

WILEY

Spectral Databases

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1H NMR – Organic Compounds (Comprehensive) Part 2 – Wiley

Spectra – 37,840

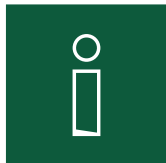
This database is only available as part of the KnowItAll NMR Spectral Library subscription



DESCRIPTION

This NMR database offers a comprehensive collection of high-resolution spectra of aromatic and heterocyclic organic compounds, complete with full chemical structure coverage, assignment information, and value-added properties. It contains high-quality, full-scan ¹H NMR spectral reference data, measured on 200 – 500 MHz NMR spectrometers.

This collection is extremely useful for identification or prediction of NMR spectra in a wide range of applications.



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
- NMR Offset
- NMR Solvent
- NMR Spectrometer Frequency
- Temperature



COMPOUND COVERAGE

Compounds containing the following elements:

- C - 37,842 compounds
- N - 36,620 compounds
- O - 35,714 compounds
- S - 15,981 compounds
- F - 6,847 compounds
- Cl - 8,470 compounds
- Br - 2,814 compounds
- I - 271 compounds
- B - 61 compounds
- Si - 14 compounds

Compound molecular weights (range - 54 to 1074 g/mol):

- < 100 g/mol - 15 compounds
- ≥ 100 and < 200 g/mol - 882 compounds
- ≥ 200 and < 300 g/mol - 6,453 compounds
- ≥ 300 and < 400 g/mol - 14,906 compounds
- ≥ 400 and < 500 g/mol - 12,244 compounds
- ≥ 500 and < 600 g/mol - 2,996 compounds
- ≥ 600 and < 700 g/mol - 317 compounds
- ≥ 700 and < 800 g/mol - 22 compounds
- ≥ 800 and < 900 g/mol - 5 compounds
- ≥ 900 and < 1000 g/mol - 1 compound
- ≥ 1000 and < 1100 g/mol - 1 compound



TECHNIQUE

All spectra were measured on NMR spectrometers with frequencies 200 – 500 MHz:

- 200 MHz - 137 spectra
- 250 MHz - 792 spectra
- 300 MHz - 5,104 spectra
- 500 MHz - 31,809 spectra

All compounds were measured in solution. NMR solvents:

- Acetone-d6 - 63 spectra
- Acetonitrile-d3 - 5 spectra
- CDCl3 - 681 spectra
- DMSO-d6 - 37,085 spectra
- No solvent reported - 8 spectra



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.

For additional information please visit www.sciencesolutions.wiley.com