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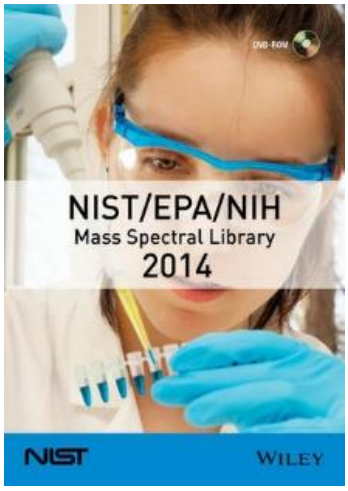

NIST / EPA / NIH Mass Spectral Library 2014

NIST, Wiley Technology

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NIST/EPA/NIH 2014 Mass Spectral Library is a trusted source of mass spectral data and software tools. The newest edition contains an expansion of the main EI library as well as significant improvements in the underlying MS Search software (2.2).

Protect Your Investment

Wiley's NIST 2014 is the most comprehensive available, with more manufacturer formats on one disc than any other source. This helps ensure transportability when switching instruments or manufacturers, and takes the guesswork out of ordering for mixed-instrument deployments.

Wiley’s NIST 2014 contains the complete NIST software suite as well as the various NIST libraries in NIST and native manufacturer formats to enable access to advanced search, analysis, and reporting methods found in the original and legacy manufacturer software systems.

NIST/EPA/NIH 2014 edition contains:

- 276,248 EI spectra for 242,466 compounds
- NIST 14 MS/MS libraries (nist_msms and nist_msms2) with 234,284 spectra of 45,298 ions
- GC Methods/Retention indices library (nist_ri) with 82,868 compounds; 56,216 compounds in the Main library have retention index data.EI-MS Spectral Library

New features and functionality included in the NIST MS Suite:

- New NIST 14 MS/MS Library. Spectra include metabolites, peptides (biologically active peptides and all di-peptides and tryptic tri-peptides), contaminants, lipids and more.
- Using Retention Index in library searching: RI deviation of a hit from the search spectrum are used to penalize the Match Factor.
- Indexing older user libraries to use saved in them RI values for library searching
- Displaying relevant RI values in the hit list
- New definitions of derivatives are used for finding replicate spectra
- Displaying derivative precursor in the Lib. Search hit list
- Displaying additional MS/MS information in hit lists
- Editing accurate peak m/z, intensities, peak annotations, and compound RI in the built-in mass spectrum editor
- All small molecule mass spectra in NIST libraries have InChIKeys linked to PubChem. These InChIKeys may also be used for searching compound information on the Web or for exact or "non-stereo" structure search in NIST libraries.
- Importing and displaying Glycan structures in KCF format; adding them to mass spectra in a user library
- In-source/EI with accurate ion m/z spectra - High resolution mass spectra
- Import of ‘in-source’ tandem or EI with accurate ion m/z spectra, which do not include a defined m/z of the precursor ion. To import these spectra, select "in-source / EI (accurate m/z)" in Spectrum Import Options.
- In-source spectra have accurate ion peak m/z and intensities. The accuracy is set in Spectrum Import Options: ion peak m/z tolerance down to 0.015 ppm or 0.00006 m/z units

- In-source/EI with accurate ion m/z spectra may be searched in In-source/EI with accurate ion m/z and/or MS/MS libraries with the new In-source HiRes search, Similarity Simple, Identity Normal or MS/MS Presearch OFF search options. For this purpose, adding Reverse Search option may useful.
- In-source/EI with accurate ion m/z spectra may be added to a user library. Currently, in-source/EI with accurate ion m/z spectra added with NIST MS Search to a user library may be searched with In-source HiRes search only with Presearch OFF option. Rebuild the library with Lib2NIST to get in-source HiRes search benefits.
- MS/MS search for small molecules (deselect Peptide Scoring in MS/MS tab of Library Search Options)
- Exact Mass Search and Constraint allows searching for exact mass of a precursor using its mass or exact m/z of a product ion. It takes into account the presence or absence of an electron, adducts or losses; accepts uncertainty in ppm or millimass units, and allows searching for isotopic or monoisotopic peaks.
- Ability to use accurate mass to search exact fragment ion mass values in NIST MS libraries mainlib, replib, and nist_msms using Exact Mass in the Any Peaks Search.
- A small portion of spectra have more than one CAS Registry number. Each CAS r.n. may be used in CAS r.n. search
- Optionally displayed columns Number of synonyms and Number of other databases and a possibility to sort by them.
- Sorting Spec List alphabetically.
- Handling and searching up to 127 MS libraries instead of 16.
- Max. number of spectra in a library has been increased from 786,420 to 1,048,560.
- Search for words in mass spectrum text information window (use context menu displayed on right mouse click.)
- Optional exclusion of Homologs from the results of Structure Similarity Search.
- Import spectra from mzXML and mzData files.
- Import MS/MS spectra from JCAMP files. See file MSMS_JCAMP_Example.JDX
- Import of ‘in-source’ tandem spectra, which do not include a defined m/z of the precursor ion. To import these spectra, select "In-source spectra" in Spectrum Import Options.
- Additional Spectrum import Options: Control the number of decimal places in the input m/z; Set peak intensity threshold; Set Prepend/Overwrite/Ask automatic mass spectrum import option.
- An alternative peak matching method has been added to improve the reliability of the score when searching noisy MS/MS spectra.
- Full compatibility with most recent NIST Peptide MS/MS libraries.
- Press Ctrl-K to copy selected lines from Hit List or Spec List into Windows Clipboard as tab-delimited Unicode text; this may be conveniently pasted into Excel.
- Multiple CAS Registry numbers for a spectrum. A small fraction of spectra in NIST MS Libraries has more than one CAS r.n. Each CAS r.n. may be found in a CAS Number search.
- Tags for searching in Spectrum Text Info have been added to Tags in Comment Constraint
- New MS/MS Instrument Type constraint.
- When a Tag from the "Comment" field is displayed separately, its display in the "Comment" field is suppressed.

Verify Coverage

Labs can freely verify compound coverage at www.compoundsearch.com

Formats

Each NIST 2014 is bundled with the following native instrument formats:

- Agilent Chemstation and MassHunter
- Shimadzu GCMS Solution
- Waters MassLynx
- ACD/Labs MS Manager
- NIST software (compatible with Leco, JEOL, Bruker, others)
- Thermo xCalibur, Chromeleon
- PerkinElmer TurboMass

Also available in MSP Kofel MassLib format.

Contact: MSP Kofel +41 31 972 31 52 info@msp.ch