C146-E292B

SHIMADZU
Excellence in Science

Gas Chromatograph Mass Spectrometer

# GC/MS Off-Flavor Analyzer

# Analytical System for Reliably Identifying Odor-Causing Substances

Solving odor problems requires identifying the substances causing the odor. However, accurate identification requires relevant knowledge, such as knowing which types of compounds can cause odors, the odor quality, and threshold levels for sensing odors. This system combines a database of the major odor-causing substances and associated sensory information (odor characteristics and threshold levels for sensing odors) with a gas chromatograph mass spectrometer (GC-MS). It provides a total solution necessary for analyzing odors.

Odor Analysis Database

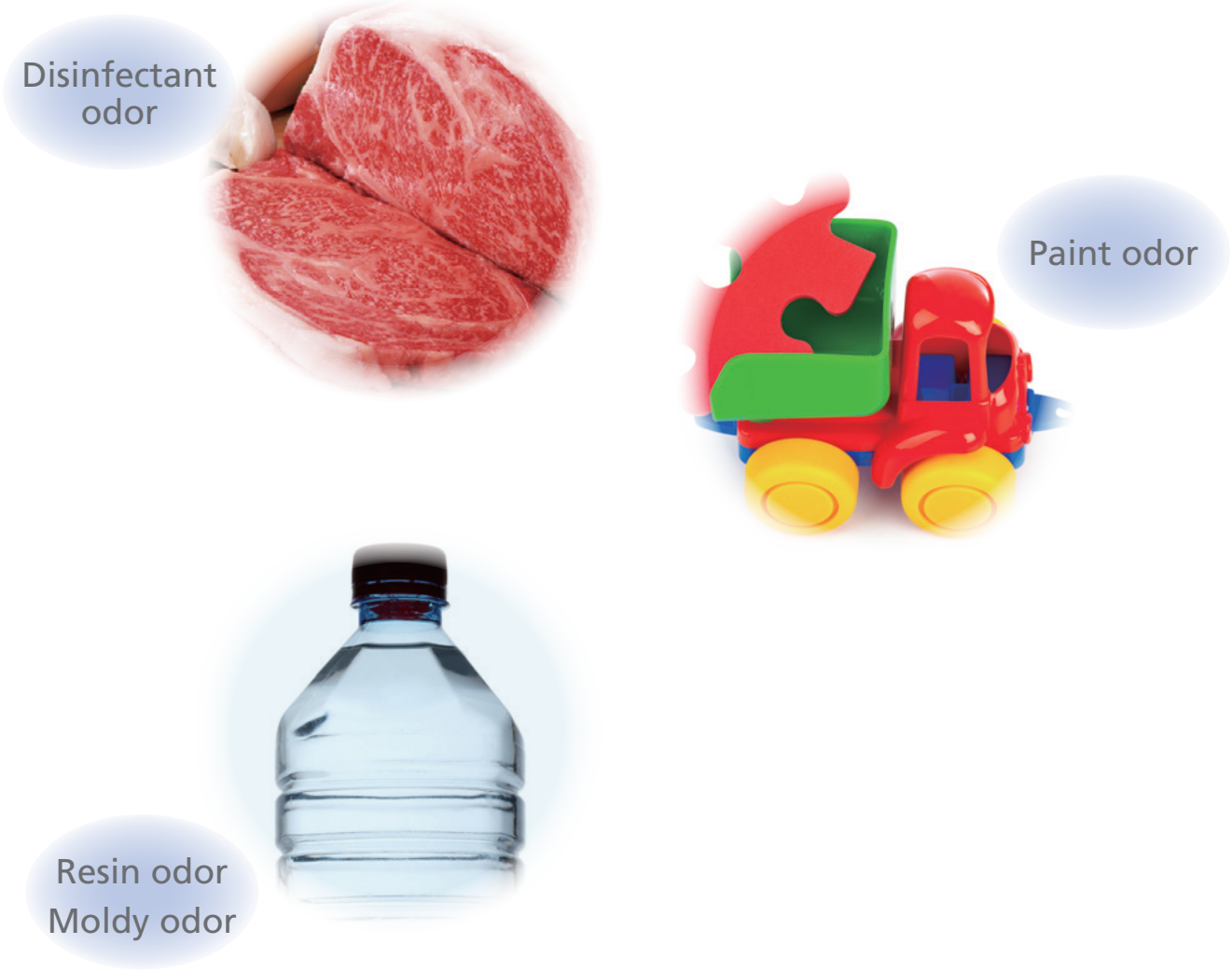
| Compound Name (E) | Ret. Index 1 (InertCap Pure-W) | Comment (E) Odor Quality | threshold Odor Threshold |
|---|---|---|---|
| Benzophenone | 2470 | Almond, Burnt sugar | 10 |
| 2,4,6-Tribromophenol | 2800 | Iodoform | 100 |
| 1-Tetradecanol | 2158 | Coconut | 1000 |
| gamma-Dodecalactone | 2364 | Sweet, Flower, Fruit | 1 |
| Dibenzyl disulfide | 3022 | Ether | 1 |

Primary odor components

GC/MS analytical conditions

Sensory information

Optimal Analytical System




## 1 Database of Expert Information for Odor Analysis

- All odor-causing substances identified from previous problems are registered.
- Accurate identification and easy quantitation are possible even without standard samples.
- Substances causing odors can be identified based on odor characteristics and odor threshold values.

## 2 Analytical System for Reliably Identifying Odor-Causing Substances

- Three different types of columns can be selected for detecting a wide variety of components with high sensitivity.
- MRM and SIM analysis can detect odor threshold concentration levels.
- Odors can be confirmed efficiently using the predicted retention time display function.

## 3 Application Solution-besed System

- An optimal system, including pretreatment unit, can be configured.

This product was developed jointly with Daiwa Can Company.

# 1 Database of Expert Information for Odor Analysis

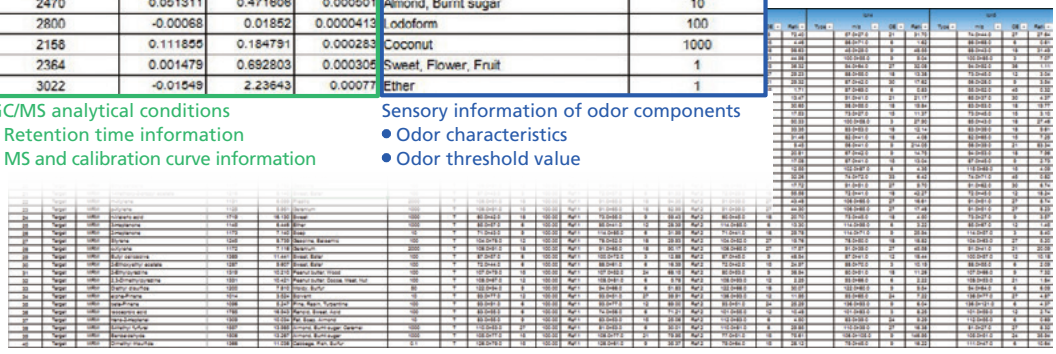
## Information Registered in Database

| Compound Name (E) | Ret. Index 1 (InertCap Pure-Wi | Quadratic Constan | Quadratic 1st | Quadratic 2nd | Comment (E) Odor Quality | threshold Odor Threshold |
|---|---|---|---|---|---|---|
| Benzophenone | 2470 | 0.051311 | 0.471606 | 0.000501 | Almond, Burnt sugar | 10 |
| 2,4,6-Tribromophenol | 2800 | -0.00068 | 0.01852 | 0.0000413 | Iodoform | 100 |
| 1-Tetradecanol | 2158 | 0.111855 | 0.184791 | 0.000283 | Coconut | 1000 |
| gamma-Dodecalactone | 2364 | 0.001479 | 0.692803 | 0.000306 | Sweet, Flower, Fruit | 1 |
| Dibenzyl disulfide | 3022 | -0.01549 | 2.23643 | 0.00077 | Ether | 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



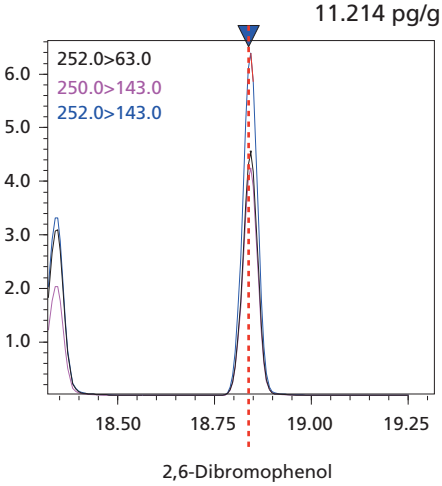
### All Odor-Causing Substances Identified from Previous Problems Are Registered.

The database includes information registered about all odor-causing substances identified from previous problems. Therefore, even if you don't know what types of compounds can cause odors, this database allows you to start analyzing them immediately.

### Accurate Identification and Easy Quantitation Are Possible Even Without Standard Samples.

Retention indices for each odor component are registered in the database. The AART function can be used to accurately identify components registered in the database by calculating their retention time using retention indices for substances with a wide range of boiling points. In addition, concentrations can be quantified easily based on the calibration curve information registered in the database.

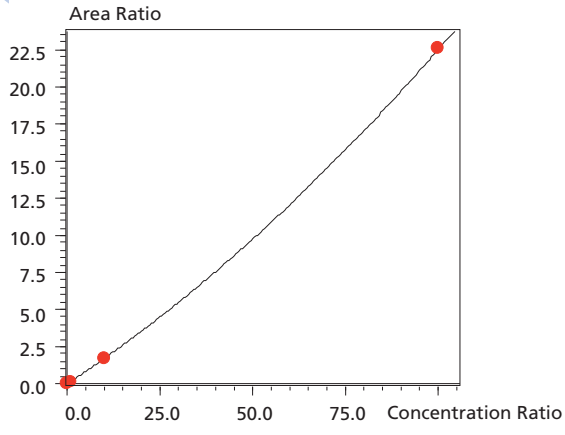
Estimated Concentration
11.214 pg/g



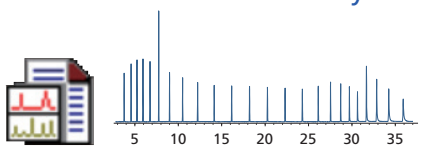

2,6-Dibromophenol

Corrected R.T.: 18.821
Identified R.T.: 18.844
Difference : 0.023 min

Easy quantitation by corrected calibration curves



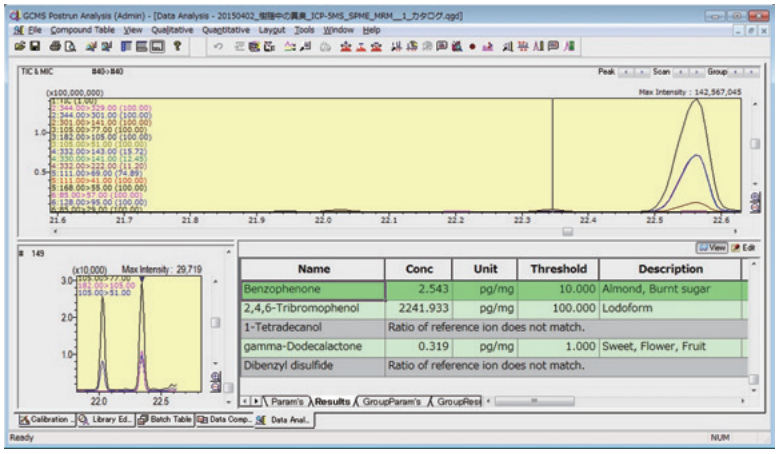

Retention time corrected by AART



## Substances Causing Odors Can Be Identified Based on Odor Characteristics and Odor Threshold Values.

Sensory information about odor components (characteristics and threshold values) is registered in the database. Therefore, by comparing the concentration of components identified in chromatograms with the threshold values, the substances causing odors can be identified. Furthermore, odor components can also be identified by actually smelling them using a sniffer unit.

### Comparison of Concentration to Odor Threshold Values




| 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 |

**Under Threshold Value**

Concentration: 2.543 pg/mg

Odor threshold value: 10.000 pg/mg

Benzophenone

**Over Threshold Value**

Concentration: 2241.933 pg/mg

Odor threshold value: 100.000 pg/mg

2,4,6-Tribromophenol

Odor components with concentrations higher than the corresponding threshold value can be identified as candidates for causing given odors.

Note: The concentration values calculated by the GC-MS off-flavor analyzer are estimates. If accurate concentration values are required, be sure to perform quantitative analysis using a method that involves creating a calibration curve.

### Confirming Odor Characteristics

| 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 |

# 2 Analytical System for Reliably Identifying Odor-Causing Substances

## Process Flow Using the GC-MS Off-Flavor Analyzer

**Step 1: Reliably identify odor components.**

**Step 2: Accurately identify the components causing the given odor.**

Collect odor components using a pretreatment unit.

1 2 Detect odor components by GC-MS analysis.

Identify odor components based on the database.

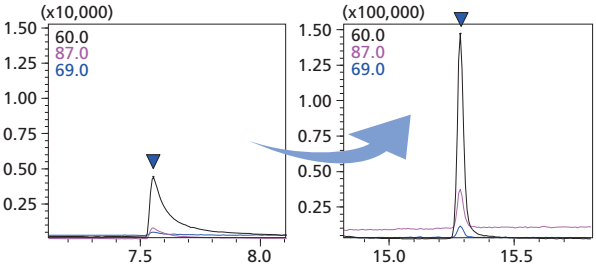
3 Reanalyze to confirm odor.

Identify odor-causing components using a sniffer unit.

## 1 Three Different Types of Columns Can Be Selected for Detecting a Wide Variety of Components with High Sensitivity.

Three types of stationary liquid-phase columns are included, so that the optimum column can be selected based on the physical properties of the target components. A handbook provided with the system lists the detection limit for each registered component using the respective columns, which makes it easy to determine which column should be selected.

Example: Comparison of peak shapes obtained using columns with slight versus high polarity




Mass Chromatograms of Isovaleric Acid
(Left: InertCap™ 5Sil/MS, Right: InertCap™ Pure-WAX)

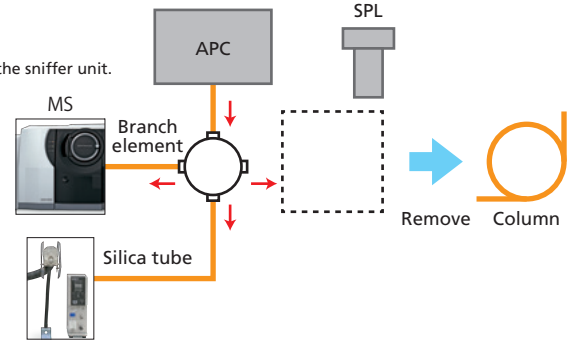
Using the slightly polar column to analyze highly acidic components, such as isovaleric acid, causes peak tailing, whereas using the highly polar column improves the peak shape, which enables measuring the component with high sensitivity.

Compatible Columns:
InertCap 5MS/Sil (30 m, 0.32 mm I.D., df = 0.5 µm)
InertCap 17MS (30 m, 0.25 mm I.D., df = 0.25 µm)
InertCap Pure-WAX (30 m, 0.25 mm I.D., df = 0.25 µm)

### Change Columns without Releasing the Vacuum

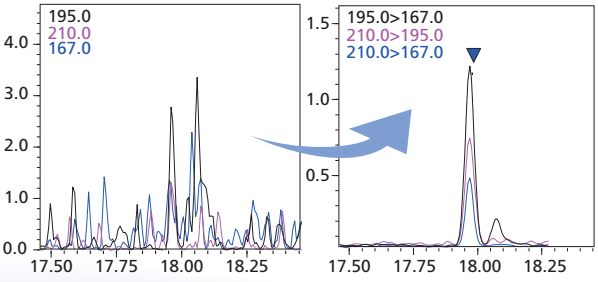
This minimizes system downtime due to changing columns.

Note: Available when using a splitter system that splits flows between detection by the MS and the sniffer unit.




## 2 MRM and SIM Analysis Can Detect Odor Threshold Concentration Levels.

Since some odor components have a low odor threshold, low concentration levels need to be detected to identify the causative substances. High-sensitivity MRM/SIM analysis by GC-MS(/MS) can reliably detect even trace components near the odor threshold (a few pg/g).

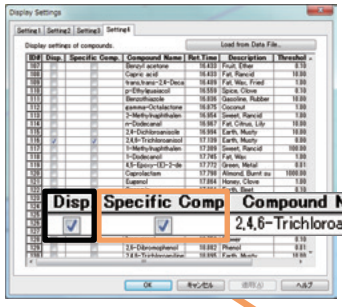



Mass Chromatograms of 2,4,6-Trichloroanisole
(estimated concentration of 18.166 pg/g) in Food with an Odd Odor
(Left: Scan analysis, Right: MRM analysis)

## 3 Odors Can Be Confirmed Efficiently Using Predicted Retention Time Display Function.

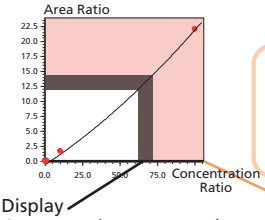
On systems with a sniffer unit, odor components identified from the database can be confirmed. The system includes a function that displays estimated retention times for detected components, so that they can be confirmed based on time.

Display Setting Window



When a data file acquired in Step 1 is loaded, components that require particular attention are automatically marked with a check mark based on semi-quantitative results and odor threshold values for identified components.

| Disp | Specific Comp | Compound Name | Ret.Time | Description | Threshold |
|---|---|---|---|---|---|
| ☑ | ☑ | 2,4,6-Trichloroanisole | 17.139 | Earth, Musty | 0.001 |




Over Threshold Value

Estimated Concentration: 18.166 pg/g

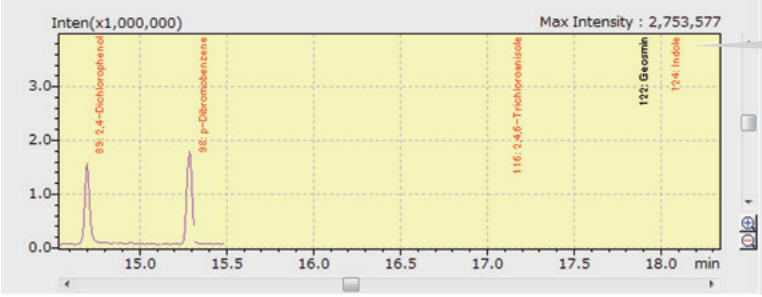
Odor threshold value: 1.000 pg/g

2,4,6-Trichloroanisole

Display
Concentrations greater than one tenth of odor threshold value

Identified Substances
Concentrations greater than the odor threshold value

Data Acquisition Window



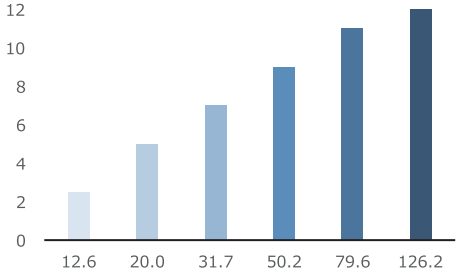

The name of components marked with a check mark are displayed near the corresponding retention time, so that in Step 2, you receive the appropriate timing for sniffing the odor.

## Confirming Odors in Matrices Prepared Using an FDL-1 Unit

The odor of detected components in a matrix can be confirmed by using an FDL-1 unit to successively add the odor in a standard sample to the odor in a matrix.

Note: This product is sold separately.

$$\text{Odor index} = 10 \log \frac{\text{Flow Rate of Matrix with Detectable Odor}}{\text{Flow Rate with Detectable Component Odor}}$$




Flow Rate with Detectable Component Odor (mL/min)

An FDL-1 unit can be used to confirm odor levels detectable in a matrix as the mixture ratio is successively changed in steps by adding different flow rates of odor components to a given flow of the matrix.

# 3 Application Solution-based System

## An Optimal System, Including Pretreatment Unit, Can Be Configured.

The following is recommended as the optimal system.
We offer total support for all systems.

AOC-6000 multifunctional autosampler :Supports injecting samples concentrated by SPME, injecting HS samples, or injecting liquid samples.
GCMS-TQ8040 NX, GCMS-TQ8040 :Enables detection of trace components by MRM analysis.
PHASER (GL Science B.V.) :If a candidate odor component is identified in a chromatogram, this unit can be used to confirm the odor.
OPTIC-4 (GL Sciences B.V.) :Supports injecting samples using a MonoTrap™.
Note 1: Sniffers other than the PHASER may be used in some cases. Contact your Shimadzu representative for details.
Note 2: The system does not support the OPTIC-4 LINEX function.

The following models may be selected depending on customer requirements.

GC/MS : GCMS-QP2020 NX, GCMS-QP2020, GCMS-QP2010 Ultra, GCMS-TQ8050 NX, GCMS-TQ8050
Autosampler : AOC-5000 Plus, AOC-20i/s

Cautions
1. Shimadzu makes no warranty regarding the accuracy of information included in the database or the usefulness of information obtained from using the database.
2. Be sure to perform tests using standard samples to confirm qualitative and quantitative information obtained using the given system.
3. To reliably identify registered substances using this database, measure samples using the instrument parameters specified in method files included with the product.



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