

# 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.

#### What's included:

- Electron Ionization (EI) MS library (*in native manufacturer formats*)
- Four NIST Tandem Mass Spectral (MS/MS) libraries
  - Small Molecule Atmospheric Pressure Chemical Ionization (APCI) High Resolution MS/MS Library
  - Small Molecule High Resolution Accurate Mass (HRAM) MS/MS Library
  - Small Molecule High Resolution Accurate Mass MS/MS Library #2
  - Small Molecule Low Resolution MS/MS Library
- 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 distributor.



## LIBRARY SPECIFICATIONS

### Electron Ionization (EI) Library

- Spectra: 394,000
- Chemical Structures: 347,100
- Unique Compounds: 341,600
- AI-RI Values for All EI Compounds

### MS/MS Libraries

- Spectra: 2.3M+
- Chemical Structures: 1.4M+
- Unique Compounds: 51,500
- Precursor Ions: 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 EI Library has added over 40,000 unique compounds with more than 43,000 spectra, in addition to AI-RI values for all EI 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 exceptional 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
- InChI/InChIKey
- Molecular Weight



## COMPOUND COVERAGE

- Drugs/Pharmaceuticals
- 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 EI and MS/MS data)
- **Even more data—plus powerful analysis tools—with KnowItAll MS Identification Pro + NIST bundles**

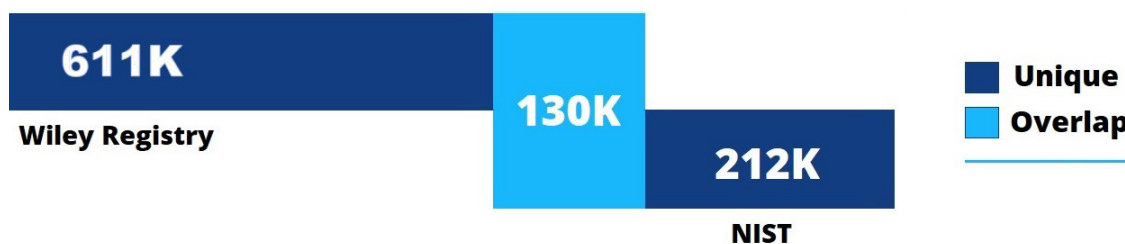
### EI Product Version Comparison Chart

Data Type	WR23 (2023)	WR Subscription	WR12 (2020)	WR11 (2017)	NIST23* (EI Spectra)	NIST20* (EI Spectra)	NIST17* (EI Spectra)	WR23/NIST23* (EI Spectra)
Mass Spectra	873,300	895,700	817,200	775,800	394,000	350,000	306,600	1,180,00
Searchable Structures	841,100	863,500	785,000	741,200	347,100	350,000	306,600	1,148,600
Unique Compounds	741,000	759,100	668,400	632,500	341,600	306,000	262,100	950,200

\* 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.

WR = Wiley Registry

### Unique EI Spectra Comparison - Wiley Registry vs NIST



### MS/MS Product Version Comparison Chart

Data Type	NIST23	NIST20	NIST17
Mass Spectra	2.3M+	1.3M+	652,400
Compounds	51,500	31,000	15,200
Ions	399,200	185,600	123,800



## COMPATIBILITY

- Compatible with most current and legacy mass spectrometry data systems
- Also available in bundles with KnowItAll software, which supports multiple instrument vendor formats

For full compatibility information, please visit

<https://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

*Be sure to ask about our MS Identification Pro Packages for access to even more spectra and tools—plus access to new data as it's added in between releases.*



## 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.