

WILEY

Spectral Databases

From the Leader in Spectral Data



LC-MS Class Rule-Based PFAS Library

Spectra – over 7,000

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



Description

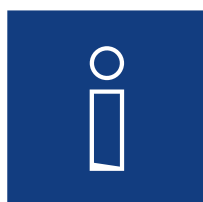
Per- and polyfluoroalkyl substances (PFAS) are a class of fluorinated organic compounds commonly known as “forever compounds” because of their environmental persistence. They can be found in many households and have contaminated drinking water and human bloodstreams after decades of use. PFAS are linked to numerous health hazards, including cancer, reproductive problems, and other diseases.

A common method of determining PFAS is through liquid chromatography-mass spectrometry (LC-MS). To aid in the identification of PFAS, Wiley offers the largest commercially available library of fluorinated organic compounds with high-resolution precision.



Applications

- Environmental analysis
- Food safety and quality control
- Cosmetics
- Biomedical
- Public Health
- Industrial manufacturing
- R&D



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



Compound Coverage

PFAS subclasses including:

- Fluorinated telomers (FTs)
- Organic perfluorinated compounds (OPFCs)
- Polyfluoroalkyl phosphates (PAPs)
- Perfluorocarboxylic acids (PFCAs)
- Perfluoroalkyl alcohols (PFOHs)
- Perfluoroalkyl sulfonates (PFSAs)
- Perfluoroalkyl sulfonamides (PFSMs)



Technique

This library was developed using class rule-based spectra using computed fragmentation across the PFAS subclasses.

To determine the fragmentation patterns for spectra, MS/MS spectra for the PFAS subclasses were measured in the laboratory using a Thermo Q-Exactive Orbitrap mass spectrometer with a negative ion polarity for over 150 standards. For each PFAS subclass, at least 2 compounds with differing chain lengths were measured. Additionally, fragmentation patterns compiled from literature were included (10.1016/j.trac.2019.02.021).

To determine fragmentation rules, the most intense fragments contained across the spectra for the subclass of compounds were chosen for annotation, and special emphasis was included for class-specific fragments.

For situations in which short-chain and long-chain species had very different fragmentation patterns, the PFAS subclass was further subdivided into two sets of 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.

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Quality Data. Results You Can Rely On.