WILEY

Spectral Databases

From the Leader in Spectral Data

LC-MS - Class Rule-Based Polymer Library

Spectra – over 202,000

This database is only available as part of the KnowItAll LC-MS Spectral Library subscription

Description

Polymers are the building blocks of most of the commonly used materials, including natural compounds such as wool and rubber, as well as synthetic compounds such as plastics, lubricants, and detergents. Some of these polymers play essential roles as drug excipients and stabilizers in various pharmaceutical applications. The interest in studying polymers has grown substantially as the notion of green chemistry rises. Accurate identification of these polymers is required to determine product quality, safety, and impacts on health.

Liquid chromatography-high resolution mass spectrometry (LC-HRMS) can be used as one method to obtain information about the structures of polymers, including their repeating unit end groups, and backbone connectivity. Wiley offers the largest commerically available library of polymers.

Applications

- Environmental analysis
- Pharmaceutical
- Biomedical and health
- Extractables and leachables (E&L)
- Food safety
- Quality control

Additional Information

When it comes to spectral analysis, the more data you have the better. Wiley spectral databases provide much more information than simply the spectrum. Database records may include valuable details when available for a record such as:

- Chemical Structure
- Compound Name
- Exact Mass
- Formula
- InChI/InChIKey
- Molecular Weight
- SMILES
- Fragment Peak Labels
- Ion Polarity
- Precursor Ion
- Precursor m/z

Compound Coverage

Polymers:

- Polysorbates
- Polysorbides
- Polyethyleneglycols (PEGs)
- Methylated PEGs
- Fatty acid substituted species

Technique

The class rule-based fragmentation spectra were generated by applying fragmentation rules determined for a series of fatty acids.

The fragmentation rules were determined by referencing the literature, as well as analyzing MS/MS measurements of standards samples and polymer mixtures measured on an Agilent 6546 LC-Q/TOF acquired using a positive ion polarity.

The fatty acids included for generating mono-, di-, tri- and tetra- substituted polymers were: caproic acid (6:0), caprylic acid (8:0), capric acid (10:0), lauric acid (12:0), myristic acid (14:0), palmitic acid (16:0), palmitoleic acid (16:1), stearic acid (18:0), oleic acid (18:1), linoleic acid (18:2), and linolenic acid (18:3). PEG units from 2 to 20 were used, with polysorbate species having up to 80 PEG possibilities.

Common fragments noted observed were the ammonium adduct ($[N^+NH_4]^+$), the three common PEG fragments ($[C_4H_9O_2]^+$, $[C_6H_{13}O_3]^+$, $[C_8H_{17}O_4]^+$), and fatty acyl (FA) fragments (e.g., $[FA^+C_2H_3]^+$).

Annotations made using the fragmentation rules do not determine the fatty acid or PEG position to the polymer backbone, nor the length of the PEGs. Multicharged features (dimers, multimers, etc.) were not included in the library.

TRUSTED DATA FROM A TRUSTED SOURCE

Wiley is the authoritative source for spectral data. Our renowned databases are processed according to rigorous protocols to ensure they are of the highest quality. Qualification procedures start at data acquisition and continue throughout the database development process. Any data acquired from trusted partners is thoroughly vetted before inclusion in our collections.