

New features in the NIST MS Search Program (version 2.0g) for the 2011 Version of the NIST/EPA/NIH Mass Spectral Library (NIST 11)

1. Search for exact precursor mass in the NIST/EPA/NIH Mass Spectral Library or any User Library and use of the exact mass as a search constraint.
2. Search for exact fragment ion mass in NIST 11 EI and MS/MS libraries.
3. Shows exact mass for spectra having chemical formulas.
4. Handles up to 127 MS libraries instead of 16, the limit in previous versions.
5. Up to 1,048,560 spectra in a single library instead of 786,420 spectra as allowed in previous versions.
6. Import mass spectra from mzXML and mzData files (in addition to mgf, msp, dta, pkl, JCAMP, etc.) – these formats are common to newer data systems
7. Import mass spectra from the Windows Clipboard.
8. Full compatibility with most recent NIST Peptide MS/MS Libraries (<http://peptide.nist.gov>).
9. View or not view option for homologs (related compounds) in a Structure Similarity Search.
10. Optional columns in Hit Lists with the number of synonyms and the number of Other Databases (reflects how commonly a compound is found) for each identifications. The Hit List can be sorted according to the values in these columns.
11. Copying selected lines from the Hit List into the Windows Clipboard.
12. Search for spectra from specified MS/MS Instrument types.
13. Tags in Comment search constraint extended to tags in the found spectrum text information view.
14. Searching in the spectrum text information view.
15. An alternative peak matching method based on dot product optimization for searching noisy MS/MS spectra.
16. The MS Interpreter program displays exact mass for both precursor and fragment ions.