SHIMADZU
Excellence in Science

Flavour & Fragrance Natural & Synthetic Compounds GC/MS Library

FFNSC3 Library

GC/MS is commonly used for flavor and fragrance analyses, and searching a library of GC/MS spectra is convenient for identifying unknown components. However, similarities in the mass spectra of some fragrant compounds makes identification difficult. The FFNSC3 library contains retention indexes using three types of columns as well as mass spectra. Shimadzu's GCMSsolution library search, utilizing the retention index, provides highly accurate identification results and makes it ideally suited for flavor and fragrance analysis.

GCMS-QP2020

3462 Mass Spectra

The FFNSC 3 library is registered with 3462 natural and synthetic chemical compounds relating to flavors, providing even greater support for analysis.

Retention Index Compatible with Three Types of Columns

The FFNCS 3 library contains retention indexes compatible with three types of columns including wax columns.
Shimadzu's GCMSsolution library search, utilizing the retention index, narrows down the search results and makes it easy to identify various fragrant compounds.

FFNSC 3 Library

Specifications

Registered Compounds:
3462 flavor and fragrance compounds

Registered Retention Indexes:

Micropolar column (SLB™-5ms)	3462[n-alkane],2516[FAMEs]
Highly-polar column (SUPELCOWAX™ 10)	1466[FAMEs],1466[FAEEs]
Non-polar column (Equity™-1)	646[n-alkane]

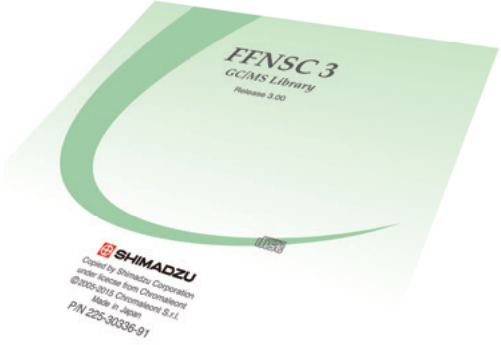
Note 1: Items in parentheses ( ) are Recommended Columns, items in brackets [ ] are reference compounds.
Note 2: SLB, SUPELCOWAX and Equity are trademarks of Sigma-Aldrich Co. LLC

Registered Information:
Mass spectrum, Retention index for each column, CAS number, compound name, molecular weight, compositional formula

Applicable models: GCMS-QP Series + GCMSsolution Ver.2.6 or later
GCMS-TQ Series + GCMSsolution Ver.4.0 or later
(single-quad mode only; does not include MS/MS spectra)

High Hit-ratio Mass Spectra

The FFNSC 3 library was developed using the Shimadzu GCMS-QP series by the skills-based group led by Prof. Mondello, (Messina Univ. in Italy). Performing analysis using Shimadzu GCMS enables obtaining mass spectra with similarities close to those registered in the library.



The mass spectra in the FFNSC library were obtained by the group led by Prof. Mondello, University of Messina, Italy.
The FFNSC library copyright is owned by Chromaleont S.r.l., a spin-off company of the University of Messina.

FFNSC3 Library

Filtering with retention index

Since flavor and fragrance components sometimes contain compounds having similar chemical structures, multiple compounds with similar mass spectra are listed as candidates when performing a library search using only the mass spectrum. Filtering with the retention index sorts the candidates by retention index, thereby providing highly accurate identification results.

Results of similarity search in mass spectrum

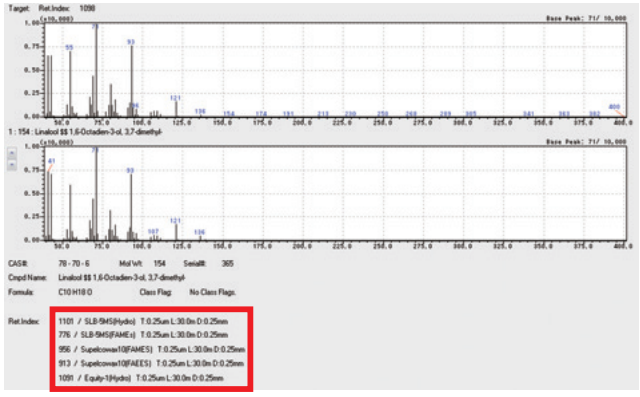
Hit	Simila	Regi	Compound Name	Mol Wt	Formula	Library Na
1	96	☑	Terpinolene $$ Cyclohexene, 1-methyl-4-(	136	C10 H16	FFNSC 3.lib
2	95	☐	Terpinene <alpha-> $$ 1,3-Cyclohexadiene	136	C10 H16	FFNSC 3.lib
3	93	☐	Carene <delta 2 > $$ Bicyclo[4.1.0]hept 2	136	C10 H16	FFNSC 3.lib
4	91	☐	Carene <delta-3-> $$ Bicyclo[4.1.0]hept-3	136	C10 H16	FFNSC 3.lib
5	90	☐	Terpinene <gamma-> $$ 1,4-Cyclohexadie	136	C10 H16	FFNSC 3.lib
6	89	☐	2,2-Dimethyl-5-methylene norbornane $$	136	C10 H16	FFNSC 3.lib
7	88	☐	Sylvestrene <iso-> $$ Cyclohexene, 1-met	136	C10 H16	FFNSC 3.lib
8	88	☐	Ocimene <(E)-, beta-> $$ 1,3,6-Octatriene,	136	C10 H16	FFNSC 3.lib

Results sorted using retention index filtering

Hit	Simila	Regi	Ret. Ind	Compound Name	Mol Wt	Formula	Library Na
1	96	☑	1086	Terpinolene $$ Cyclohexene, 1-methyl-4-(	136	C10 H16	FFNSC 3.lib

Multi-column compatible

All of the column retention indexes can be confirmed at the same time, which assists in close investigation of identification results.



Provides greater support for flavor and fragrance analysis

Gas Chromatograph Mass Spectrometer

GCMS-QP2020

Enables high-sensitivity and high-speed analysis
Single Quadrupole Mass Spectrometer

Various System Configurations*

Headspace Analysis System

Thermal Desorption Analysis System**

GC/MS Off-Flavor Analysis System

* The accuracy of the retention indexes differes depending on the sample introduction method.
** Not available in the U.S.

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