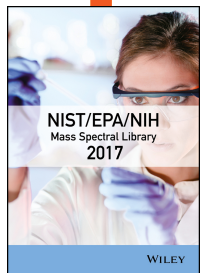


NIST / EPA / NIH Mass Spectral Library 2017



Introduction

Thoroughly updated and more comprehensive than ever, the 2017 release of NIST/EPA/NIH Mass Spectral Library is the one of the most trusted, versatile mass spectral data collections ever published. It is made up of three libraries, an Electron Ionization (EI) mass spectral library, a MS/MS library, and a GC Retention Index library. This new edition contains 306,622 EI spectra for over 262,150 compounds, 652,475 MS/MS spectra for over 15,243 compounds, and 404,045 retention index values for over 99,400 compounds. The library showcases an expansion of the main EI library, the MS/MS library, as well as significant improvements in the underlying MS Search software (2.3g).

New spectra cover a wide range of compound types, with special emphasis afforded to human and plant metabolites, drugs, peptides, and compounds of industrial and environmental importance. Data fields accompanying most spectra are chemical name, formula, chemical structure, molecular weight, CAS number, contributor name, list of peaks, synonyms, and estimated and/or measured retention index.

Wiley's NIST 2017 is the most comprehensive available, compatible with all of the leading manufacturer formats. This helps ensure transportability when switching instruments or manufacturers, and takes the guesswork out of ordering for mixed-instrument deployments.

Compound Classification

- Drugs, metabolites
- Poisons, pesticides, fungicides
- Organics present in soil, water and air
- Amino acids
- Di and tri peptides
- Sample contaminants and more

Specifications

	EI Library Counts	MS/MS Library Counts	GC Retention Library Counts
Spectra	306,622	652,475	---
Compounds	267,376	15,243	99,400
Retention Index Values	---	---	404,045

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Compound Coverage

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

What's New

- Increased coverage and quality in all libraries (EI MS, MS/MS, and GC RI). Nearly 3x increase in MS/MS.
- New and improved search algorithms for NIST MS Search 2.3 (e.g. hybrid search)
- Presearch for EI Similarity/Neutral Loss search. Eliminates restrictions on the maximum loss considered
- Added 'InChIKey' presearch for all library spectrum searches. Finds all spectra which have the same first InChIKey segment as the search spectrum, and compares them to the search spectrum.

Compatibility

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

- NIST MS Search (GC, MS/MS)
- Thermo Xcalibur
- Shimadzu GCMS Solution
- Agilent (Chemstation, MassHunter)
- PerkinElmer TurboMass
- Waters MassLynx
- ACD/Labs MS Manager

Ordering Information

NIST / EPA / NIH Mass Spectral Library 2017

ISBN: 978-1-119-37674-3

NIST / EPA / NIH Mass Spectral Library 2017, Upgrade

ISBN: 978-1-119-37675-0

To order: Call 1.800.245.6217 or email dbinquiry@wiley.com

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