SHIMADZU
Excellence in Science

Elevate efficiency

Special libraries for GC-MS analysis

FFNSC, pesticides, lipids

Elevate efficiency

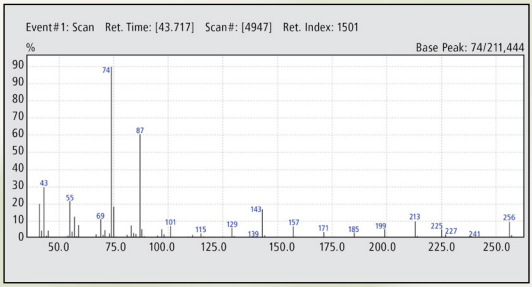
Simplified routine applications, time-saving processes, efficient workflows: MS-libraries support accurate results. Based on the fragmentation pattern after separation, this “fingerprint” can be compared with spectra in the library to identify the substance detected.

Shimadzu offers solutions for flavour & fragrance analysis, for food and beverage applications as well as clinical and medical applications.

Pesticides GC-MS Library Version 2

For food and beverage products

The GC-MS library efficiently supports precise identification of pesticide components for regulatory compliance and quality assurance needs.



SPECFICATIONS

- **Registered compounds**
  1,300 Pesticide compounds
- **Linear Retention Indices (LRI)**
  Non-polar column (SLB®-5ms)
  Non-polar column (Equity®-1)
- **Registered information**
  Mass spectrum, retention index for each column, CAS number, compound name, molecular weight, compositional formula

FFNSC4 Library

Flavour & Fragrance Natural & Synthetic Compounds

GC-MS technology is commonly used for flavour 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 challenging.

SPECFICATIONS

- **Registered compounds**
  4,030 flavor and fragrances compounds

- **Linear Retention Indices (LRI)**
  Non-polar column (SLB®-5ms)
  Highly-polar column (SUPELCOWAX® 10)
  Non-polar column (Equity®-1)

- **Registered information**
  Mass spectrum, retention index for each column, CAS number, compound name, molecular weight, compositional formula

Performing analysis using Shimadzu GC-MS enables obtaining mass spectra with similarities close to those registered in the library. The FFNSC4 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 flavour and fragrance analysis.

Lipids GC-MS Library

For food analysis, clinical and medical applications

Lipids are one of the major constituents of food, and play an essential role in human diet, metabolism, physiological and pathological processes. Mass spectrometry is the most important technology for lipid analysis. The Lipids Library provides significant support in peak assignment of complex mixtures and can be a valuable tool in many research fields such as food analysis, clinical and medical applications.

GCMS-QP2020 NX
This single quadrupole mass spectrometer provides high-speed and high-sensitivity analysis.

SPECFICATIONS

- **Registered compounds**
  430 lipid-like molecules classified in 11 different classes

- **Linear Retention Indices (LRI)**
  Non-polar column (SLB®-5ms)
  Non-polar column (Equity®-1)
  Highly-polar column (SUPELCOWAX® 10)

- **Registered information**
  Mass spectrum, retention index for each column, CAS number, compound name, molecular weight, compositional formula

All of the retention indices have been verified with data reported in the specific literature and underwent repeatability testing. The compounds were checked three times during a six month period.

Filtering with retention index

Greater assurance and efficiency of identification

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

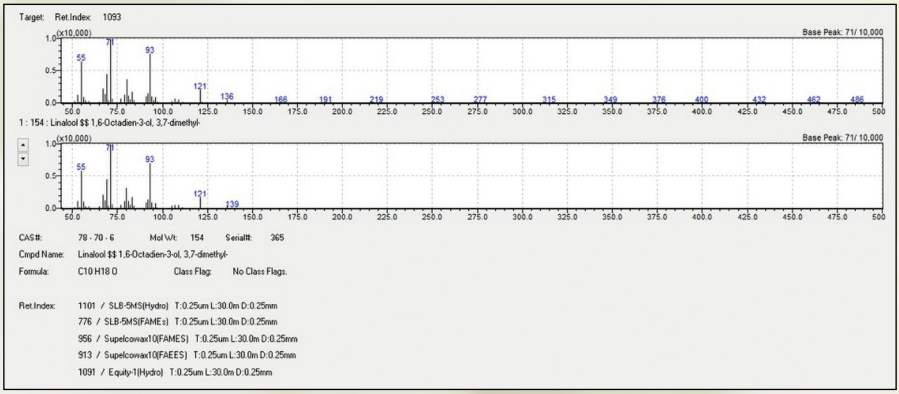
Hit#	Similarity	Register	Compound Name	Mol Wt	Formula	Library Name
1	98	☑	Linalool $$ 1,6-Octadien-3-ol, 3,7-dimethyl-	154	C10 H18 O	FFNSC 4.0.lib
2	98	☐	Linalyl anthranilate $$ 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-(2-aminobenzoate)-	273	C17 H23 N O	FFNSC 4.0.lib
3	89	☐	Linalool <ethyl-, (E)-> $$ 1,6-Nonadien-3-ol, 3,7-dimethyl-, (E)-	168	C11 H20 O	FFNSC 4.0.lib
4	89	☐	Linalool <ethyl-, (Z)-> $$ 1,6-Nonadien-3-ol, 3,7-dimethyl-, (6Z)-	168	C11 H20 O	FFNSC 4.0.lib
5	86	☐	Linalyl formate $$ 1,6-Octadien-3-ol, 3,7-dimethyl-, formate	182	C11 H18 O2	FFNSC 4.0.lib
6	86	☐	Linalool isobutyrate $$ Propanoic acid, 2-methyl-, 1-ethenyl-1,5-dimethyl-4-hexenyl ester	224	C14 H24 O2	FFNSC 4.0.lib
7	86	☐	Terpineol <beta-, cis-> $$ Cyclohexanol, 1-methyl-4-(1-methylethenyl)-, cis-	154	C10 H18 O	FFNSC 4.0.lib
8	86	☐	Linalyl acetate $$ 1,6-Octadien-3-ol, 3,7-dimethyl-, acetate	196	C12 H20 O2	FFNSC 4.0.lib

Results sorted using retention index filtering

Hit#	Similarity	Register	Ret. Index	Compound Name	Mol Wt	Formula	Library Name
1	98	☑	1091	Linalool $$ 1,6-Octadien-3-ol, 3,7-dimethyl-	154	C10 H18 O	FFNSC 4.0.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.



Various System Configurations

Through a choice of modules, detectors, components and accessories, dedicated application-specific GC-MS solutions are adjusted to the goal of a certain analytical task. Users can be sure to contribute to consumers and patients as well as environmental protection.

Headspace Analysis System

Thermal Desorption Analysis System

GC-MS Off-Flavor Analysis System

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The FFNSC4, Pesticides and LIPIDs libraries were developed using the Shimadzu GCMS series by the skills-based group led by Prof. Mondello, (Messina University, Italy). Its copyright is owned by Chromaleont S.r.l., a spin-off company of the University of Messina.