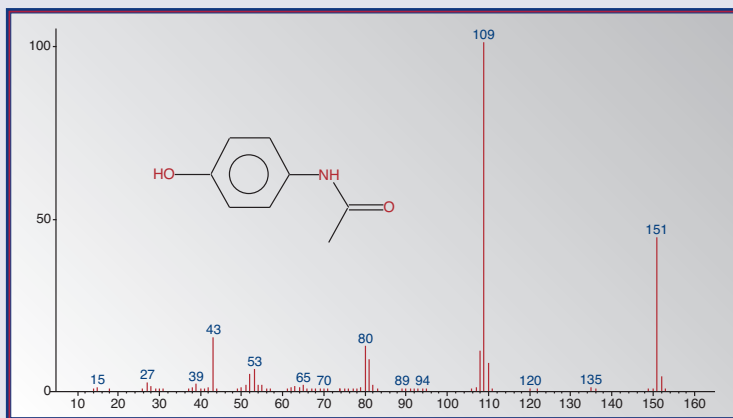


NIST '08

NIST/EPA/NIH Mass Spectral Library - Version 2008

A Major NEW Release of the world's most widely used, fully evaluated, and trusted mass spectral reference library.

NIST '08 is a collection of electron ionization (EI) mass spectra. It also includes MS/MS spectra, GC data, and software for mass spectral analysis.



NIST '08 Components

NIST Data Libraries

Electron Ionization (EI) Mass Spectral Library:

220,460 spectra of 192,108 compounds, with identification and chemical structures (**new salts database included**).

Gas Chromatography (GC) Data Library:

224,038 retention indices of 44,008 compounds (21,847 in the EI library), with corresponding **GC column conditions and literature citations** on both non-polar and polar columns.

MS/MS Spectral Library:

14,802 spectra of 5,308 precursor ions (3,898 positive ions and 1,410 negative ions).

NIST Mass Spectral Software:

NIST MS Search Program

Searching and Browsing of the database, which now includes the display of compound derivatives in the database with replicated spectra.

MS Interpretation Program

Assists in mass spectra analysis and interpretation. Includes ability to predict fragmentation based on structure input.

AMDIS

Extracts noise-free component spectra from GC/MS data of mixtures by deconvolution.



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NIST Data Libraries

Summary:

The NIST '08 Mass Spectral Database, the successor to the NIST '05, is a collection of electron ionization (EI) mass spectra. It also contains MS/MS spectra, GC data, and software for mass spectral analysis. The NIST Database is known for its high quality. It is the product of a two decade, comprehensive evaluation and expansion of the world's most widely used mass spectral reference library by a team of experienced mass spectrometrists in which each spectrum was examined for correctness.

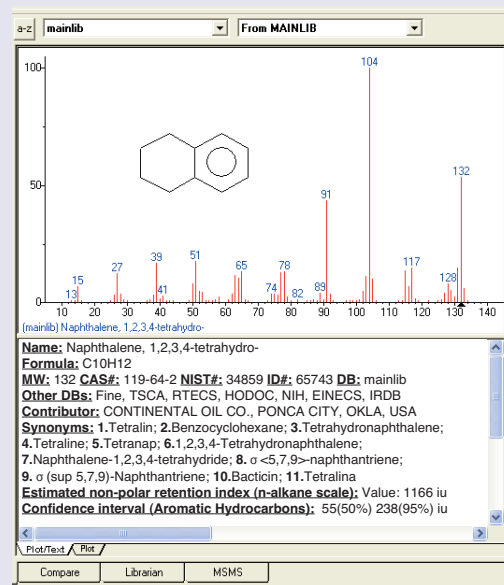
These data libraries are included:

1. Electron Ionization (EI) Mass Spectral Library:

220,460 spectra of 192,108 compounds, with name, list of synonyms, CAS registry number, molecular formula/weight, chemical structure, contributor name, list of peaks, and estimated GC retention index. The size **increased 15% over NIST '05**, with continued improvement in library quality. Thousands of spectra of common derivatives and contaminants have been reexamined. It now also includes a separable library of 717 spectra of 672 low-volatile salts (nist-salts). Libraries are provided in NIST format, usable with the NIST search software and certain data systems. Other formats, including Agilent ChemStation .L are also available.

1. Value: 1153.9 iu; Column Type: Capillary; Column Class: Standard non-polar; Active Phase: Petrocol DH; Column Length: 50 m; Carrier Gas: He; Column Diameter: 0.25 mm; Phase Thickness: 0.5 um; Data Type: Linear RI; Program Type: Ramp; Start T: 35 C; End T: 200 C; Heat Rate: 3 K/min; Start Time: 10 min; End Time: 10 min; Source: Censullo, A.C.; Jones, D.R.; Wills, M.T., Speciation of the volatile organic compounds (VOCs) in solventborne aerosol coatings by solid phase microextraction-gas chromatography, J. Coat. Technol., 75(936), 2003, 47-53

GC Library Example Data



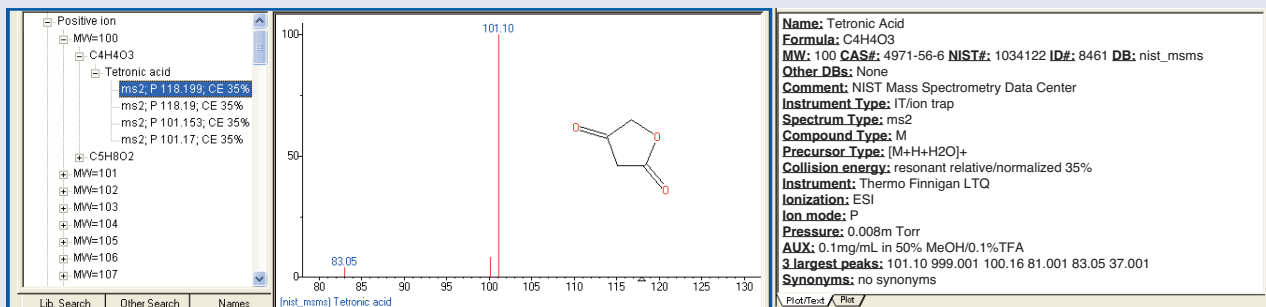
EI Library Example Spectrum

2. Gas Chromatography (GC) Data Library:

224,038 retention indices, with corresponding **GC column conditions and literature citations**, on both non-polar and polar columns, **for 44,008 compounds (21,847 in the EI library)**. The size increased 50% over NIST '05, and it now includes polar columns.

3. MS/MS Spectral Library:

14,802 spectra of 5,308 precursor ions (3,898 positive ions and 1,410 negative ions). The size increased 250% over NIST '05, with contaminants and metabolites forming a large fraction of the new spectra. Spectra were primarily measured on ion-trap and collision cell instruments using electrospray ionization, though other methods are represented.

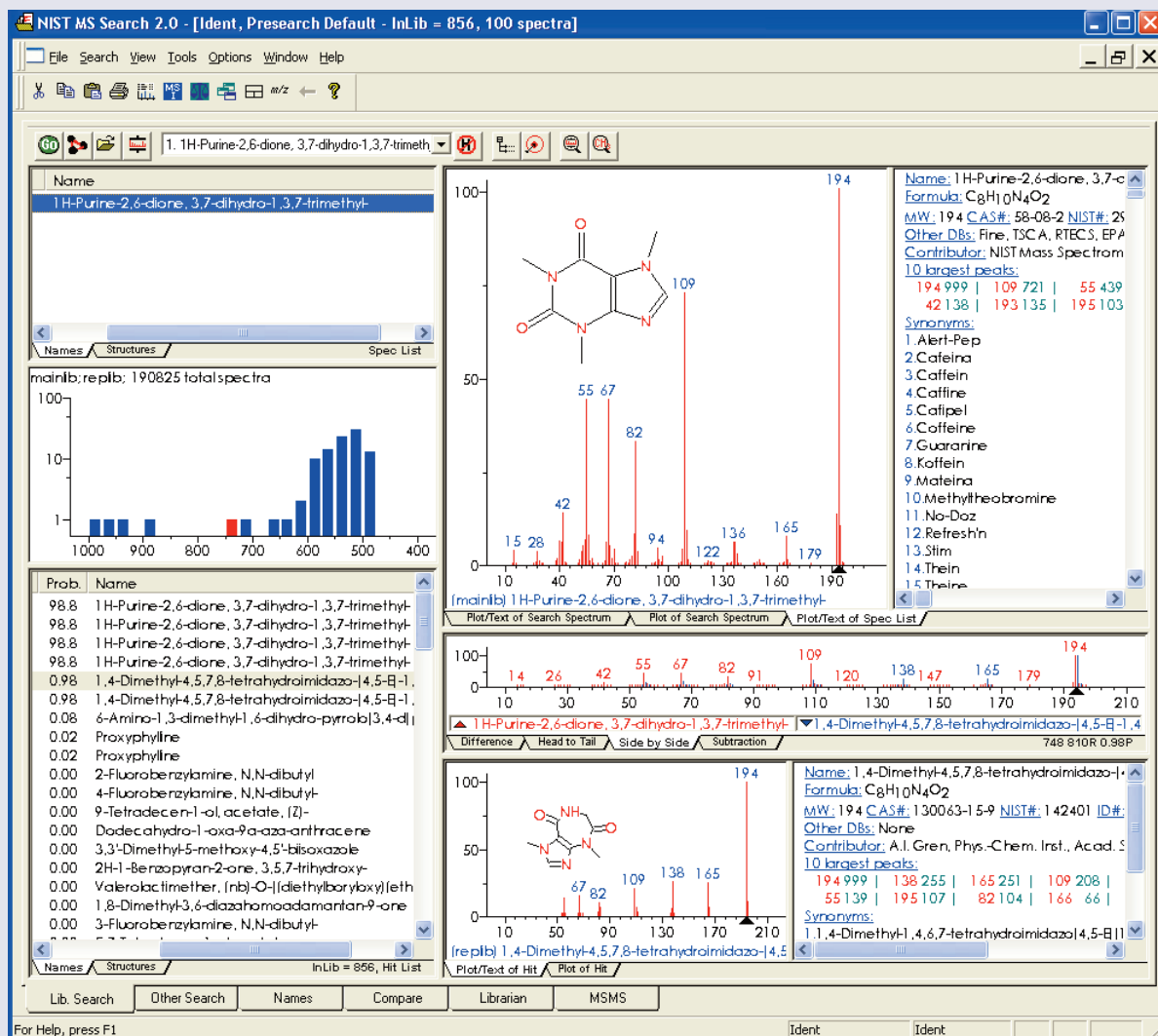


MS/MS Library Example Data

A more detailed list of changes is available at <http://www.sisweb.com/nist#whatsnew>

NIST MS Search Program

The NIST '08 Database can be browsed and searched using the included NIST MS Search software (below).



NIST MS Search Software showing comparison of caffeine spectra (top) with list of Database matches sorted by probability (lower left). Spectra can be compared side-by-side (center), and data on spectra compounds can be examined (upper and lower right).

Features:

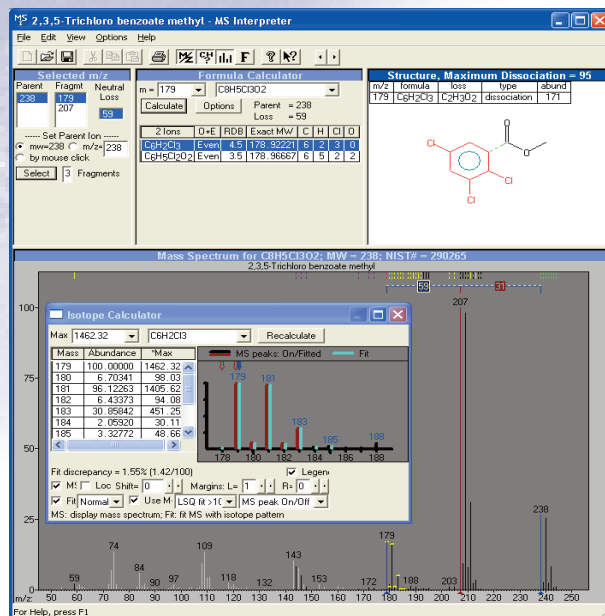
- **Browsing:** Browse all spectra in the NIST Database or user created databases. Data include MS peaks, structures, formulas, CAS registry number, synonyms, estimated and measured GC retention indices, and GC column data.
- **Spectral searching:** Given user provided (unknown) spectra, search for the best matching spectra in the NIST or user libraries. Searches may add a variety of constraints (name, elements present, common compound, etc.). Searching is also possible from various mass spectral data systems from Agilent, Thermo Finnigan, Varian, and others.
- **Structure searching:** Find all chemical structures similar to the structure of the search spectrum, using the structural data from the NIST MS database or from user structures drawn in most chemical drawing packages.
- **Datasystem interfaces:** Directly transfer data between a number of commercial data systems.
- **Compare views:** Visually compare two spectra in a variety of ways.
- **MS/MS browsing window and MS/MS library:** The MS/MS identity search is a new type of search for searching for MS/MS spectra in MS/MS libraries.

NIST Mass Spectrum Interpreter

NIST '08 also includes a Mass Spectrum Interpreter utility to assist the evaluation of mass spectra. You can examine neutral losses, isotope patterns and possible chemical formulas, along with computer-assisted chemical structure/spectra analysis.

Features:

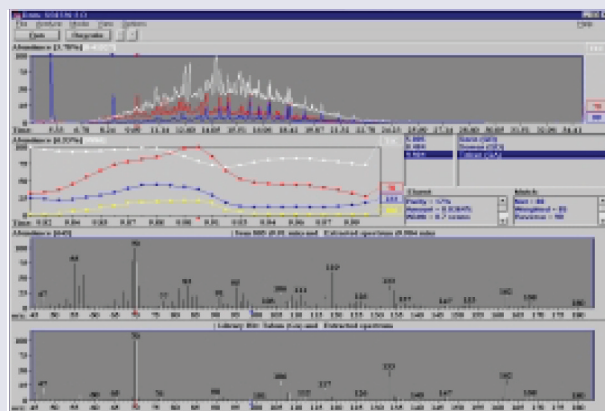
- **Spectrum-structure consistency:** After importing a structure and a mass spectrum, each peak is marked as either consistent or inconsistent with fragmentation rules, and molecular formulas of consistent peaks are highlighted.
- **Neutral loss analysis:** Examine fragmentation stating from the molecular ion or any secondary ion.
- **Isotopic cluster analysis:** Calculate theoretical isotopic profiles and compare with spectra.
- **Chemical formula for each peak:** Rapidly find possible elemental formulas for any peak or neutral loss in a spectrum.
- **Interfaced to the NIST MS Search software.**



Automated MS Deconvolution and Identification System (AMDIS)

NIST '08 also bundles the AMDIS utility, which extracts the spectrum of each component in a mixture analyzed by GC/MS or LC/MS and identifies target compounds.

- **GC/MS deconvolution:** Preprocesses GC/MS or LC/MS data, 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.
- **Interfaced to the NIST MS Search software.**



Part No.	Description	Price
641010	NIST 08 Library & Search Program, Standard Version	
641010UG	NIST 08 Library & Search Program, Standard Version (Upgrade)	
641010HP	NIST 08 Library & Search Program, Agilent ChemStation Version	
641010HPUG	NIST 08 Library & Search Program, Agilent ChemStation Version (Upgrade)	

For Additional Information Please Visit Our Web Site At <http://www.sisweb.com/nist>



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