

# A92 NIST MS Library and Software

## NIST 05 - NIST/EPA/NIH Mass Spectral Library

*A new major release of the NIST/EPA/NIH Mass Spectral Library*

*Available with the enhanced, full featured NIST MS Search Program for Windows, with integrated tools for GC/MS Deconvolution, MS Interpretation, and Chemical Substructure Identification*

### Library of EI Spectra

- 10% increase in coverage and quality improvements over NIST 02 (45% increase over NIST 98)
- 190,825 fully evaluated spectra of 163,198 compounds with structures
- 27,627 Replicate Spectra
- Approximately 100 peaks/spectrum

**NEW!**

### Library of Retention Index Values

121,112 Kovats Retention Index values for 25,893 compounds on nonpolar columns

**NEW!**

### Library of MS/MS Spectra

5,191 spectra of 1,943 different ions (1,671 positive and 341 negative ions)

### Data Sources Include:

- Chemical Concepts - including Prof. Henneberg's industrial chemicals collection
- Georgia and Virginia Crime Laboratories
- TNO Flavors and Fragrances
- AAFS Toxicology Section, Drug Library
- Association of Official Racing Chemists St. Louis University Urinary Acids
- VERIFIN & CBDCOM Chemical Weapons

**N**IST 05 is a fully evaluated collection of electron ionization (EI) mass spectra. 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 experience mass spectrometrists in which each spectrum was examined for correctness. This has led to thousands of selections, deletions and modifications to produce an optimal reference library of compound identification by spectrum matching and library searching. All decisions required agreement by two evaluators, as described in presentations at major conferences.

The NIST/EPA/NIH Main Library now contains spectra of more than 163,000 compounds along with associated chemical identification data including chemical structures, synonyms, and other of relevant information. The best quality spectra are placed in the Main Library; and good-quality, alternate spectra are provided in the Selected Replicates Library, bringing the total number of spectra to over 190,825. Each spectrum has been carefully evaluated, and all decisions regarding selection or deletion were made only after agreement of two experienced mass spectral evaluators. While computer methods assisted in finding chemical identification errors and inconsistencies, and revealed certain varieties of mass spectral errors, manual interpretation was the principal basis for this evaluation effort. All erroneous spectra from pre-

vious versions were removed or replaced. Efforts were also made to remove duplication of the same or edited forms of a single spectrum and to limit the replicate library to spectra showing a meaningful degree of variability. This release represents an increase in both quality and coverage in the 30-year history of the NIST/EPA/NIH Mass Spectral Database—the world's most widely used reference MS database—and the library has been fully evaluated. The objective of this effort was to provide the best possible reference library for compound identification by mass spectral library searching.

## NIST 05 Software

**T**he new full-featured NIST MS Search Program for Windows has a full range of integrated tools. The new updated version of this widely used, full-featured software is designed for identifying compounds from their mass spectra and for exploring mass spectral libraries. It contains new tools for deconvoluting gas/liquid chromatograms and interpreting mass spectra.

- Library Searching via Multiple Search Modes
- Chemical Identity
- Structure Similarity
- Impurity Reduction
- Neutral Loss
- Four Peak Types
- Library Building
- GC/MS Deconvolution
- MS Interpretation
- Chemical Substructure Analysis
- Chemical Substructure Identification
- Molecular Weight Estimation
- Chlorine/Bromine Analysis
- Isotope/Formula Generator
- Integration with multiple Instrument Data Systems

*This software provides a flexible means of accessing data in the NIST and User libraries including:*

- Chemical identification by optimized, documented spectrum-matching methods.
- Analyzing mass spectra of compounds not in the library using library data.
- Finding spectra with pre-selected characteristics.
- Viewing spectra by name, formula, CAS registry number, molecular weight, or ID number.
- User library building and maintenance and integration with a number of commercial GC/MS data systems and spectral analysis tools.

**Library Searching** - Identify unknown compounds and substructures using fully documented and optimized procedures, or search by a wide range of compound and spectral properties.

**Library Building** - Maintain your own libraries, add your own chemical structures and search using the same optimized procedures developed for NIST 98/02.

**Flexible User Interface** - Set multiple Desktop configurations with up to seven independently configured windows to examine search results and match your needs.

**Use with Your Instrument Data Systems** - Direct transfer between a number of commercial data systems (including Agilent, Thermo, Varian, Waters, and Shimadzu) and the NIST Search Program.

**A special Agilent Chemstation (.L) version of the database** is available with full Chemstation PBM search integration.