SHIMADZU
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GC/MS Mass Spectra Library

Polymer Additives Library Ver.2

The analysis of additives contained in polymer materials is essential for managing and improving the quality of these materials, and for complying with regulations dealing with chemical substances. The Polymer Additives Library Ver.2 is a GC/MS mass spectral library containing information on a wide range of additives utilized in polymer materials.
In addition to mass spectra and retention indices, it contains information on the classification of additives to enable detailed analysis of additives.

GCMS-QP2050

Contains Approximately 5,800 Mass Spectra

This library consists of a library*, which contains 5,775 mass spectra for 590 types of polymer additives and GC/MS pyrolysates from the pyrolysis GC/MS analysis of additives, and a library containing the mass spectra for 65 compounds often targeted for analysis, selected based on their usage in the commercial market, and chemical substance regulatory information. In total, this product contains 5,840 mass spectra, which provides strong support for the analysis of polymer additives. In Ver.2, the compound registration has been newly enhanced, for example vulcanizing accelerators utilized in the rubber filed. Approximately 1,000 spectra have been added.

*ADD-MS22B F-Search Additives Library from Frontier Laboratories

Ready-to-Use Methods

This library provides GC/MS and PY methods; both contain all necessary conditions and measurement parameters. Anyone can easily start analysis with optimal analysis conditions.

Includes Retention Indices and Classification Information of Additives

Retention indices are registered for all compounds. Compounds can be identified with a high degree of accuracy by reducing the library search results using retention indices. In addition, information on the classification of additives is included, so even without detailed knowledge of additives, users can see which additive is associated with a compound found in the library.

Can Be Used with a Variety of GC/MS Systems

The library can be used for a variety of GC/MS applications, including pyrolysis GC/MS, which is widely used for the analysis of additives in polymer materials, and liquid sample injection GC/MS. It supports a wide range of additive analysis for customers.

▌Library Specifications

Registered compounds*: 5,775+65
Registered information: Mass spectrum, retention index for each analytical condition, compound name, molecular weight, compositional formula, structural formula, classification of additives
Applicable models: GCMS-QP™ series, GCMS-TQ™ series (This library does not include MS/MS spectra.)
Pyrolyzer (Pyrolysis analysis system): PY-2020D, PY-2020iD, and EGA/PY-3030D
Workstations: GCMSsolution™ Ver. 4.6 and later, LabSolutions™ GCMS™ Ver. 5.131 and later, LabSolutions DB/CS GCMS Ver. 6.131 and later

*: This consists of two types of libraries. The library with 5,775 compounds consists of the ADD-MS22B F-Search Additives Library developed by Frontier Laboratories, which has been converted to the Shimadzu mass spectral library format, and prepared for use with GCMSsolution and LabSolutions GCMS. The library with 65 compounds registered is an additive library developed exclusively by Shimadzu. It contains additives often targeted for analysis, selected based on their usage in the commercial market, and chemical substance regulatory information. Using these two libraries in combination enables the analysis of an even wider range of additives.

Polymer Additives Library Ver.2

Filtering with Retention Index

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 using mass spectrum

Hit#	Similarity	Register	Ret. Index	Compound Name		Mol Wt	Formula	Library
1	95	☑	1729	Ethylhexyl benzoate	[Original Additive: Bi	234	C15H22O2	FLAB_ADD1
2	81	☐	2042	Undecyl benzoate	[Original Additive: Diu	276	C18H28O2	FLAB_ADD1
3	81	☐	1796	Octyl benzoate	[Original Additive: Tri-n-	234	C15H22O2	FLAB_ADD1
4	79	☐	2109	Tridecyl benzoate	[Original Additive: Diun	304	C20H32O2	FLAB_ADD1
5	66	☐	793	1-Octene	[Original Additive: Alkyl phosp	112	C8H16	FLAB_ADD1
6	65	☐	791	Isomer of C8H16	[Original Additive: Alkyl	112	C8H16	FLAB_ADD1

Results sorted using retention index filtering

| Hit#	Similarity	Register	Ret. Index	Compound Name		Mol Wt	Formula	Library
1	95	☑	1729	Ethylhexyl benzoate	[Original Additive: Bi	234	C15H22O2	FLAB_ADD1

Confirming the Additive Classification Information

The additive classification information (such as plasticizers and flame retardants) registered in the library plays a role in confirming the type of additive associated with the compounds included in search results.
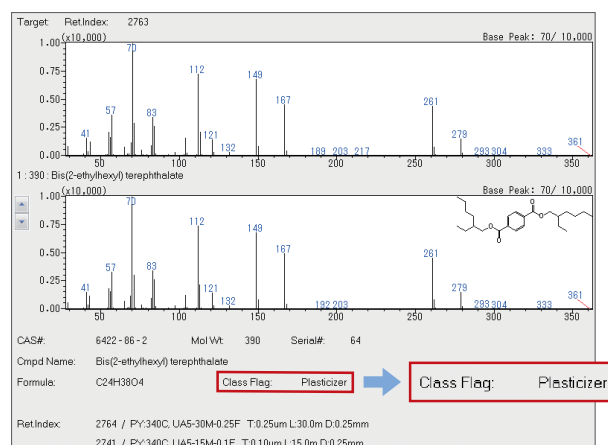
Deconvolution Analysis with LabSolutions Insight Explore™ GCMS

Even more accurate additive analysis is achieved by combining deconvolution analysis, which is capable of separating out impurities and detecting trace compounds, with this library.
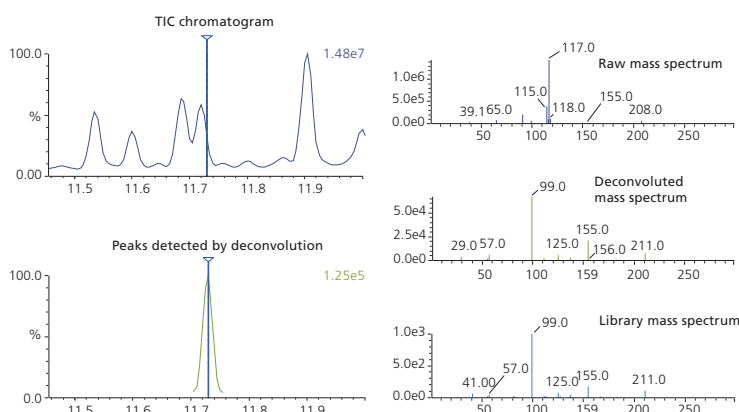
Example of System Configuration*

Pyrolysis Analysis System: EGA/PY-3030D, GCMS-QP2050
Liquid Injection Analysis System: AOC-30i, GCMS-QP2050

*: The accuracy of the retention indexes differs depending on the sample introduction method. Some of the pyrolysates may only be seen using a pyrolysis GC/MS analysis.

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