

What's New in NIST 11 MS Library (May 2011)

NIST 11 consists of the 2011 release of the **NIST/EPA/NIH Electron Ionization (EI) Mass Spectral Library**, the **NIST MS/MS Library**, and the **NIST GC Methods and Retention Index Library**, along with a new version of the **NIST Mass Spectral Search (MS Search) Program** (version 2.0g). Enhanced versions of **MS Interpreter** and **AMDIS** are also included with NIST 11.

The **NIST/EPA/NIH Library of Electron Ionization Mass Spectra** now contains **243,893** carefully evaluated spectra for **212,961** compounds, an increase of nearly 10% from the 2008 version. This includes **23,433** new spectra of metabolites, drugs of abuse, derivatives of the above, common compounds and many more; most of them measured specifically for this library. Other major enhancements have been made to the prior version including many replacements with higher quality spectra, a thorough review of chemical names and merging of the previous salts library into the main and replicates libraries.

The **NIST Library of MS/MS spectra** has undergone an even greater enhancement. The new collection more than doubles the number of compounds represented. Further, most spectra have been acquired on both ion trap and qtof/triple quad instruments, thereby increasing the number of spectra by over a **factor of six** compared to the 2008 version. Spectra for the latter instrument classes have been acquired over a wide range of energies to ensure matching regardless of instrument collision settings. Also, when available, **high mass accuracy spectra** are stored. New spectra include metabolites, peptides (biologically active peptides and all di-peptides and tryptic tri-peptides), contaminants, lipids and more. The 2011 version contains **10,065 ion trap spectra** for **9,194 different ions** of **4,628 compounds**, and **85,344 collision cell spectra** (qtof and tandem quad) for **7,172 different ions** of **3,877 compounds**.

The **GC Methods and Retention Index Library** contains **346,757** GC Methods with Retention Index (RI) values for **70,835** compounds, a 61% increase in the number of compounds compared to the previous version. The annotations include literature source and measurement conditions. The number of compounds with RI data in the EI Library is **38,648**, an increase of 76%. In addition, for many compounds in the database an **Estimated Kovats Retention Index (RI)** together with a confidence interval is displayed based on the structure associated with the spectrum. MS Search will also calculate RI values for structures submitted by users.

Since the introduction of the **NIST MS Search Program** as a Windows 32-bit version (v.2.0), it has evolved into a power tool for not only the matching of spectra of unknown compounds against spectra for that compound in the **EI** and **MS/MS Libraries**, but also the identification of unknowns encountered in toxicology, forensic, quality control, flavor and fragrances, environmental and many other fields through their mass spectra, regardless of the type of ionization or the analyzer used to determine the intensities of ions. The **EI Library** contains much more than just the mass spectra of compounds. It contains a primary and in many cases multiple synonyms including common and trade names. It contains names of other databases where specific compounds can be found, the name of the contributor, the compound's elemental composition, its nominal and exact mass, and the compound's chemical structure.

New features in NIST MS Search version 2.0g (May 2011 release)

1. Search for the exact mass value in the NIST/EPA/NIH Mass Spectral Library or any User Library and use of the accurate or exact mass as a search constraint.
2. Search for exact fragment ion mass values in NIST 11 libraries mainlib, replib, and nist_msms.
3. Display of the exact mass with any spectrum that has an associated chemical formula.
4. Optional columns in Hit Lists containing the number of synonyms and the number of Other Databases in which the Hit appears. The Hit List can be sorted according to the values in these columns.
5. Managing and searching as many as 127 separate MS libraries instead of 16, which was the limit in previous versions.
6. Up to 1,048,560 spectra in a single library instead of 786,420 spectra allowed in the previous versions.
7. Import spectra from mzXML and mzData MS and MS/MS files (in addition to mgf, msp, dta, pkl, JCAMP, etc.)
8. Option to turn off homolog hits in a Structure Similarity Search.
9. Full compatibility with most recent NIST Peptide MS/MS Libraries.
10. Sorting the Spec List alphabetically and by the accession numbers.
11. Copying selected lines from Hit List or Spec List into Windows Clipboard as tab-delimited Unicode text; this may be conveniently pasted into Excel.
12. MS/MS Instrument Type constraint.
13. Tags in Comment constraint has been enhanced to include Tags in Text Information window.
14. When a Tagged item from the Comment is displayed separately in Text Information window its display in the Comment is suppressed.
15. Searching for a text in a Text Information window of a spectrum.
16. Spectra in the MSP text format can be imported from the Windows Clipboard into the Spec List.
17. Default view of Constraints and Other Searches dialog boxes changed to provide more convenience to the users.
18. An alternative peak matching method has been added to improve the reliability of the score when searching noisy MS/MS spectra.
19. The MS Interpreter program displays high accuracy mass for both molecular ions and product ions.