

Mass spectra library NIST 2020



Product information

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With version 2020, the **N**ational **I**nstitute of **S**tandard and **T**echnology provides a new version of its mass spectra library.

The library contains 350,643 spectra of 306,869 components. Each spectrum has been checked for conclusive fragmentation patterns by at least two experts. Thus, NIST defines a new quality standard for identification for MS libraries. In order to be able to use the retention information of substances, the database also contains retention indices of over 139,498 components, 111,788 of which also contain MS spectra. In addition, the structural formula of almost every substance is also included. Another highlight is a special library with over 1.3 million MS/MS spectra of 186,000 precursor ions based on 31,000 components.

Both the database with the retention indices and the MS/MS database are available separately.

In addition to the database, the NIST 2020 package includes software packages that simplify data handling. The browser makes it very easy to search the database. A search for trivial names is possible as well as searches for elemental compositions, CAS numbers, molecular weight etc. Of course the browser software allows the comparison of unknown spectra with the database.

The also included AMDIS data system can be used for the evaluation and deconvolution of GC-MS chromatograms from different manufacturers. 18 different data formats can be read in.

Small auxiliary programs for the interpretation of mass spectra and the calculation of isotope patterns complete the package. A detailed documentation is included.

Note: An English manual is available for the MS library NIST.

Subject to technical changes

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