Access to your success
SHIMADZU

FAMEs GC/MS Library

Fatty Acid Methyl Esters Library ver 1.0
For Shimadzu GCMS-QP2010 Series

For Flavor & Fragrance, Food and Beverage Products

Powerful Backup to Identification of Fatty Acid Methyl Esters

240 Compounds:

Mass Spectra and Retention Indices Contained in Special Library

Through Linking with Similarity Search with Retention Index supported by GCMSsolution

Highly Reliable and Efficient Identification is Achieved for Fatty Acid Methyl Esters

Similarity Search with Retention Index

- The retention index is calculated automatically by GCMSsolution.
- Similarity search with retention index enables greater reliability of search results by matching retention indices with those of compounds contained within the mass spectral libraries.

Unequivocal Identification for Compounds with Similar Mass Spectra such as Isomers and Homologs.

FAMEs GC/MS Library

FAMEs GC/MS Library

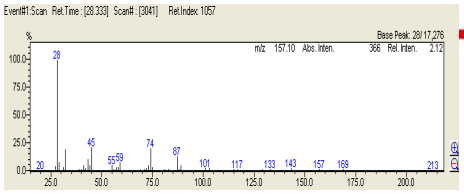
- The FAMEs GC/MS Library is a special mass spectral library in which mass spectra and retention indices (LRI) are registered. Each hit in the library has been obtained from the injection of pure chemicals and registered with the information relative to the official CAS information. The LRI have been calculated relatively to alkanes, FAMEs and FAEEs. All the retention indices reported have been verified with data reported in the specific literature, and tested for repeatability.
- The mass spectra and retention indices registered in the FAMEs GC/MS Library were obtained using the Shimadzu GCMS-QP2010.

* The FAMEs GC/MS Library was obtained by the Prof. Mondello group of the University of Messina in Italy. This was done using the SLB-5ms and the Supelcowax-10 columns (length 30m x inner diameter 0.25mm x film thickness 0.25 m) made by Supelco. The copyright is owned by Chromaleont S.r.l.

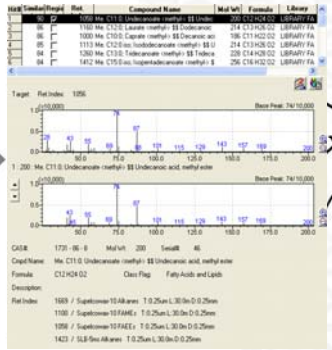
Retention Index Search - Greater Assurance and Efficiency of Identification -

Target Spectrum

Retention Index Automatic Calculation
Retention Index : 1057



Until Now:
Similarity Search



Similarity 80 or more

Many hits, but Identification is difficult

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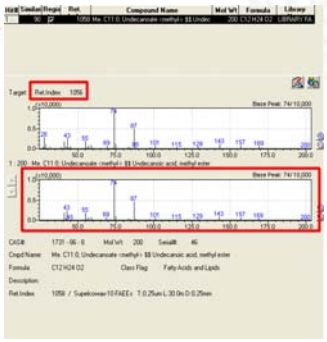
FAMEs GC/MS Library :
Similarity Search
+ Retention Index Search



Similarity 80 or more
+
Retention Index calculated against FAEEs:

Tolerance Range : ± 10

Identification Is Easy!

Conventional library search, making use of solely spectral similarity, often indicates so many probable candidates for an unknown that it is hard to identify it, especially in the case that sample includes isomers and much matrix. GCMSsolution provides “similarity search with retention index”, using retention indices registered in FAMEs GC/MS Library. This function makes it possible to perform more reliable and easier search even for complex samples. The results can be output as reports in electronic or hardcopy.

*FAMEs GC/MS Library can be used for GCMSsolution Ver 2.4 or higher.

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The retention index allowance windows and the tolerance range have been calculated by means of multiple injections of compounds for testing the repeatability. 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.
In table are reported LRI repeatability data (expressed as difference between the LRIs), calculated for a series of randomly-selected compounds.

Hit	COMMON NAME	CAS NAME	LRI FAEEs	Inj 1	Inj 2	Dif. Inj 1	Dif. Inj 2
46	Me, C11:0, Undecanoate <methyl>	Undecanoic acid, methyl ester	1058	1059	1058	-1	0
49	Me, C15:0, Pentadecanoate <methyl>	Pentadecanoic acid, methyl ester	1462	1462	1462	0	0
68	Me, C19:0, Nonadecanoate <methyl>	Nonadecanoic acid, methyl ester	1867	1869	1865	-2	2

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