SHIMADZU
Excellence in Science

Lipids GC-MS Library Version 1

For food analysis, clinical and medical applications

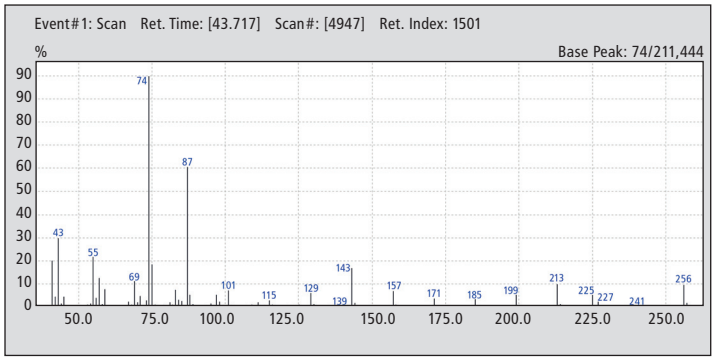
Lipids GC-MS Library Version 1.0 for GCMS-QP2020 single quadrupole and GCMS-TQ triple quadrupole series

430 lipid-like molecules classified in 11 different classes:
Mass spectra and retention indices contained in special library

Lipids are one of the major constituents of food. They 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.

Supported by GCMSsolution through linking with a similarity search for retention index
Highly reliable and efficient identification achieved for Lipids

Similarity search using retention index
- GCMSsolution automatically calculates the retention index
- A similarity search using retention index increases the reliability of search results by matching retention indices with those of compounds contained in the mass spectral libraries.



Lipids GC-MS Library

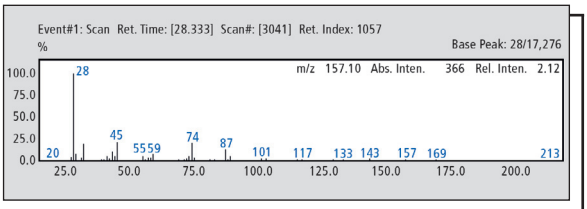
The Lipids GC-MS Library is a special mass spectral library in which mass spectra and retention indices (LRI) are registered. Mass spectra, relative to standard and well-known simple matrix components, were obtained and recorded through GC-qMS separation/identification. Furthermore, associated information relative to each component (CAS number, common name, systematic name, nominal mass (as Mol Wt), compound formula, chemical class) plus Linear Retention Index (LRI) values were added. The LRI have been calculated relative to alkanes, FAMEs and FAEEs.

Prof. Luigi Mondello and his team of the University of Messina, Italy developed the Lipids GC-MS library. The mass spectra and retention indices registered in the library were obtained using the Shimadzu GCMS-QP2020 equipped with an SLB-5MS (5 % diphenyl + 95 % dimethyl polysiloxane) 30 m x 0.25 mm ID x 0.25 µm film thickness (Supelco, #28471-U), Supelcowax-10 30 m x 0.25 mm ID x 0.25 µm film thickness (Supelco, #24079) and Equity-1 30 m x 0.25 mm ID x 0.25 µm film thickness (Supelco, #28046-U) columns.

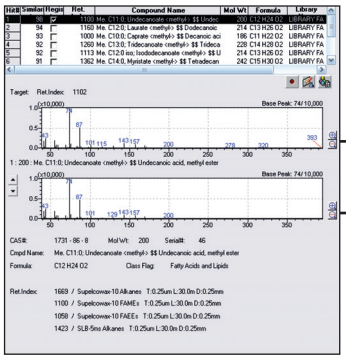
Retention Index Search – Higher reliability and efficiency of identification

Target Spectrum

Retention Index Automatic Calculation → **Until Now:**
Retention Index : 1057 **Similarity Search**

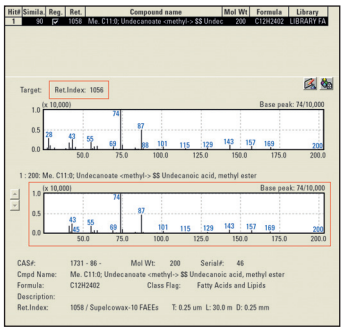


FAMEs GC/MS Library:
Similarity Search
+Retention Index Search



Similarity 80 or more

Many hits, but Identificationis difficult?



Similarity 80 or more
+
Retention Index calculated against FAEEs:
Tolerance Range: ± 10

Identification is easy!

A conventional library search using spectral similarity often indicates probable candidates only for an unknown compound and makes it hard to identify substances, particularly when isomers and a complex matrix are included.

In comparison, the GCMSsolution software provides a "similarity search with retention index" registered in the Lipids GC-MS library. This function enables a more reliable and easier search, even for complex samples. Results can be exported as reports in either electronic or hardcopy form.

*Lipids GC-MS Library can be used for GCMSsolution Ver 2.4 or higher.

To test the repeatability, the retention index allowance windows and the tolerance range have been calculated by means of multiple injections of compounds. Due to the low solubility of n-alkanes in the polar stationary phase, FAMEs and FAEEs standard mixtures have been used to calculate LRIs on the Supelcowax-10 column.

LRI repeatability data (expressed as difference between the LRIs) reported and calculated for a series of randomly selected compounds are shown in the table on the right.

Hit	Common Name	CAS Name	LRI FAEEs	Inj. 1	Inj. 2	Dif. Inj.1	Dif. Inj.2
46	Me, C11:0, Undeconate <methyl>	Undeconate acid methyl ester	1058	1059	1058	-1	0
49	Me, C15:0, Pentadeconate <methyl>	Pentadeconate acid methyl ester	1462	1462	1462	0	0
68	Me, C19:0, Nonadeconate <methyl>	Nonadeconate acid methyl ester	1867	1869	1865	-2	2

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