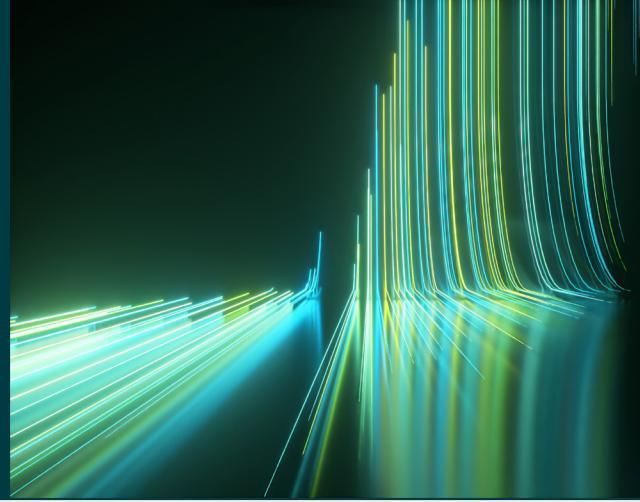


Spectral Databases

From the leader in spectral data



LC-MS - Metabolites Library - Wiley

Spectra – 16,578

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



Description

Metabolomics is essential for translating molecular knowledge into clinical impact, discovering new therapies, and understanding the complex interplay between genetics, the environment, and health. Applications span drug and biomarker discovery, food safety monitoring, and clinical research.

The LC-MS - Metabolites Library contains over 16,500 spectra of various metabolites. To ensure comprehensive compound coverage and confident identification, spectra are available in positive and negative ion modes and at different collision energies where possible. The database enables faster dereplication and facilitates discovery of novel bioactive compounds from both clinical and natural product sources.



Applications

- Drug discovery and development
- Metabolomics
- Food safety and agriculture
- Clinical and biomedical
- Environmental chemistry
- 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 include the following valuable details when available:

- Chemical structure
- Chemical name
- Exact mass
- Formula
- InChI/InChIKey
- Molecular weight
- SMILES
- Ion polarity
- Precursor ion
- Precursor m/z
- Technique
- Collision energy
- Retention time
- Convenient links to related references such as Human Metabolome Database (HMD), ZINC, KEGG, ChEMBL



Compound coverage

- Primary and secondary metabolites
- Lipids
- Lichens
- Phenolics
- Natural products



Compatibility

For full compatibility information, please visit sciencesolutions.wiley.com/compatibility.



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.