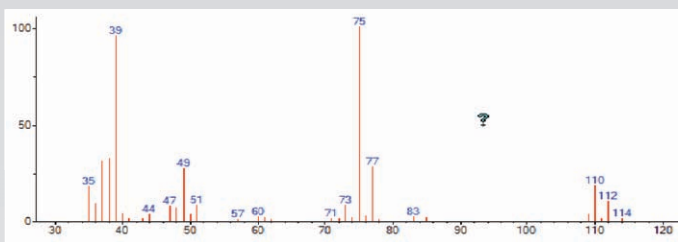


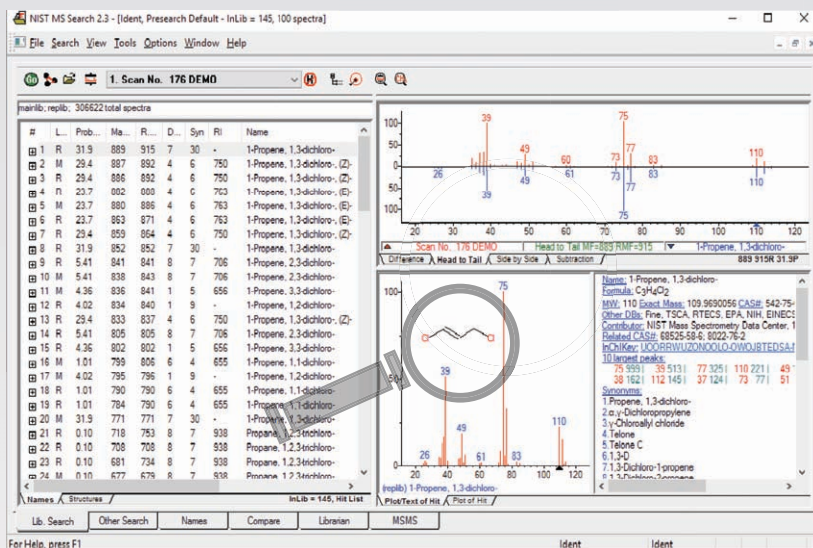
# NIST 17

Mass Spectral Library &  
Search Software  
Version 2017

## What is this mass spectrum?



Identify it with NIST 17, the world's most widely trusted mass spectral library!



## Improvements since 2014

- Increased coverage and quality in all libraries:
  - Nearly 3x increase in MS/MS spectra.
  - 30,000+ new EI spectra
  - 16,000+ more compounds with GC & retention index citations
- Improved search software (v. 2.3)
  - New search methods and algorithms, such as our new “hybrid” search type for MS/MS and EI.
  - See back for details.

Upgrade discount for any previous version. Agilent format option.

Compatible with most mass spectral data systems, including Agilent ChemStation/ MassHunter, Thermo Xcalibur, Waters MassLynx, Shimadzu GC/MS Solutions, and others.

*Quality, broad coverage, and accessibility* — these are what the NIST MS Library is known for, a product of a three decade, comprehensive evaluation, where each spectrum is validated for correctness by a team of experienced mass spectrometrists.

Additional utilities bundled with NIST 17:

*AMDIS* - extracts noise-free component spectra from GC/MS data files and can library search them with NIST MS Search

*MS Interpreter* - assists in analysis and interpretation of mass spectra (New Version)

## NIST 17 contains nearly a million mass spectra:

306,000+ electron ionization (EI) spectra for 267,000+ compounds.

652,000+ tandem MS/MS spectra:

176,000+ ion trap spectra for 120,000+ ions of 14,000+ compounds

475,000+ collision cell spectra for 39,000+ ions of 14,000+ compounds

NIST 17 also contains search software to match your spectra against spectral libraries.

Each spectrum has corresponding information, such as

- chemical formula, structure, and mass
- chemical names, synonyms, CAS#, InChiKey (PubChem)
- GC method and retention indices if applicable (72,000+ in EI library)



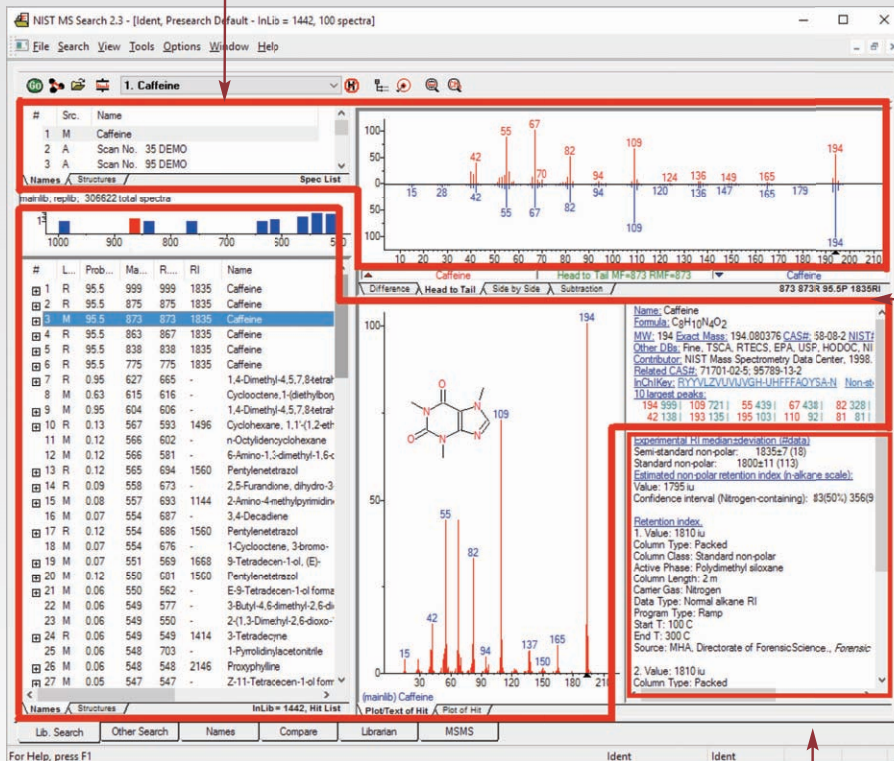
Scientific Instrument Services, Inc.™

[www.sisweb.com/nist](http://www.sisweb.com/nist)

# NIST Libraries & Search Software

The included NIST MS Search Software allows browsing and searching the EI MS, MS/MS, and GC libraries.

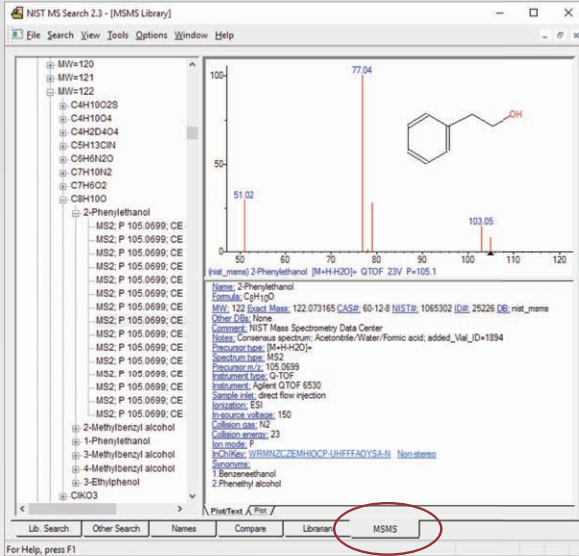
Given a user provided (unknown) spectrum, library search for the best matching spectra in the NIST and user libraries. Matches are ranked. Searches may add a variety of constraints (name, elements present, structural similarity, etc.). Searching is also possible from most mass spectral data systems, including Agilent ChemStation/MassHunter, Thermo Xcalibur, and others.



The **Electron Ionization (EI) mass spectral library** consists of 306,622 spectra of 267,376 unique compounds, each with name, formula, molecular structure (mol), molecular weight, CAS#/InChIKey, contributor name, list of peaks, and synonyms.

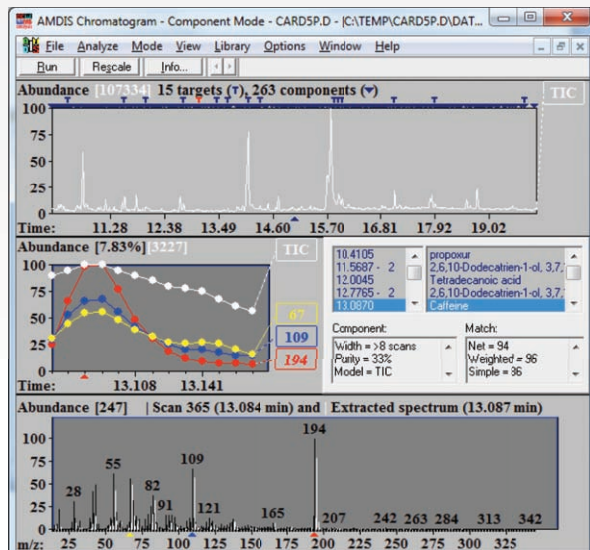
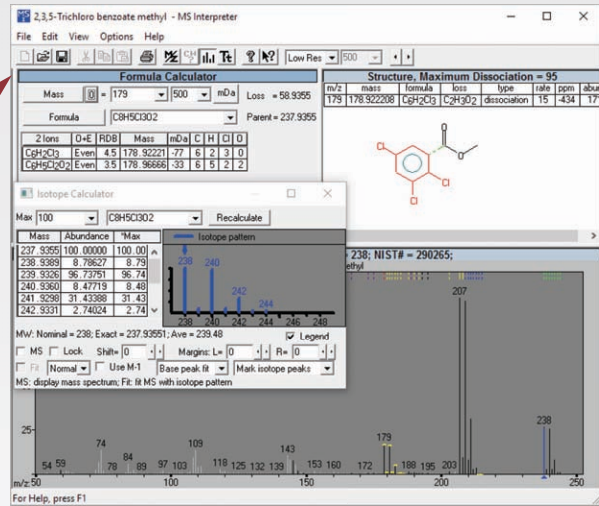
The **GC library** contains 404,045 citations of retention indices (Kovats or Lee) RI and GC methods for 99,400 compounds (72,361 in the EI library) with structures, covering both polar and non-polar columns. When available, this data is displayed with the spectrum search results. RI values can now be displayed in the hit list and used for scoring.

The **MS/MS library** contains 652,475 tandem spectra from ion trap, qTOF, HCD, and tandem QQQ collision cell instruments, most acquired under electrospray. Spectra can be browsed by mass, formula, and energy from the MS/MS tab or library searched against your own spectra or search criteria. Details on experimental conditions on each library spectrum are displayed.



MS/MS Library		#spectra	#ions	#compounds
small molecules, di- and tri-peptides	ion trap	163,532	114,925	12,992
	collision cell	411,294	34,517	12,728
commercial peptides	ion trap	13,062	6,422	1,828
	collision cell	77,182	5,637	1,814
<b>total</b>		<b>652,475</b>	<b>123,881</b>	

The **Mass Spectrum Interpreter** utility assists in the evaluation of mass spectra. You can examine neutral losses, isotope patterns and possible chemical formulas, along with computer-assisted chemical structure/spectra analysis.



The **NIST AMDIS** utility integrates with NIST MS Search for

- **GC/MS deconvolution:** Preprocesses GC/MS or LC/MS data files, automatically reconstructing spectra from complex mixtures. Selected compounds can then be sent to the NIST MS Search software for library searching.
- **Chemical Identification:** Can also act as a “black box” chemical identifier, displaying all chemical identifications that meet a user-selectable degree of confidence. Identification can be aided by internal standards and retention times.

# New in NIST 17

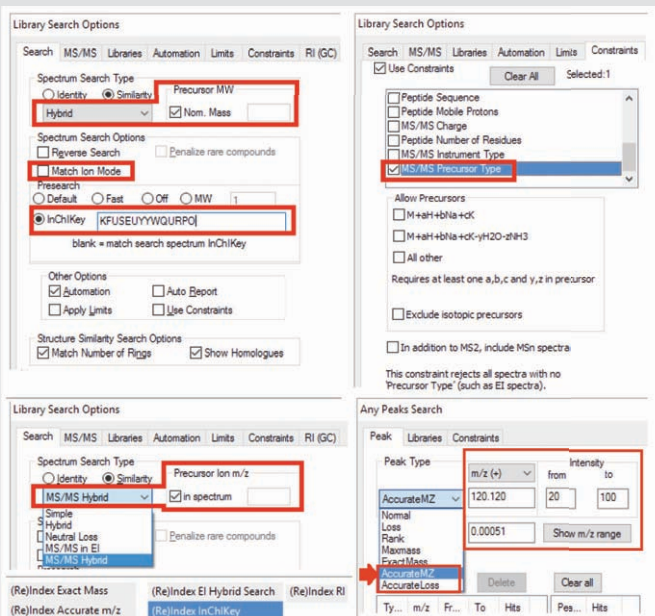
All libraries have undergone substantial enhancements in the 2017 release.

- **EI MS Library:** 30,000+ new EI spectra. Expands coverage of metabolites and designer drugs, as well as the application of new computer-assisted evaluation methods for removal of low quality spectra.
- **MS/MS Library:** Nearly 3x increase in the MS/MS library. Spectra include metabolites, peptides (biologically active peptides and all di-peptides and tryptic tri-peptides), contaminants, metabolites, lipids and more.
- **GC RI Library:** 16,000+ more compounds have GC data method and retention indexes.

Version	#EI Spectra	#MS/MS Spectra	#GC RI	Software
2017	306,622	652,475	404,045	v.2.3
2014	276,248	234,284	387,463	v.2.2
2012		121,586		
2011	243,893	95,409	349,757	v.2.0g
2008	220,460	14,802	224,038	v.2.0f
2005	190,825	5,191	121,112	v.2.0d
2002	179,948	0	0	v.2.0a

Updated software - some major new features include

- **MS/MS Searching**
    - New HiRes MS/MS Hybrid search type uses the logic of normal searching and the logic of neutral loss searching to find many more similar compounds in the hit list (requires a precursor mass).
    - AnyPeak search: New accurate mass peak and loss types.
    - MS/MS Precursor m/z search
    - Precursor type constraint to restrict results to specific precursor types, exclude isotopic precursors, and display MS2 and higher spectra in addition to MS2.
    - Spectrum polarity filter
  - **EI MS Searching**
    - New EI Hybrid Search (Similarity / Hybrid) type uses both the logic of normal searching plus the logic of neutral loss searching. Same algorithm as MS/MS Hybrid search with unit charges and nominal MW instead of precursor m/z.
    - Presearch for EI Similarity/Neutral Loss search. Eliminates restrictions on the maximum loss considered.
  - **All Searching**
    - An 'InChIKey' presearch for all library spectrum searches. Finds all spectra which have the same first InChIKey segment as the search spectrum, and compares them to the search spectrum.
    - Improved algorithms for scoring high mass accuracy searches that account for sparse spectra.
    - User interface enhancements.
    - New version of MS Interpreter software.
- See "What's New" on our web page for additional details.



Visit <http://www.sisweb.com/nist> for more details, to contact us, or to order online.

Part No.	Description
941010	NIST 17 Library & Search Program, Standard Version
941010UG	NIST 17 Library & Search Program, Standard Version (Upgrade)
941010HP	NIST 17 Library & Search Program, Agilent Format Version
941010HPUG	NIST 17 Library & Search Program, Agilent Format Version (Upgrade)
941010MF	NIST 17 Library & Search Program, Multifformat/Shimadzu Version
941010MFUG	NIST 17 Library & Search Program, Multifformat/Shimadzu Version (Upgrade)
941010GC	NIST 17 Library & Search Program, GC RI Only
941010MSMS	NIST 17 Library & Search Program, MS/MS Only

Upgrade discount available for users of any previous version of NIST MS.



**Scientific Instrument Services, Inc.**<sup>TM</sup>

1027 Old York Rd. Ringoes, NJ 08551-1039

Phone: (908)788-5550

[www.sisweb.com](http://www.sisweb.com)

[us@sisweb.com](mailto:us@sisweb.com)