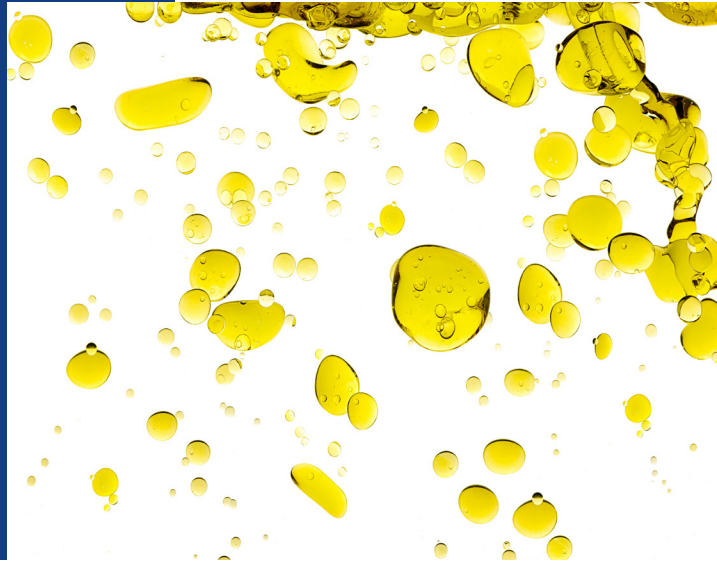
WILEY

# Spectral Databases

From the Leader in Spectral Data



## LC-MS - Class Rule-Based Lipids Library

Spectra – over 2.5 million

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

### Description

Lipids are a group of naturally occurring organic compounds that can vary greatly in their structural makeup, and thus the roles they play. Notably, lipids have the ability to serve as biomarkers for several diseases because of the critical role they play in organisms. The functionality of the lipid depends on its overall chemical structure. When taking into account the overall molecular variations of lipids such as to the backbone, degree of saturation, and stereochemistry, there are millions of potential structures of lipids.

Liquid chromatography-mass spectrometry (LC-MS) can be used as one method to analyze complex lipids. Wiley offers a large library of class rules-based lipid compounds with high resolution precision.

### Applications

- Food safety and quality control
- Cosmetics
- Metabolomics
- Consumer Goods
- Biomedical
- Pharmaceutical
- Clinical Sciences
- Natural Products

### 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

Over 56 lipid classes:

- Fatty acyls
- Glycerolipids
- Glycerolphospholipids
- Sphingolipids
- Sterol lipids
- Prenol lipids
- Saccharolipids

## Technique

Class rule-based spectral libraries were created using fragmentation rules. A script was used to generate a list of fatty acid combinations with 2 or 3 fatty acids, 39 possible endogenous fatty acids, and 214 potential oxidized fatty acids. A list of 126 possible long chain fatty acids were generated by the addition of one or more O-atom (as a ketone or epoxy), -OH (as hydroxyl radical), and -OOH (as a perhydroxyl radical), according to the degree of unsaturation. A list of 88 possible short chain oxidized fatty acids were generated by cleavage of unsaturated fatty acids and with the additional terminal -CHO (aldehyde) or -COOH (carboxylic acid). Oxidized fatty acyl chains were combined with the original list of fatty acyl chains to generate possible fatty acyl combinations for oxidized lipids.

For each lipid class, structurally indicative fragments were compiled from publicly available MS/MS databases to provide fragmentation rules from literature, and by analyzing acquired MS/MS spectra of standards. The MS/MS spectra were acquired in both positive and negative ion polarities using high energy collision dissociation (HCD) with internal standards on a high resolution orbitrap mass spectrometer. Using multiple sources to obtain fragmentation allowed for cross-validation of fragments and generation of lipid class-specific fragmentation rules.

## 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.