## WILEY

# NIST/EPA/NIH Mass Spectral Library 2023

From the Leader in Spectral Data

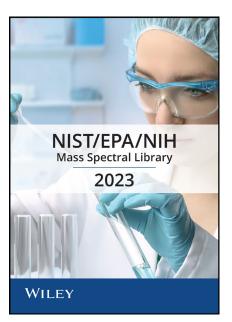


# Maximize analysis workflow with expanded coverage in latest release of this essential resource

One of the most trusted mass spectral libraries has once more been extensively updated. The *NIST/ EPA/NIH Mass Spectral Library 2023*, developed by the experienced mass spectrometry team at the National Institute of Standards and Technology (NIST), represents the culmination of more than four decades of comprehensive evaluation and expansion, making it an essential resource for those analyzing mass spectra.



- Electron Ionization (EI) MS library (in native manufacturer formats)
- 4 MS/MS libraries
- GC Retention Index (RI) library
- NIST 2023 Software: MS Search, AMDIS, MS Interpreter



### Take the guesswork out of compatibility.

Wiley supports more instrument software than any other NIST 2023 distribution.



#### LIBRARY SPECIFICATIONS

#### **Electron Ionization (EI) Library**

Spectra: 394,000

Chemical Structures: 347,100

• Unique Compounds: 341,600

Al-RI Values for All El Compounds

#### **MS/MS Libraries**

• Spectra: 2.3M+

Chemical Structures: 1.4M+Unique Compounds: 51,500

Precursor lons: 399,200

#### GC Retention Index (RI) Library

RI Values: 491,700

• Unique Compounds: 180,600

153,400 compounds from the GC-RI Library are also in the NIST EI Library.



#### WHAT'S NEW IN THIS RELEASE

Be sure your lab is up to date with the latest release of this evolving collection. Take advantage of all the benefits in the 2023 release:

- The El Library has added over 40,000 unique compounds with more than 43,000 spectra, in addition to Al-Rl values for all El data.
- The MS/MS Library has added 60% more compounds than the 2020 release, now covering over 51,000 compounds and over 399,000 precursor ions.
- The GC RI Library added over 40,000 compounds.



#### **APPLICATIONS**

This collection offers exception reliability as a comprehensive resource for the analysis, identification, classification, and verification of compounds by mass spectrometry in a wide range of applications such as **environmental**, **forensics/toxicology**, **metabolomics**, **pharmaceutical**, **biotech**, **food/cosmetics**, and many more.



#### **ADDITIONAL INFORMATION**

When it comes to spectral analysis, the more data you have the better. The NIST spectral database provides much more information than simply the spectrum to give you a fuller picture of your results. Database records may include valuable details when available for a record such as:

- Chemical Structure
- Chemical Name
- Exact Mass
- Formula
- InChl/InChlKey
- Molecular Weight



#### COMPOUND COVERAGE

- Drugs/Pharmaceuticals
   Extractables &
- Industrial Surfactants
- Pesticides/Pollutants
- Metabolites
- Extractables & Leachables
- Peptides
- Glycans-Lipids-Sugars



#### **ABOUT THE NIST STANDARD REFERENCE DATA CENTER**

For over 50 years, NIST has developed and distributed standard reference data in chemistry, engineering, fluids and condensed phases, material sciences, mathematical and computer sciences and physics.



#### ACCELERATE YOUR WORKFLOW WITH THESE OPTIONS

#### Be sure to ask about our NIST bundles!

- More data with the Wiley Registry/NIST 2023 combined library.
  Comprehensive coverage with over 3 million spectra (includes El and MS-MS data)
- More data and powerful analysis tools with KnowltAll™ Wiley MS Identification Pro + NIST bundles.

#### Includes:

- 1. NIST library/NIST software\*
- 2. Annual subscription to:
  - KnowItAll Mass Spectral Library collection with access to Wiley Registry plus additional databases, and access to new data as it's added to the collection
  - KnowItAll's software tools for automated non-targeted GC-MS analysis, MS adaptive search to aid with novel compounds, processing, structure drawing, and more

#### PRODUCT & VERSION COMPARISON CHART

Data Type	WR23 (2023)	WR12 (2020)	WR11 (2017)	WR10 (2014)	NIST23* (El Spectra)	NIST20* (El Spectra)	NIST17* (El Spectra)	NIST14* (El Spectra)	WR23/NIST23* (El Spectra)
Mass Spectra	873,300	817,200	775,800	719,400	394,000	350,000	306,600	276,200	1,180,00
Searchable Structures	841,100	785,000	741,200	684,700	347,100	350,000	306,600	276,200	1,148,600
Unique Compounds	741,000	668,400	632,500	583,700	341,600	306,000	262,100	237,400	950,200

<sup>\*</sup> Note: Table above does not include MS-MS data counts from NIST and WR/NIST libraries. Wiley Registry/NIST EI database counts = Wiley Registry and NIST, minus any overlap.

<sup>\*</sup> Per license to be used on the same computer as KnowltAll license.



#### COMPATIBILITY

Wiley's NIST 2023 works seamlessly with most current and legacy mass spectrometry data systems. For full compatibility information, please visit **sciencesolutions.wiley.com/compatibility** 



#### ORDERING INFORMATION

NIST/EPA /NIH Mass Spectral Library 2023 -

**USB:** 9781394198726

**DOWNLOAD: 978EALDB05727** 

NIST/EPA/NIH Mass Spectral Library 2023 Upgrade

**USB:** 9781394198733

DOWNLOAD: 978EALDB05734

Wiley Registry/NIST Mass Spectral Library 2023 -

**USB:** 9781394197972

DOWNLOAD: 978EALDB05741

• Wiley Registry/NIST Mass Spectral Library 2023 Upgrade -

**USB:** 9781394197989

**DOWNLOAD: 978EALDB05758** 

The NIST database is also available as a bundle with Wiley's KnowltAll Software & Mass Spectral Library. Ask us for details.



#### TRUSTED DATA FROM A TRUSTED SOURCE

Wiley is the authoritative source for spectral data. Our renowned databases are processed according to rigorous protocols to ensure they are of the highest quality. Qualification procedures start at data acquisition and continue throughout the database development process. Any data acquired from trusted partners is thoroughly vetted before inclusion in our collections.

https://sciencesolutions.wiley.com/

Quality Data. Results You Can Rely On.

