C146-E452

SHIMADZU
Excellence in Science

Database for GC-MS(/MS) Aroma Analysis

# Smart Aroma Database 1.8.2

# Provides Efficient and Accurate Aroma Analysis Using GC-MS(/MS)

1.8.2 Information on more than 500 compounds that contribute to aroma is registered in Smart Aroma Database™, enabling the objective evaluation and analysis of aroma compounds using GC-MS(/MS).

## 1. Automatically Detects Aroma Compounds from Scan Measurements with High Accuracy

In conventional aroma analysis, measurements are performed using the GC-MS scan method, and the peaks detected for the compounds are then identified from the mass spectrum. With this method, however, there are a number of problems, including the inability to detect a trace peak or identify isomers with similar mass spectra.

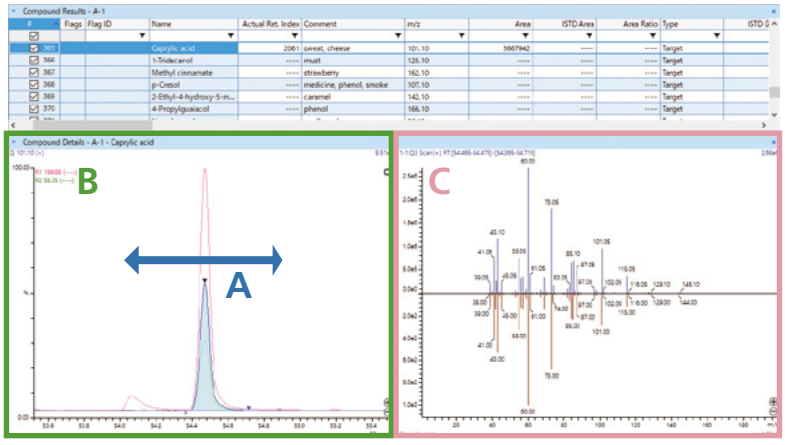
With Smart Aroma Database, even aroma compounds that are hard to analyze with conventional methods can be detected easily and reliably using information on characteristic ions, retention times, and mass spectra.

Containing more than 500 aroma compounds, Smart Aroma Database supports the aroma analysis of a wide range of samples.

**A Retention Time**
Peaks are found from the corrected retention time.

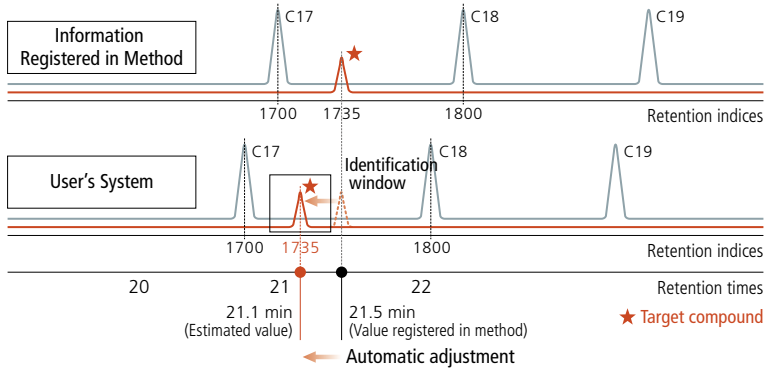
**B Mass Chromatogram**
Peaks are identified from the registered characteristic ions and ion ratios.

**C Mass Spectrum**
Spectra are evaluated for degree of similarity to the mass spectra of standard samples registered in the database.

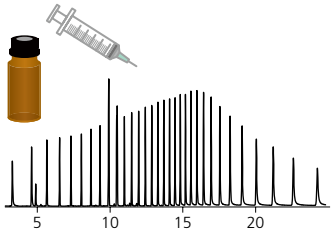


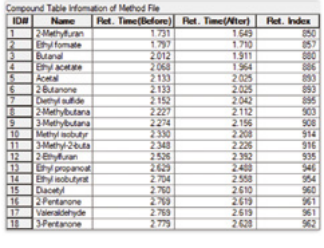

### Automatic Adjustment of Retention Time (AART) of the Compound

AART function adjusts the retention times of target compounds using retention indices and the retention times for *n*-alkanes.




1. Analysis of *n*-alkanes ›››
2. Automatic adjustment of retention time using the AART function ›››
3. Analysis of samples using the adjusted method

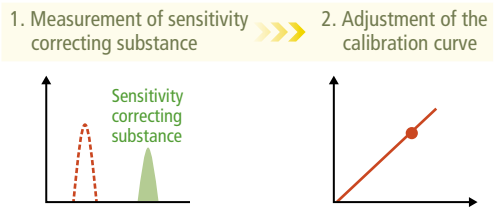



## 2. Easily Narrows Down the Compounds that Contribute to the Aroma

1.8.2

Sensory information is registered for each registered compound. In addition, a sensitivity coefficient for each compound is registered in the database, so semi-quantitative concentration can be calculated for the detected compounds by measuring a sensitivity correcting substance. Using this information, the compounds that contribute to the aroma can be analyzed from the detected compounds.



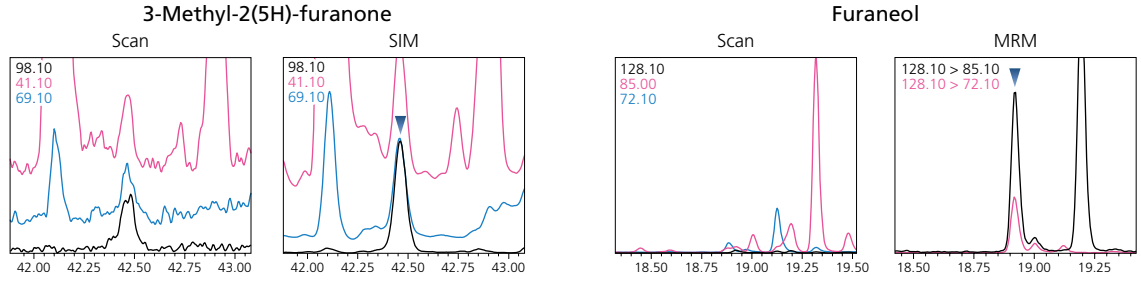

| Name | Conc. | Unit | Comment |
|---|---|---|---|
| delta-Undecalactone | 0.6 | ng | peach |
| Geranic acid | 1.2 | ng | wood, flower |

Semi-quantitative concentration

Sensory information

## 3. Enables High-Sensitivity Target Analysis Using MRM and SIM

Using Smart Aroma Database, measurement methods and data analysis methods for MRM mode and SIM mode can be created automatically. The sensitivity in a scan analysis may be insufficient for compounds that contribute to an aroma, even in trace quantities. However, a high-sensitivity target analysis is possible using MRM mode and SIM mode. MRM mode in particular enables a high-accuracy analysis in which the effects of impurities in a sample are eliminated.




## 4. Supports a Variety of Systems

Various sampling methods are used for aroma analysis depending on the sample configuration and the compound concentrations. Smart Aroma Database supports a variety of samplers used in aroma analysis. In addition, it can be used in combination with a sniffer GC-MS, so the aromas of the compounds actually detected can be checked.

# Database Configuration

## Number of Registered Compounds

| Column | Analysis Time | Number of Registered Compounds |
|---|---|---|
| SH-I-5Sil MS (30 m, 0.25 mm I.D., df = 0.25 µm) | 35 min | 492 |
| SH-PolarWax (60 m, 0.25 mm I.D., df = 0.25 µm) | 90 min | 506 |
| InertCap Pure-WAX (30 m, 0.25 mm I.D., df = 0.25 µm) | 35 min | 501 |

* For some compounds, the MRM information and sensitivity coefficients are not registered.

** Semi-quantitative results can vary significantly from the true value depending on the system status and pretreatment method. Be sure to perform a quantitative test using standards if accurate quantitative results are required.

*** The HS-20 autosampler series is not compatible with the semi-quantitative function.

## Product Configuration

Database file (Excel®), method file, library file

## Supported Models

GC-MS: GCMS NX series, GCMS-QP2020, GCMS-TQ™ series, GCMS-QP2010 SE

Autosampler: AOC-20/30 series, AOC-6000 series, HS-20 series, TD-30 series, OPTIC-4

Excel®: Microsoft® Excel® 2019 (32-bit/64-bit), 2016 (32-bit)

## Recommended Consumables

*N*-alkanes:

C7–C30 Saturated Alkanes (Sigma-Aldrich, Cat: 49451-U)

Sensitivity Correcting Sample:

Internal standards/surrogate standard substances Mix EPA 524.1, EPA 524.2 (Sigma-Aldrich, Cat: 47358-U)

Acenaphthene-*d*10 Solution (Sigma-Aldrich, Cat: 48417)

Analysis Column:

SH-I-5Sil MS (30 m, 0.25 mm I.D., df = 0.25 µm) (Shimadzu Corporation, P/N 221-75954-30)

SH-PolarWax (60 m, 0.25 mm I.D., df = 0.25 µm) (Shimadzu Corporation, P/N 227-36247-02)

InertCap Pure-WAX (30 m, 0.25 mm I.D., df = 0.25 µm) (GL Sciences, P/N 1010-68142)

**Cautions**

1. Absolutely no assurances are offered regarding the accuracy of the information contained in the database as well as the utility of the information obtained as a result of its use.
2. Be sure to perform tests using standards in order to confirm the qualitative and quantitative information obtained with this system.
3. When performing measurements, use the instrument parameters in the method files included with this product in order to reliably identify registered substances using this database.



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