



## NIST 2017 Mass Spectral Reference Libraries

NIST

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The NIST 17 mass spectral database, the successor to the NIST 14, is a set of fully evaluated collections of electron impact (EI) mass spectra, tandem MS (MS/MS) mass spectra and retention index (RI) data. It is the product of a thirty year, comprehensive evaluation and expansion of the world's most widely used mass spectral reference libraries by experienced mass spectrometrists in which each spectrum was examined for correctness.

### **NIST/EPA/NIH Mass Spectral Library of Electron Ionization Spectra**

This release contains 306,622 electron ionization (EI) spectra of 267,376 different chemical compounds - an increase of over 30,000 spectra and nearly 25,000 compounds from the previous release (NIST 14). For this release, special effort has been made to add spectra for human and plant metabolites as well as for illicit 'designer drugs', leading to the addition of 1000s of spectra. The evaluation of this library has employed newly-developed search methods, some of which are implemented in the accompanying software and described below.

### **NIST Tandem MS Library**

This library consists of two sub-libraries:

- Small molecules: Includes 574,826 spectra of 118,082 precursor ions for 13,808 different compounds – a 2/3 increase in numbers of compounds over NIST 14! Spectra of all identifiable precursor ions are included, including fragments, adducts, and isotopic chlorine and bromine peaks. We continue to include spectra for both positive and negative charge states, with fragmentation in both ion trap (at multiple msn levels) and in beam-type collision cells (over a range of energies).
- Biologically relevant peptides: Includes 77,649 spectra of 1,435 biologically relevant peptides. Also included are 12,595 spectra of 469 dipeptides also in small molecules library.

### **NIST Gas Chromatography Retention Index and GC Methods Library**

This contains 404,045 retention indices for 99,400 compounds, including 72,361 of which are in the EI library. This is an increase of 16,582 RI values.

### **NIST Search Software**

The capabilities of the NIST MSSearch user-interface software were greatly enhanced. It features a new, powerful search method, the 'Hybrid Search', which can find many more matching spectra in both the EI and tandem libraries. Another new search method enables the quick comparison of all spectra of a single compound, in both EI and tandem libraries. Multiple enhancements were made for handling high mass accuracy spectra, including a new version of the Mass Spectrum Interpreter, and improved filtering of the multitude of ions and instruments encountered in high mass accuracy ESI ionization.

### **NIST 17 is available as full version and also as upgrade for owners of a previous edition:**

NIST17	NIST 2017 Mass Spectral Libraries, Single User
NIST17U	NIST 2017 Mass Spectral Libraries, Single User, Upgrade

These items include the library in NIST format. Please note that the library is also available in various other formats, e.g. MassLib, ChemStation, etc. Please contact us for a quote.