



Presenting the New NIST Mass Spectral Libraries for 2017

NIST/EPA/NIH Mass Spectral Library

An electron ionization library

- 306,622 spectra
- 267,376 compounds

Library growth concentrated in

- Human metabolites
- Plant metabolites
- Legal & illicit drugs

NIST LC-MS Tandem Mass Spectral Libraries

**An electrospray ionization library for small
molecules**

- 13,808 compounds
- 118,082 precursor ions
- 574,826 spectra
- Spectra of all identifiable precursor ions are included
- Spectra for both positive and negative charge states
- Fragmentation in both ion trap (at multiple MS_n levels) and in beam-type collision cells (over a range of energies)

**An electrospray ionization library for
biologically relevant peptides**

- 80,328 spectra
- 1488 peptides

NEW LIBRARIES

NIST

**National Institute of
Standards and Technology**
U.S. Department of Commerce

Gas Chromatography Retention Index and Methods Library

- 404,045 RI values
- 99,400 compounds

Software

MS Search v. 2.3

- Main library search program
- Features the new hybrid search (EI & Tandem)
- New search by chemical structure (InChI Key)

AMDIS

- GC-MS deconvolution program

MS Interpreter

- A thermochemical fragmentation predictor
- Now processes high mass accuracy spectra

Order Today from our Distributors

Distributors List

www.nist.gov/srd/nistepanih-mass-spectral-library-distributors

Email

massspec@nist.gov

Web

chemdata.nist.gov

NIST

National Institute of
Standards and Technology
U.S. Department of Commerce

