SHIMADZU
Excellence in Science

GC/MS Mass Spectra Library

Polymer Additives Library

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 is a GCMS 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-QP2020 NX

Contains Approximately 4,900 Mass Spectra

In addition to the existing library*, which contains 4,804 mass spectra for 494 types of polymer material additives and GC/MS pyrolysates from the pyrolysis GC/MS analysis of additives, a library has been added 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 4,869 mass spectra, which provides strong support for the analysis of polymer additives.

*ADD-MS16B F-Search Additives Library from Frontier Laboratories

Ready-to-Use Methods

This library provides GCMS 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*: 4,804+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 + GCMSsolution™ ver. 2.6 or later
GCMS-TQ™ series + GCMSsolution ver. 4.0 or later (This library does not include MS/MS spectra.)
Pyrolyzer (Pyrolysis analysis system): PY-2020D, PY-2020iD, EGA/PY-3030D

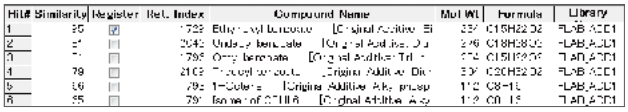
*: This consists of two types of libraries. The library with 4,804 compounds consists of the ADD-MS16B F-Search Additives Library (Ver. 16B.02) developed by Frontier Laboratories, which has been converted to the Shimadzu mass spectral library format, and prepared for use with GCMSsolution. The library 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

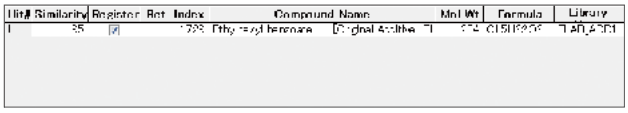
Filtering with Retention Index

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

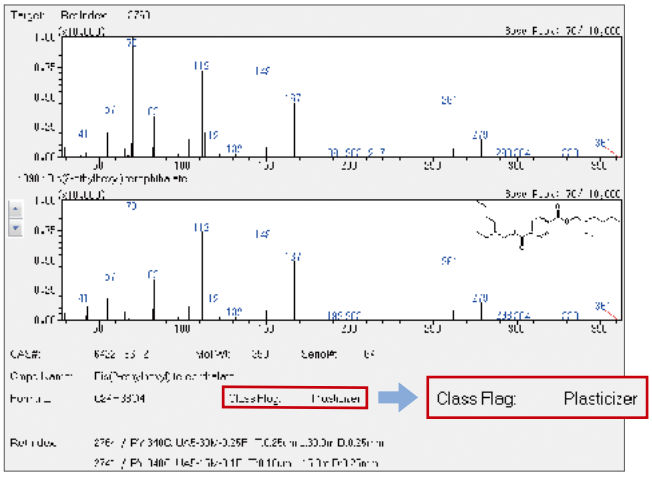


Results sorted using retention index filtering



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.



Screening System for Phthalate Esters

Can be Used in Combination with Py-Screener™

In addition to screening for phthalate esters, using this product in combination with Py-Screener enables the analysis of a wide range of other additives.

Example of System Configuration*

Pyrolysis Analysis System

Liquid Injection Analysis System

*: 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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