

NIST/ EPA / NIH MS / MS Mass Spectral Library 2017



Introduction

Newly expanded for its 2017 release, NIST MS/MS Spectral Library contains more than twice the spectra of the 2014 release at 652,475 and more than two times the number of ions at 123,881. The MS/MS library was expanded to now cover small molecules, di and tri peptides, metabolites, designer drugs, surfactants, and commercially available peptides. Of the included 123,881 ions there are 1,436 biologically-relevant peptides.

The NIST 2017 MS/MS library provides a variety of new methods for identifying target compounds or compound classes. Featured spectra have been provided by contributors, measured at NIST, and extracted from the literature.

Specifications

- | | | |
|---------------------------------|---------------------------|----------------------------|
| • Collision Cell Counts: | • Ion Trap Counts: | • TOTAL Counts: |
| • Spectra: 475,881 | • Spectra: 176,594 | • Spectra: 652,475 |
| • Compounds: 14,073 | • Compounds: 14,351 | • Unique Compounds: 15,243 |
| • Ions: 39,158 | • Precursor Ions: 120,346 | • Unique Ions: 123,881 |

Key Benefits

- New 2017 MS/MS spectra include metabolites, drugs, peptides (biologically active peptides and all di-peptides and tryptic tri-peptides), surfactants, commercially available peptides, contaminants, sugars, lipids, and more.
- Restrict MS/MS spectra in search results to specific precursor types, charge, instrument, msn, and mass accuracy
- New HiRes MS/MS Hybrid Search type. Uses the logic of normal searching and the logic of neutral loss searching.
- Types of Any Peak search: HiRes peak and HiRes loss

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Compound Coverage

Compound coverage for individual compounds can be verified at www.compoundsearch.com

Measurement Specifications

- **Precursor Types:**
- [M+H]⁺
- [M+2H]²⁺
- [M-H]⁻
- [M+Na]⁺
- [M+NH₄]⁺
- [Cat]⁺
- [An]⁻
- [p-H₂O]
- [p-NH₃] and more

Compatibility

Compatible with most current and legacy mass spectrometry data systems, including:

- NIST Software (MS Search 2.2)
- Thermo XCalibur
- Bruker
- Waters MassLynx
- PerkinElmer TurboMass
- LECO
- JEOL
- Agilent (ChemStation, MassHunter)
- Shimadzu GC-MS Solution

Ordering Information

NIST / EPA / NIH MS / MS Mass Spectral Library 2017

ISBN: 978-1-119-37673-6

To order:

Call **1.800.245.6217**

or email dbinquiry@wiley.com

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