WILEY Spectral Databases

From the Leader in Spectral Data



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.



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

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
- InChl/InChlKey

- Molecular Weight
- NMR Offset
- NMR Solvent
- NMR Spectrometer Frequency
- Temperature



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



ABOUT THE AUTHOR

Dr. Alexander Yarkov, born in 1954 in Russia, attended Lomonosov Moscow State University in the department of chemistry from 1971 to 1976. He then continued as a postgraduate student in the physical chemistry department, working in a molecular spectroscopy laboratory until 1979. In 1982, he was a candidate of chemistry for Moscow State University. Dr. Yarkov is now the senior scientist for the Applied Spectroscopy Laboratory at the Institute of Physiologically Active Compounds at the Russian Academy of Science. His research areas of interest include molecular spectroscopy, NMR spectroscopy, mass spectroscopy, identification of chemicals using spectral databases, and QSAR.



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.