is generally used as a means of compound identification. However, experience with compound identification is required if the compound is not registered in the mass spectral library, or there are a number of compounds with similar structures. With the GCMS-QP2020, in addition to the mass spectrum, three kinds of value-added compound information are used in combination to support high-accuracy qualitative analysis.



* Accurate mass refers to the accurate mass calculated mathematically by MassWorks.

❖ Databases Containing High Value-Added Retention Indices

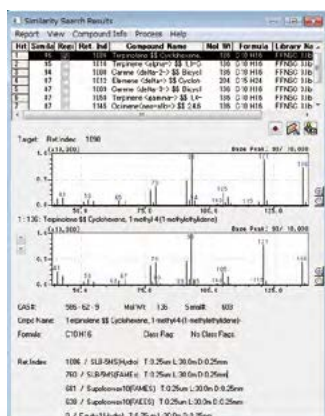
Databases are available with retention indices specific to a variety of application fields, including foods, fragrances, forensics, and metabolite component analysis. In addition to mass spectra, searches are performed in combination with retention indices, which are very highly compound specific, so isomers and compounds with similar structures are accurately identified.



Other Mass Spectra Libraries

- NIST Mass Spectral Library
Registered with 306,622 spectra.
- WILEY Mass Spectral Library
Registered with 719,000 spectra.
- GC/MS MPW DRUG Library
Drugs, toxicants, pesticides, environmental pollutants (8,650 compounds)

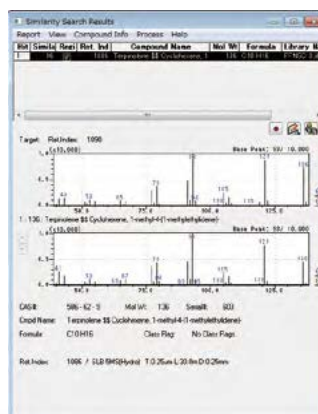
Up to 10 library files can be configured. In addition to the public NIST and Wiley libraries, a variety of library files can be configured. In addition, there is a function to easily create private libraries.



Ret. Index Allowance

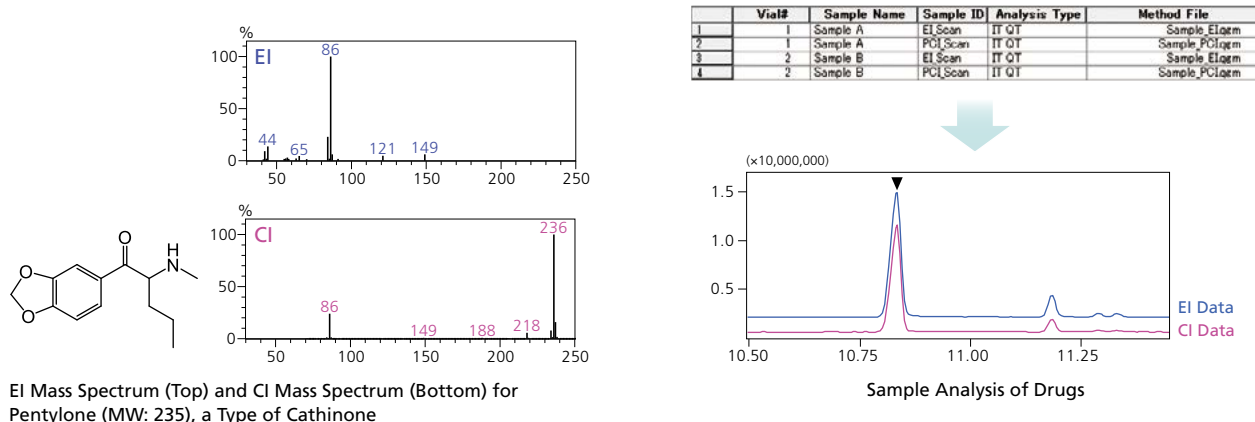
- 10 + 10

Narrowed by retention index



Quick-Cl Switches Easily Between the EI and CI Method

Quick-Cl can switch between the EI and CI method with the same ion source, allowing EI and CI data to be collected on the same sample. Although confirmation of molecular ions is difficult with the EI method, molecular weight information can be obtained from the CI data.

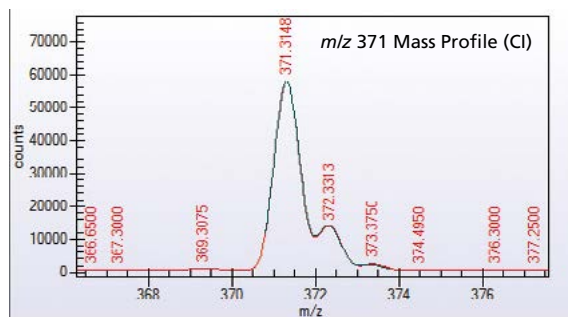


EI Mass Spectrum (Top) and CI Mass Spectrum (Bottom) for Pentylone (MW: 235), a Type of Cathinone

Estimating Composition Using Accurate Mass

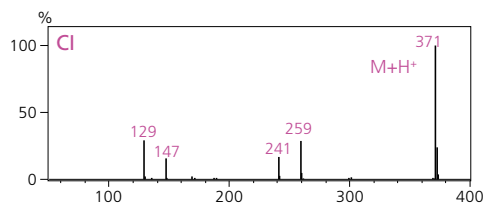
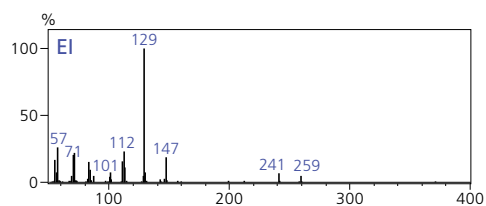
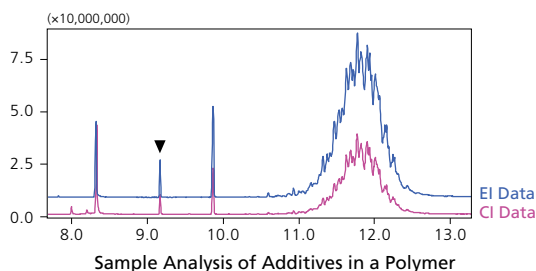
The MassWorks software calculates the theoretical accurate mass from the quadrupole MS mass profile. It then outputs candidate compositional formulas based on isotopic ratios and the theoretical accurate mass. This software is useful for estimating the composition of compounds that are not registered in a mass spectral library.

The GCMSolution software can simultaneously output GC/MS data and mass profile data. The majority of compounds detected with the GC/MS data can be identified from a mass spectral library. MassWorks is then used to estimate the composition of any compounds that are not identified, further increasing the quality of the qualitative analysis.



| CLIPS Results | | | | | | |
|---------------|---|--------------|------------------|------------------|-------------------|-------|
| | Formula | Mono Isotope | Mass Error (mDa) | Mass Error (PPM) | Spectral Accuracy | RMSE |
| 1 | C ₂₂ H ₄₂ O ₄ | 371.3158 | -0.7863 | -2.1176 | 98.9772 | 256 |
| 2 | C ₁₉ H ₅₀ P ₃ | 371.3120 | 2.8124 | 7.5743 | 98.7149 | 321 |
| 3 | C ₁₉ H ₄₈ O ₂ P ₅ | 371.3107 | 4.0856 | 11.0030 | 97.8758 | 531 |
| 4 | C ₁₉ H ₄₇ O ₄ S | 371.3190 | -4.1571 | -11.1956 | 97.6479 | 500 |
| 5 | C ₁₉ H ₄₉ O ₂ P ₂ | 371.3202 | -5.4303 | -14.6244 | 98.0709 | 282 |
| 6 | C ₂₂ H ₄₄ O ₂ P | 371.3073 | 7.4564 | 20.0611 | 98.0498 | 287 |
| 7 | C ₁₉ H ₄₉ P ₂ S | 371.3025 | 12.3283 | 33.2017 | 98.0968 | 478 |
| 8 | C ₁₉ H ₄₇ O ₂ S ₂ | 371.3012 | 13.6014 | 36.8305 | 95.1422 | 1,214 |

It is predicted to be diethylhexyl adipate (C₂₂H₄₂O₄) based on the candidate compositional formula and the mass spectral pattern.



Dramatic Improvement in the Efficiency of Multicomponent Simultaneous Analysis

GCMS Insight Software Package

This new software packages an automatic method creation function and a multi-data processing program to dramatically improve 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.



The optimal MS table is automatically created

- 41: Chlorpropham
- 42: Ethafluralin
- 43: Dichloflumid metabolite
- 44: Italed
- 45: Flusilazole metabolite
- 46: Dicyctophos
- 47: Trifluralin
- 48: 2,6-Dichlorobenzamide
- 49: Bendiocarb
- 50: Dioxabenzofos
- 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: Thiometon
- 61: Hexachlorobenzene
- 62: Diclolan
- 63: Dimethoate
- 64: Simazine
- 65: Fuziazole
- 66: Carbofuran
- 67: Chlorbutam
- 68: Atrazine

Smart SIM

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

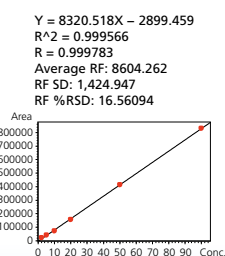
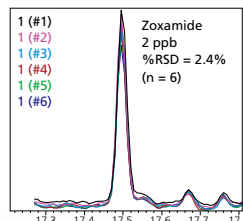
| Index# | Type | Acq. Mode | Method No. | Compound Name (Jp) | Type | m/z | Ratio | Type | m/z | Ratio | Type | m/z | Ratio | Type | m/z | Ratio |
|--------|--------|-----------|------------|--------------------|------|-------|--------|-------|-------|--------|-------|--------|--------|------|-----|-------|
| 1 | Target | SIM | 1 | Azinphos-meg | T | 110.0 | 100.00 | Ref.1 | 130.0 | 68.35 | Ref.1 | 152.05 | 100.00 | | | |
| 2 | Target | SIM | 1 | DCIP | T | 121.0 | 100.00 | Ref.1 | 177.0 | 89.47 | Ref.1 | 79.0 | 100.00 | | | |
| 3 | Target | SIM | 1 | Metolachlor deg | T | 68.0 | 100.00 | Ref.1 | 85.0 | 100.00 | Ref.1 | 65.0 | 100.00 | | | |
| 4 | Target | SIM | 1 | Chlorfentazine deg | T | 137.0 | 100.00 | Ref.1 | 139.0 | 33.20 | Ref.1 | 152.0 | 88.80 | | | |
| 5 | Target | SIM | 1 | Hydroxyazido | T | 86.0 | 100.00 | Ref.1 | 71.0 | 18.40 | Ref.1 | 100.0 | 14.40 | | | |
| 6 | Target | SIM | 1 | Metolachlor deg | T | 143.0 | 100.00 | Ref.1 | 84.0 | 32.34 | Ref.1 | 95.0 | 206.11 | | | |
| 7 | Target | SIM | 1 | Dicyctophos | T | 180.0 | 100.00 | Ref.1 | 130.0 | 400.20 | Ref.1 | 220.0 | 16.13 | | | |
| 8 | Target | SIM | 1 | Thiometon | T | 70.0 | 100.00 | Ref.1 | 140.0 | 3.20 | Ref.1 | 100.0 | 20.00 | | | |
| 9 | Target | SIM | 1 | Azinphos-meg | T | 100.0 | 100.00 | Ref.1 | 170.0 | 6.88 | Ref.1 | 66.0 | 294.88 | | | |
| 10 | Target | SIM | 1 | Surfactant | T | 171.0 | 100.00 | Ref.1 | 170.0 | 76.00 | Ref.1 | 180.0 | 22.00 | | | |
| 11 | Target | SIM | 1 | SEPC | T | 120.0 | 100.00 | Ref.1 | 180.0 | 24.80 | Ref.1 | 130.0 | 22.40 | | | |
| 12 | Target | SIM | 1 | Surfactant | T | 160.0 | 100.00 | Ref.1 | 150.0 | 37.80 | Ref.1 | 160.0 | 20.00 | | | |
| 13 | Target | SIM | 1 | Butyltin | T | 140.0 | 100.00 | Ref.1 | 150.0 | 10.10 | Ref.1 | 170.0 | 60.90 | | | |
| 14 | Target | SIM | 1 | Metolachlor | T | 127.0 | 100.00 | Ref.1 | 152.0 | 27.80 | Ref.1 | 180.0 | 10.00 | | | |



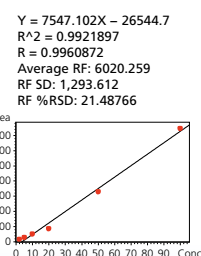
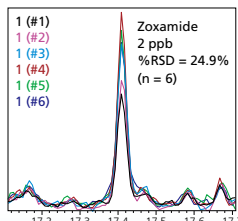
High-sensitivity, high-accuracy analysis is enabled in comparison to the group measurement method. In a batch analysis of 434 components, favorable repeatability and calibration curves were obtained, even down to the trace-quantity region, improving quantitative performance.



Smart SIM



Conventional Method (Group Measurement)

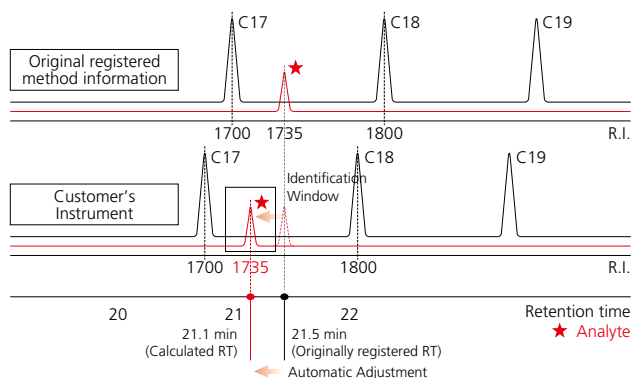


Functions Using Retention Indices

Automatic Adjustment of Compound Retention Time (AART)

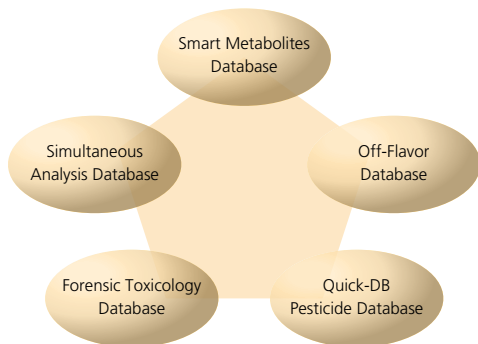
The AART (Automatic Adjustment of Retention Time) function can estimate the retention times of target components from retention indices and the retention times of an alkane standard mix*.

* Requires alkane mix which is sold separately.

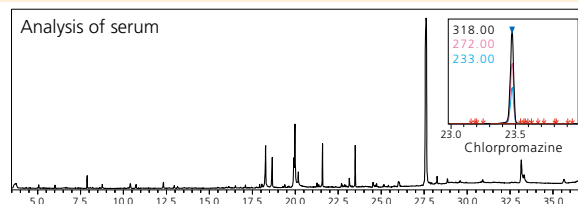


Databases Specific to All Kinds of Industries

Databases are available for a variety of industries, and contain analysis conditions optimized for multicomponent batch analysis. Analysis can start immediately just by automatically correcting the retention times utilizing the AART function.

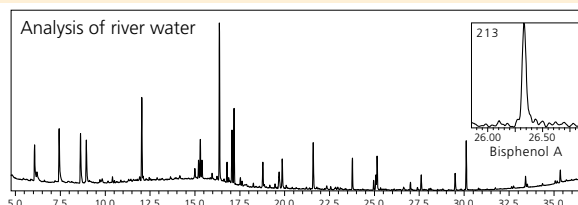


GC/MS Forensic Toxicological Database



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)

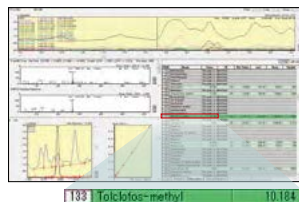


Simultaneous GC/MS analysis supporting identification and quantification of 942 environmental pollutants can be performed. The retention times and calibration curve information of environmentally hazardous chemical substances are registered, so approximate concentrations can be obtained, even when it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

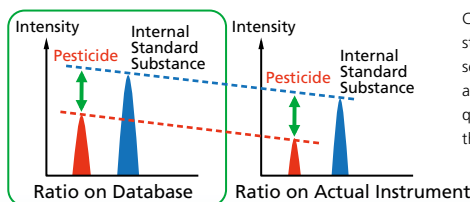
Quantitation Analysis Without Using Standard Samples

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 474 components (for scan or SIM mode) 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.

LabSolutions Insight Heightening the Efficiency of Multi-Analyte Data Analysis

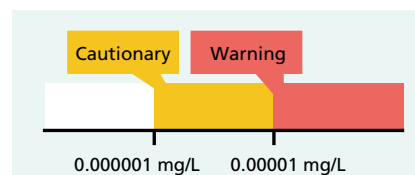
With LabSolutions Insight software, quantitative results for a complete series of data files can be displayed side-by-side for comparison and QC review. All of the chromatograms for a selected target compound can be displayed simultaneously, making it easy to review the detected peaks and confirm the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

Color-coded Quantitative 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

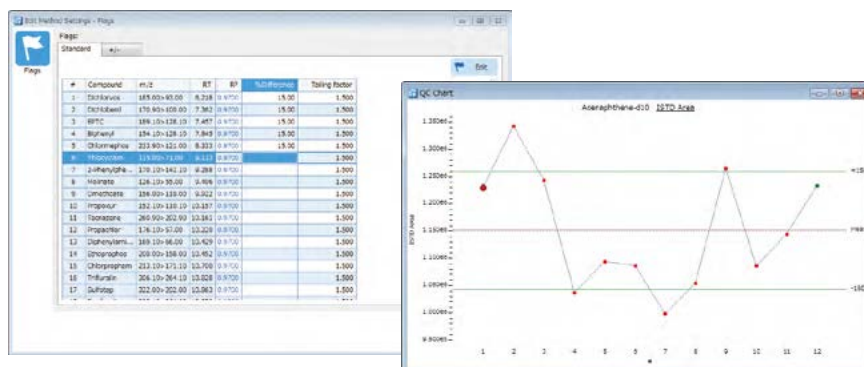
The following example illustrates how an orange flag was set to identify moldy odor compound concentrations that exceeded a defined cautionary limit of 1.0 ppt (part-per-trillion), and a red flag was used as a warning to identify those which had exceeded 10 ppt. In the figure below, quantitative results 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.



Enhanced Accuracy Controls

Accuracy control results such as retention time differences, calibration curve linearity and peak shapes (tailing) can be assessed visually.

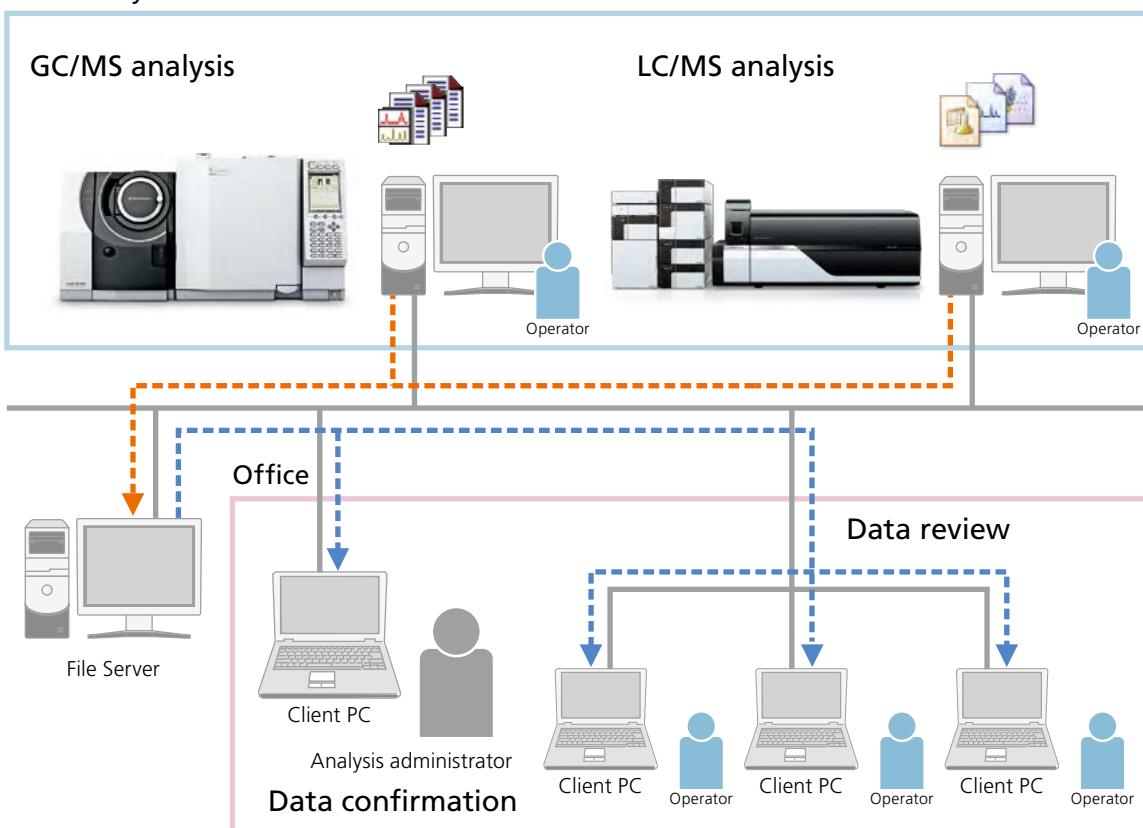
In addition, the QC chart function in LabSolutions Insight allows visual confirmation of variations in target compounds across multiple data sets. This is useful when evaluating variations in internal standard substances between samples, for example.



System Configurations Using Multiple Client Computers

Data acquired from multiple systems 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.

Laboratory



File management on a file server is recommended for systems with more than 5 users.

Configure Optimal Analysis Systems to Meet Your Needs

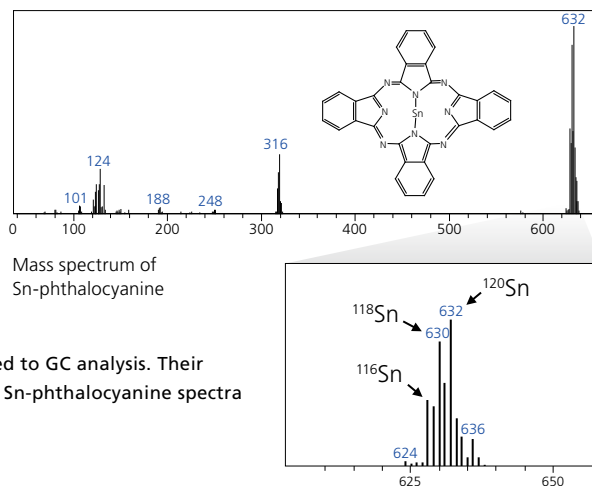
Various System Configurations

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 System

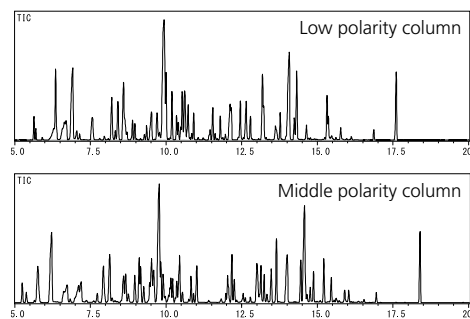
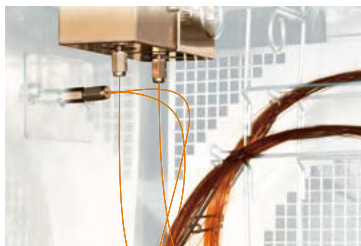
The DI probe allows a sample to be introduced directly into the ion source without passing through a GC column. It is an effective technique for obtaining mass spectra of synthetic compounds that do not chromatograph well. A DI system can be incorporated into a standard GC-MS configuration without making 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.

Twin Line MS System Eliminates the Need to Swap Columns

The GCMS-QP2020 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.



Analysis of flavor and fragrance components using complementary column phases

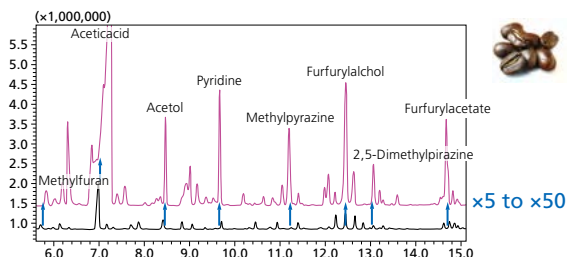
Headspace Analysis System



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

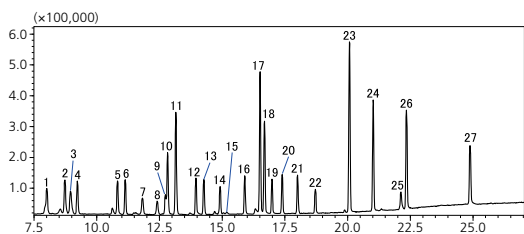
There is a loop model capable of static headspace analysis, and a trap model capable of trap headspace analysis.

High-Sensitivity Analysis of Fragrant Components in Coffee



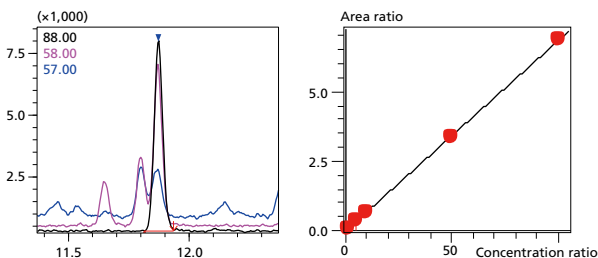
Trace quantities of fragrant components undetectable with conventional headspace samplers can be qualified and quantified by combining the high-sensitivity, electronically cooled trap with GCMS.

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.



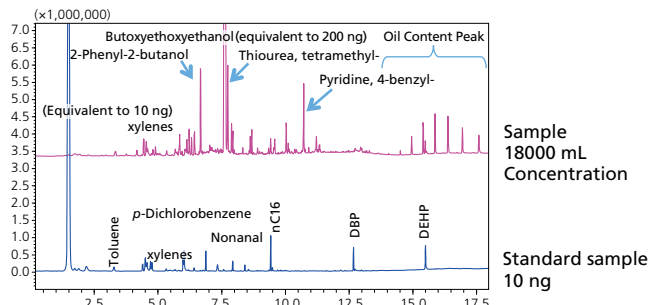
SIM Chromatogram (5 µg/L) and Calibration Curve (1–100 µg/L) of 1,4-Dioxane

Thermal Desorption Analysis System



TD-30 series was developed as the optimal solution for gas and materials analysis. Its outstanding processing ability and excellent expandability provide strong support for all types of analysis, from diffusion gas to environmental air. TD-30 standard model with 60 sample tubes and TD-30R high-end model with 120 sample tubes, retrapping function and internal standard added function are now available in this system.

Analysis of Gas Generated from Electrical Parts

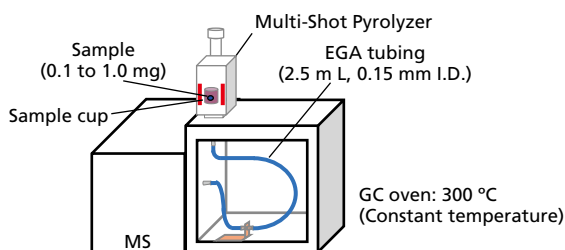


Components Detected with 18 L Outgas (Concentrated) from Electronic Parts Maintained at 70 °C

Pyrolysis System

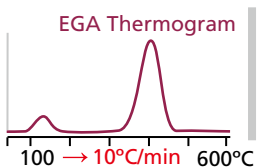
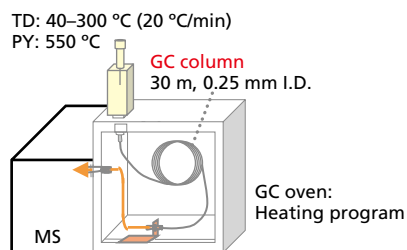


EGA-MS



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. Search software utilizing a pyrolysis library assists in the identification.

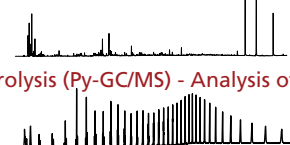
Single-Shot (Thermal Desorption, TD)
Double Shot (Pyrolysis, PY)-GC/MS



Analysis of thermogram corresponding to temperature
Qualitative analysis using the MS spectrum

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

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



GC×GC-MS System

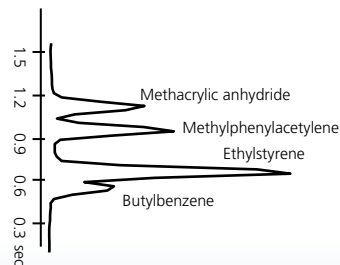
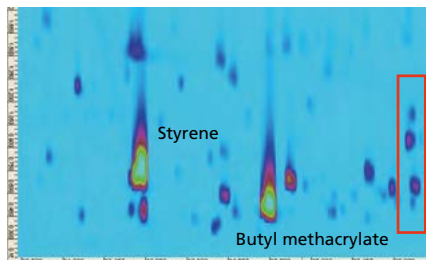


With comprehensive 2D chromatography (GC×GC), chromatographic separation of complex samples is achieved via 2D separation. The Py-GC/MS chromatogram is very complex, but GC×GC separation enables a higher degree of separation and qualitative confirmation.

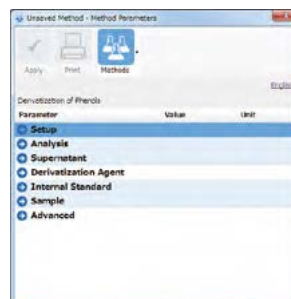
Analysis of Styrene-Butyl Methacrylate by Py-GC×GC-MS



ChromSquare Analysis Software



❖ AOC-6000 Multifunctional Autosampler System

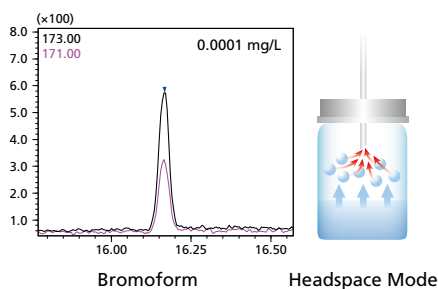


AOC-6000 Control Software

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

The overlap function, which improves the efficiency of continuous analysis, can also be used. Automatic syringe replacement (10 µL to 1000 µL) 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

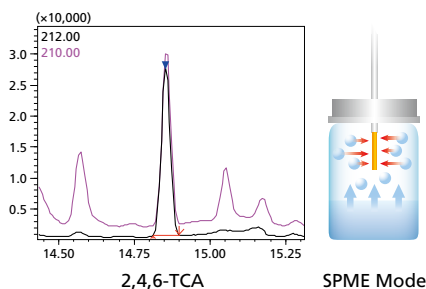


Bromoform

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



2,4,6-TCA

SPME Mode

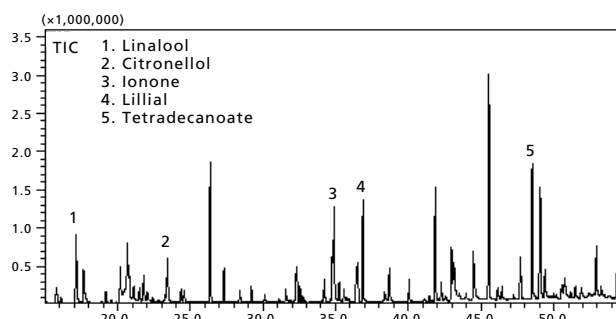
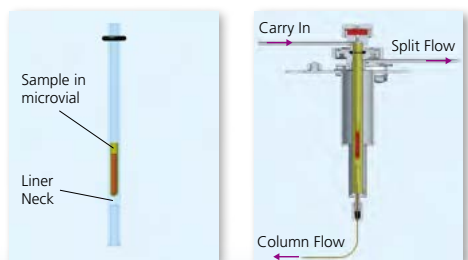
A trace amount of odor compounds was detected by concentration effect with SPME mode at high sensitivity. (5 ng/L)

❖ 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.

GC/MS Off-Flavor Analyzer



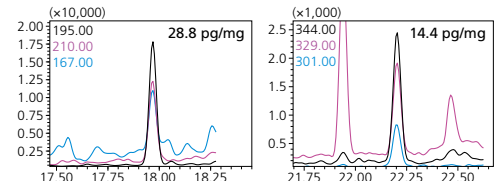
Information Registered in Database

| Compound Name (C) | Ret. Index (I) | Quadrant | Quadrant | Quadrant | Comment (E) | Threshold |
|---------------------------|----------------|----------|----------|----------|---------------------|-----------|
| Benzophenone | 2470 | 6.68-811 | 6.44-608 | 0.0000 | Almond, Burnt sugar | 10 |
| 2,4,6-Tribromophenol | 2801 | 0.0000 | 0.0000 | 0.0000 | Lodoform | 100 |
| 1-Trichloroanisole | 2168 | 0.11-056 | 0.10-051 | 0.0000 | Chemical | 1000 |
| Gamma-Chlorobutyrolactone | 2362 | 0.00-470 | 0.00-000 | 0.0000 | Musty Flower, Fruit | 1 |
| Diethyl disulfide | 822 | 0.00-048 | 0.00-043 | 0.0000 | Fear | 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.

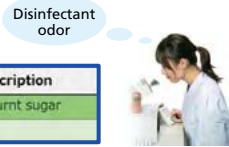
This product was developed in cooperation with Daiwa Can Company.



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

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 |



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

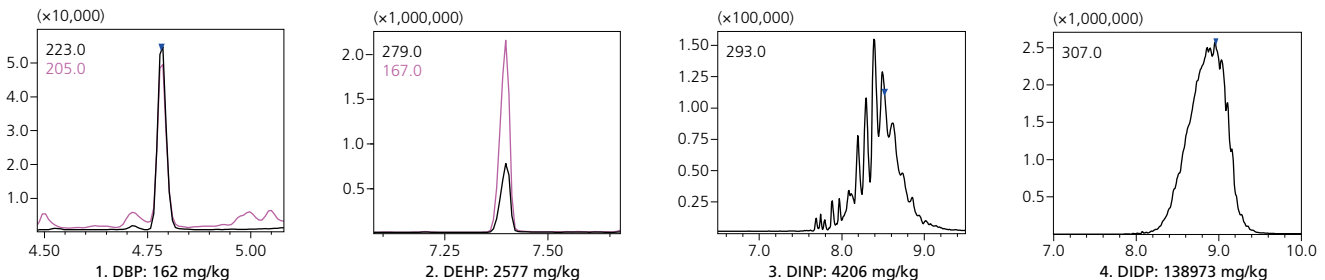
Standard samples and test samples can be prepared without using organic solvents.



Standard Samples Containing Phthalate Ester for Py-GC/MS



Preparation of Resin Standard Samples



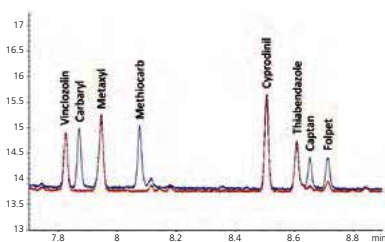
Mass Chromatogram of Compounds Detected When Measuring a PVC Cable

Inert Flow Path Achieves High-Sensitivity GC/MS Flow Path

Minimizing adsorption and other losses in the flow path from sample injection to the detector is important for stable, high-sensitivity measurements using GC/MS. The flow lines in the GCMS-QP series and the TQ series consist of high-quality, highly reliable consumable parts, so even trace concentrations of components can be detected with high sensitivity and favorable repeatability.

Glass liner

The Restek glass liner recommended for GCMS analysis uses a proprietary inactivation technology to dramatically suppress active sites. After packing into the insert, the wool is subjected to a complete inactivation treatment. This product is controlled throughout from production to final inspection to provide 100 % satisfaction.



Blue: Sky liner (with wool)
Red: A liner other than Sky liner (with wool)

Micro-syringe



Autosampler syringes feature improved durability, clarity, and accuracy, achieving reliable injection accuracy.

GC septum



Our lineup now includes low bleed septa, which maintain optimal seal performance even when the injection cycles are increased, and can be used even at high temperatures. This reduces sensitivity variations due to leaks.

Ferrules and gold gasket



The high-quality Vespel ferrule is easily attached and designed to resist leaking. The gold gasket is inactive, and adsorption does not occur.

Ion source

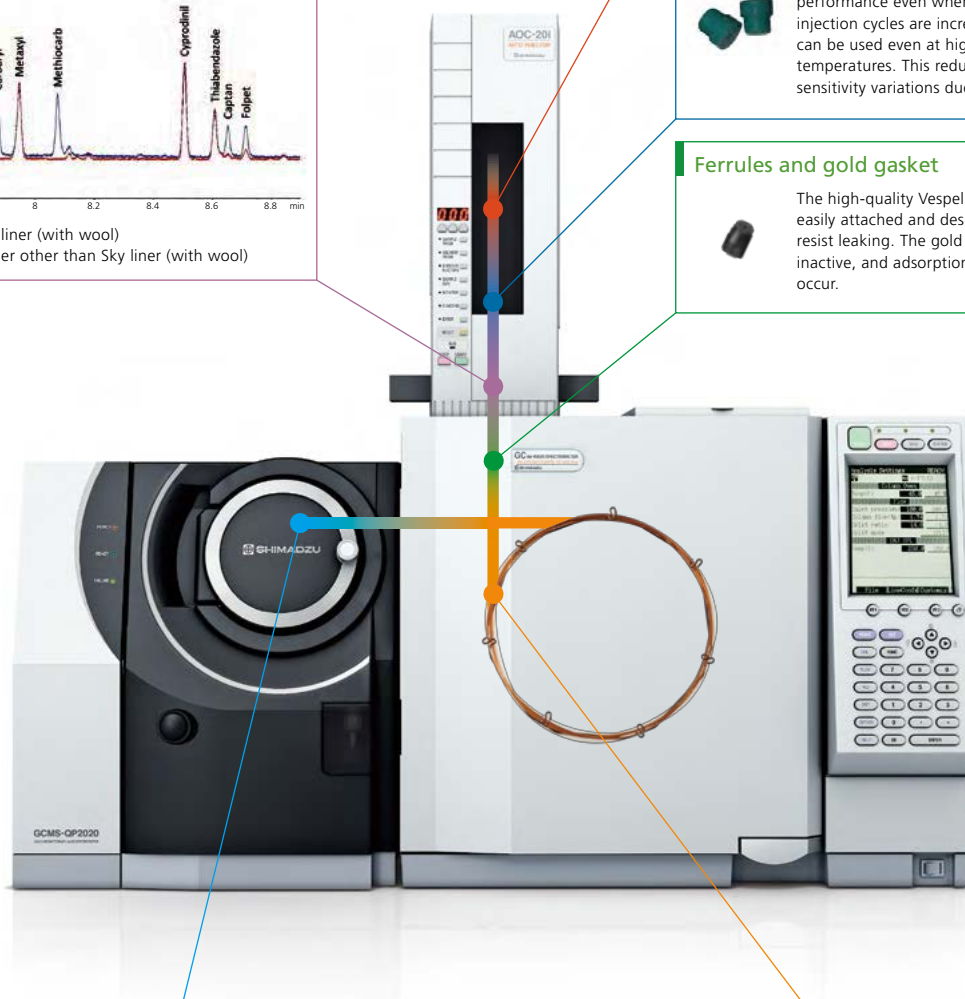


Designed with a shield that blocks radiant heat generated by the filament, and an ion source treated with an oxide coating, active spots inside the ion source are not prone to occur, which enables high-sensitivity analysis with long-term stability.

Capillary columns



For the SH-Rxi series, a high-quality fused silica like no other is used as the raw material. Our proprietary surface inactivation technology and optimal process to mask silanol groups result in a low-bleed column with very impressive inactivation performance, even with respect to polar compounds comparable to acidic and basic substances.





Shimadzu Corporation
www.shimadzu.com/an/

For Research Use Only. Not for use in diagnostic procedures.

This publication may contain references to products that are not available in your country. Please contact us to check the availability of these products in your country.

Company names, products/service names and logos used in this publication are trademarks and trade names of Shimadzu Corporation, its subsidiaries or its affiliates, whether or not they are used with trademark symbol "TM" or "®".

Third-party trademarks and trade names may be used in this publication to refer to either the entities or their products/services, whether or not they are used with trademark symbol "TM" or "®".

Shimadzu disclaims any proprietary interest in trademarks and trade names other than its own.

The contents of this publication are provided to you "as is" without warranty of any kind, and are subject to change without notice. Shimadzu does not assume any responsibility or liability for any damage, whether direct or indirect, relating to the use of this publication.