



NIST 2020 Mass Spectral Reference Libraries

NIST

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The NIST 20 mass spectral database, the successor to the NIST 17, is a set of fully evaluated collections of electron impact (EI) mass spectra, tandem MS (MS/MS) mass spectra and retention index (RI) data. It is the product of a thirty year, comprehensive evaluation and expansion of the world's most widely used mass spectral reference libraries by experienced mass spectrometrists in which each spectrum was examined for correctness.

NIST/EPA/NIH Mass Spectral Library of Electron Ionization Spectra

This release contains 350,643 electron ionization (EI) spectra of 306,869 different chemical compounds - an increase of over 44,000 spectra and nearly 30,000 compounds from the previous release (NIST 17). For this release, for the first time nearly all new spectra were run at NIST based on their analytical importance and then individually evaluated with the aid of newly developed software.

NIST Tandem MS Library

This library consists of four sub-libraries with a total of 1,320,389 spectra of 185,608 ions for 30,999 compounds (>2x increase) including spectra for both positive and negative charge states, with fragmentation in both ion trap (at multiple msn levels) and in beam-type collision cells (over a range of energies):

Small Molecule High Resolution MS/MS Library (1,026,712 spectra of 94,472 ions of 27,840 compounds)

Small Molecule Low Resolution MS/MS Library (215,649 spectra of 163,512 ions of 28,559 compounds)

Small Molecule APCI High Resolution MS/MS Library (3,555 spectra of 605 ions of 246 compounds)

Biological Peptide MS/MS Library (90,244 spectra of 6,803 ions of 1,904 compounds)

NIST Gas Chromatography Retention Index and GC Methods Library

This library contains 447,285 retention indices for 139,963 compounds, including 112,253 of which are in the EI library. This is an increase of about 40,000 compounds.

NIST Search Software

The capabilities of the NIST MSSearch user-interface software were again enhanced. The entire library is now based on chemical structures using the NIST-developed InChIKey representation. A new search type, the 'Hybrid Search' enables finding many more similar compounds in the hit list. It requires a precursor mass. A new neutral loss search is available that eliminates restrictions on the maximum loss considered. The greatly improved MS Interpreter program allows for enhanced quality control by linking ions to originating structures in the precursor molecule.

NIST 20 is available as full version and also as upgrade for owners of a previous edition:

NIST20 NIST 2020 Mass Spectral Libraries, Single User

NIST20U NIST 2020 Mass Spectral Libraries, Single User, Upgrade

These items include the library in NIST format. Please note that the library is also available in various other formats, e.g. MassLib, ChemStation, etc. Please contact us for a quote.