

NIST 14

Mass Spectral Library & Search Software - Version 2014

Identify your mass spectra with the NIST 14 Mass Spectral Library and Search Software. NIST 14, the successor to NIST 11, is a collection of electron ionization (EI) mass spectra, tandem MS/MS spectra, GC data, and software for searching and identifying your mass spectra. NIST 14 is integrated with most mass spectral data systems, including Agilent ChemStation/MassHunter, Thermo Xcalibur, and others. The NIST Library is known for its high quality, broad coverage, and accessibility. It is a product of a three decade, comprehensive evaluation and expansion of the world's most widely used and trusted mass spectral reference library compiled by a team of experienced mass spectrometrists in which each spectrum was examined for correctness.

Components

Electron Ionization (EI) Mass Spectral Library:

- 276,248 carefully evaluated 70 eV spectra of 242,466 unique compounds common in GC/MS, with identifications and chemical structures.

MS/MS Tandem Spectral Library:

- 234,284 tandem spectra: 51,216 ion trap spectra (42,126 ions / 8,171 compounds) and 183,068 qTOF, HCD and tandem quad collision cell spectra (14,835 ions / 7,692 compounds).

Gas Chromatography (GC) Data Library:

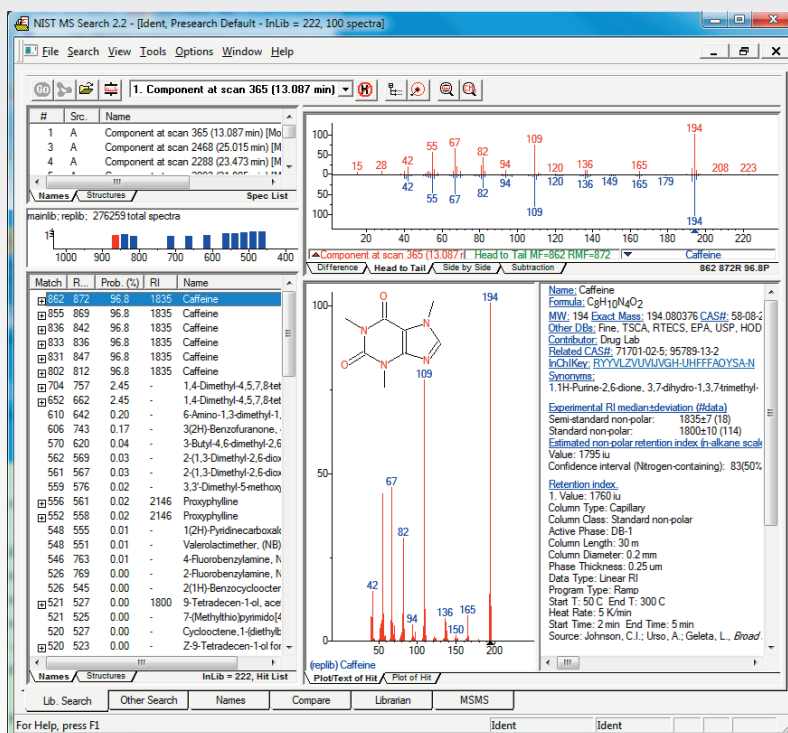
- 387,463 citations of retention indices (Kovats or Lee) and GC methods for 82,868 compounds with structures (56,216 in the EI library) covering both polar and non-polar columns.

Improvements from 2011

- Increased coverage in all libraries (EI MS, MS/MS, and GC RI)
- 32,355 more EI spectra
- 138,875 more MS/MS spectra
- 37,706 more GC RI citations
- Retention index usable in match scoring
- Metadata improvements, including InChIKey, derivatives, and user libraries
- Upgrade discount for any previous version
- Lowest Agilent format price available

NIST Mass Spectral Software:

- NIST MS Search Program v2.2:**
Searching and browsing of the database
- AMDIS Program:**
Extracts noise-free component spectra from GC/MS data files
- MS Interpreter Program:**
Assists in mass spectra analysis and interpretation



The GC and MS/MS databases are included in the full library or can be purchased separately.



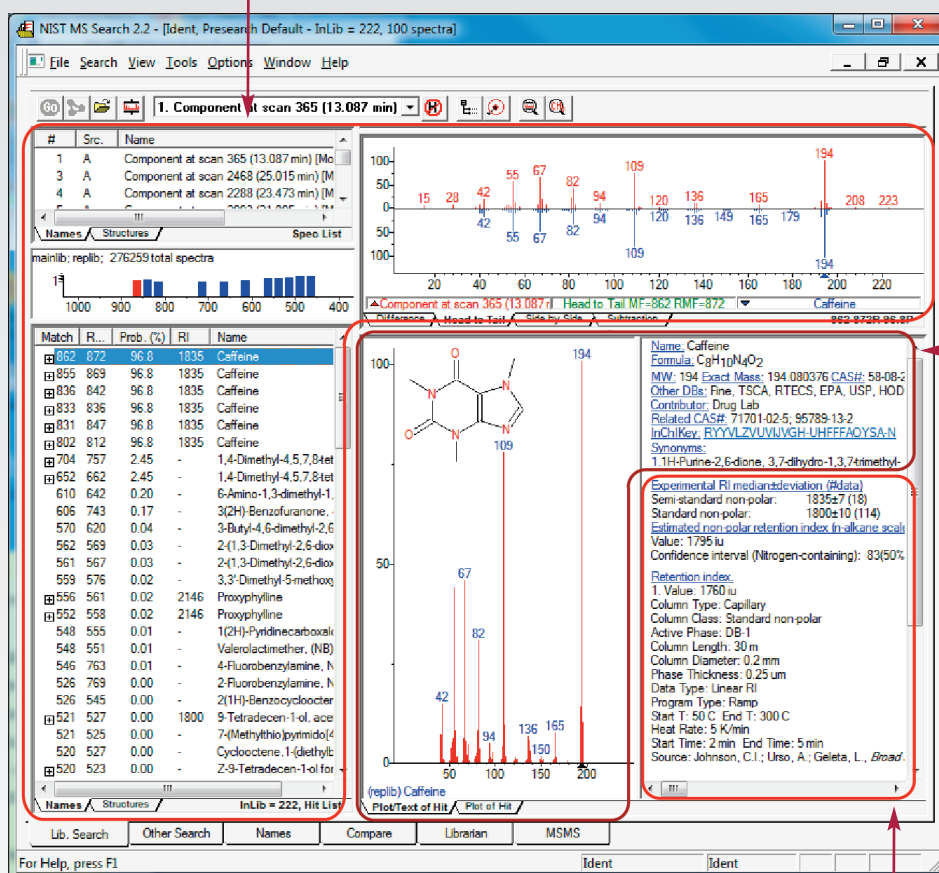
Scientific Instrument Services, Inc.™

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.

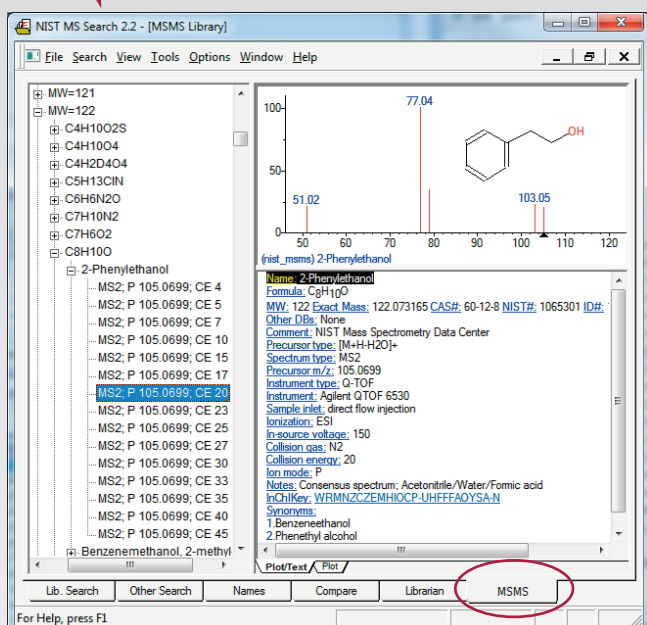
Given a user provided (unknown) spectrum, library search for the best matching spectra in the NIST and user libraries. Matches are ranked. Searches may add a variety of constraints (name, elements present, structural similarity, etc.). Searching is also possible from most mass spectral data systems,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



The **Electron Ionization (EI)** mass spectral library consists of 276,248 spectra of 242,466 unique compounds, each with name, formula, molecular structure (mol), molecular weight, CAS# /InChIKey, contributor name, list of peaks, and synonyms.

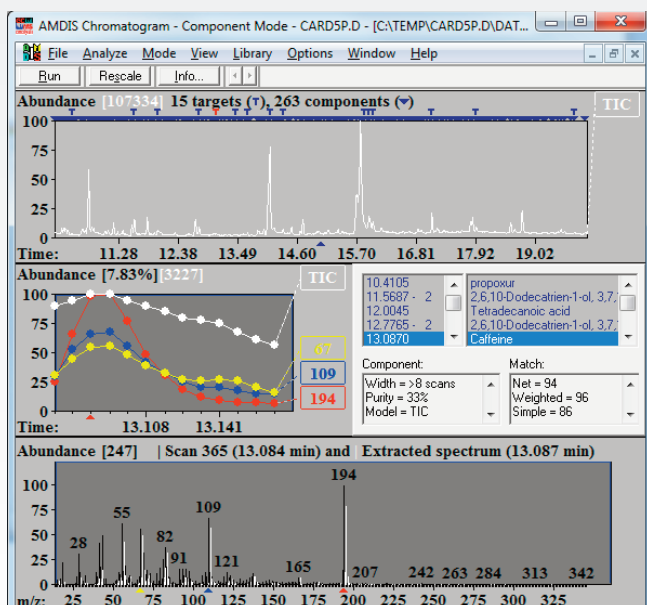
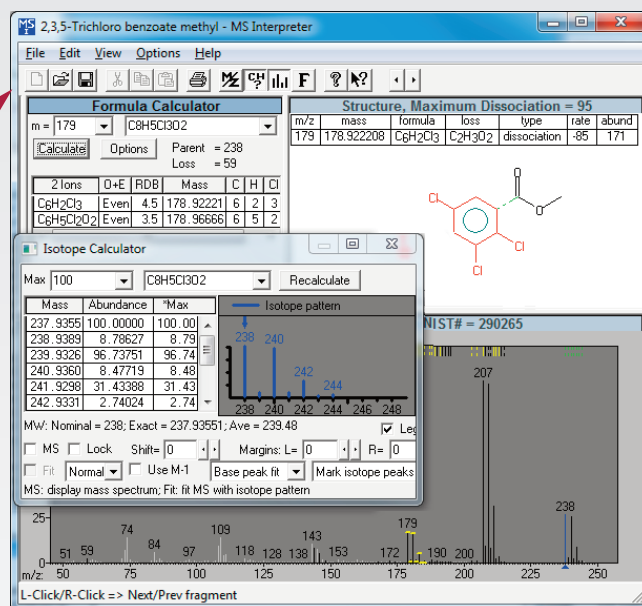
The **GC library** contains 387,463 citations of retention indices (Kovats or Lee) RI and GC methods for 82,868 compounds (56,216 in the EI library) with structures, covering both polar and non-polar columns. When available, this data is displayed with the spectrum search results. RI values can now be displayed in the hit list and used for scoring.

The **MS/MS library** contains 234,284 spectra: 51,216 ion trap spectra (of 42,126 ions/8,171 compounds) and 183,068 qTOF, HCD, and tandem QQQ collision cell spectra (of 14,835 ions/7,692 compounds), 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	ion trap	48,238	39,148	7,254
	collision cell	144,881	12,133	6,793
	- QTOF	42,588	4,379	2,783
	- QQQ	33,325	3,236	2,333
commercial peptides	ion trap	2,978	2,978	917
	collision cell	38,187	2,702	899
total		234,284	45,298	9,344

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 or confidence. Identification can be aided by internal standards and retention times.

New in NIST 14

All libraries have all undergone substantial enhancements in the 2014 release.

Version	#EI Spectra	#MS/MS Spectra	#GC RI Citations	Search Software
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

EI MS Library: Spectra for nearly 30,000 new compounds have been added since the 2011 version, with special effort devoted to metabolites (plant and human), drugs and compounds of industrial and environmental importance. Thousands of improvements in chemical names, structures and replicate spectra have also been made, with special attention to improving naming for derivatives.

MS/MS Library: The number of compounds from the 2012 version has increased by 30% to 9,344 (a 60% increase from 2011 version). With an increased focus on adding all possible precursor ions, this had led to an increase in the number of precursor ions by a factor of three relative to the 2012 version with a near doubling of the total number of spectra to 232K. All new spectra were acquired at high accuracy and resolving power, over a range of energies, and in both collision cells (beam type) and ion traps (up to MS3) in both positive- and negative-ion mode, when appropriate. A large proportion of these new compounds are metabolites, both from plants and humans. This includes significant numbers of glycans. Advanced noise removal processes have improved the quality of a number of spectra added to earlier versions.

GC RI Library: GC data method and retention index are provided for over 82,000 compounds, an increase of over 12,000 compounds from the 2011 version.

Updated Software A number of major new features have been added to the search software. The most significant are

EI MS Library

- Use of retention index (RI) values for a column type in the hit list and for scoring when the submitted spectrum has a known RI.
- Derivative structures optionally can be displayed as the precursor compound with the derivative name (TMS, for example).

MS/MS Library

- Precursor ion, instrument and energy shown in the hit lists and mass spectrum plots.
- Improved search scoring for spectra with few peaks.

All Libraries

- The InChI chemical identifier added to each compound and linked to PubChem (NIH).
- Significant enhancements to the spectrum editor and the spectrum-import function to improve the development of user libraries.

Additional Information: <http://www.sisweb.com/nist>

Part No.	Description
841010	NIST 14 Library & Search Program, Standard Version
841010UG	NIST 14 Library & Search Program, Standard Version (Upgrade)
841010HP	NIST 14 Library & Search Program, Agilent Format Version
841010HPUG	NIST 14 Library & Search Program, Agilent Format Version (Upgrade)
841010MF	NIST 14 Library & Search Program, Multiformat/Shimadzu Version
841010MFUG	NIST 14 Library & Search Program, Multiformat/Shimadzu Version (Upgrade)
841010GC	NIST 14 Library & Search Program, GC RI Only
841010MSMS	NIST 14 Library & Search Program, MS/MS Only

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



Scientific Instrument Services, Inc.

1027 Old York Rd. Ringoes, NJ 08551-1039

Phone: (908)788-5550 www.sisweb.com/nist Fax: (908) 806-6631