

Database for GC-MS(/MS) Aroma Analysis

Smart Aroma Database



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

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

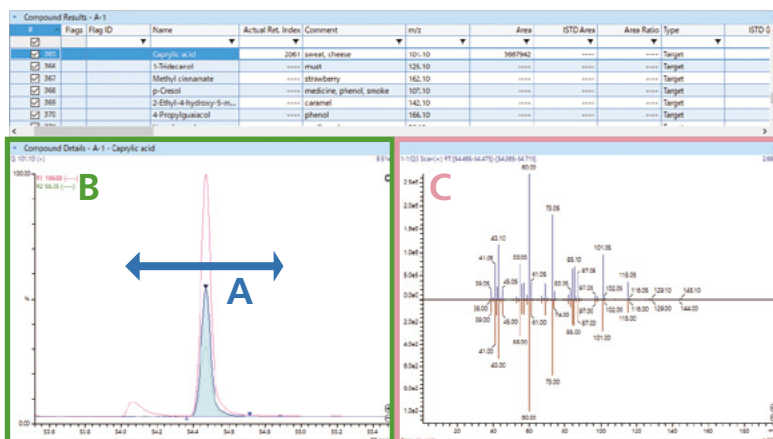
Peaks are found from the corrected retention time.

B Mass Chromatogram

Peaks are identified from the registered characteristic ions and ion ratios.

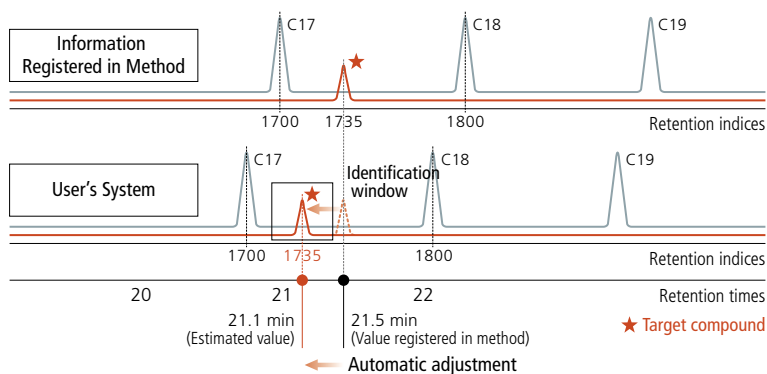
C Mass Spectrum

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

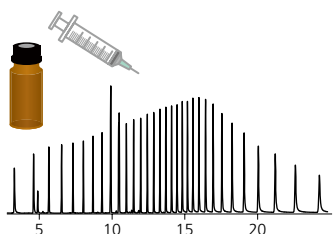


Automatic Adjustment of Retention Time (AART) of the Compound

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

ID#	Name	Ret. Time(Before)	Ret. Time(After)	Ret. Index
1	2-Methylfuran	1.731	1.649	850
2	Bihyl formate	1.797	1.710	857
3	Butanal	2.012	1.911	885
4	Ethyl acetate	2.065	1.964	886
5	Acetal	2.133	2.025	893
6	2-Butanone	2.133	2.025	893
7	Diethyl sulfide	2.152	2.042	895
8	2-Methylbutane	2.227	2.112	903
9	2-Methylbutane	2.274	2.156	909
10	Methyl isobutyl	2.336	2.209	914
11	3-Methyl-2-butene	2.348	2.226	918
12	2-Ethylfuran	2.526	2.392	925
13	Ethyl propionate	2.629	2.488	945
14	Bihyl isobutyl	2.704	2.558	954
15	Diacetyl	2.760	2.610	960
16	2-Pentanone	2.769	2.619	961
17	Valeraldehyde	2.769	2.619	961
18	3-Pentanone	2.779	2.628	962

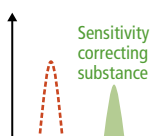
3. Analysis of samples using the adjusted method



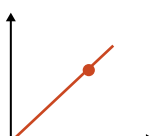
2. Easily Narrows Down the Compounds that Contribute to the Aroma

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.

1. Measurement of sensitivity correcting substance



2. Adjustment of the calibration curve



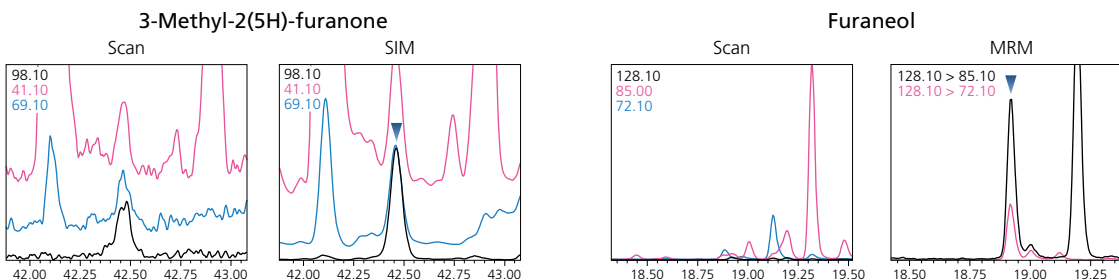
Name	Conc.	Unit	Comment
delta-Undecalactone	0.6	ng	peach
Geranic acid	1.2	ng	wood, flower

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® 2021, 2019 (64-bit/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.

Smart Aroma Database and GCMS-TQ are trademarks of Shimadzu Corporation and affiliated companies in Japan and/or other countries.
Excel and Microsoft are trademarks or registered trademarks of Microsoft Corporation in the United States and/or other countries.



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.