

# WILEY

## Wiley Registry/NIST Mass Spectral Library 2023

From the Leader in Spectral Data



### Comprehensive compound coverage for confident results

*Experience the combined power of two essential libraries for mass spectral analysis*

The **Wiley Registry/NIST Mass Spectral Library 2023** is the most comprehensive combined mass spectral library commercially available, with **over 3 million spectra** (including EI and tandem MS data), making it the clear choice for general unknown compound identification. Broad, up-to-date compound coverage ensures identification across multiple use cases and a wide variety of analytes.

- **Broad range of compounds** for targeted and non-targeted analyses.
- **Spectral records contain additional information** that's searchable such as physical properties, structures, and other fields to help narrow your results even further.
- **Data is carefully curated and reviewed** by Wiley's internal and external experts to ensure it meets quality standards for results you can rely on.
- **Spectra are segmented into separate libraries** including excess replicate spectra to enable robust searching across varied laboratory settings.
- **Take the guesswork out of compatibility.** Available in the most common manufacturer formats to work the way you do.
- **Includes the NIST 2023 Software** (MS Search, AMDIS, MS Interpreter) to keep your lab up to date with the latest tools.



---

**Increase the speed and likelihood of MS identification with expanded coverage in the latest release of this trusted resource.**

---

- **Expansive chemical structure coverage enables focused searching based on cheminformatic features in addition to spectrometry features.**

Replicate spectra and over 4 million chemical names and synonyms can help to provide a higher rate of correct identification and ensure that this library can aid in classical EI, exact mass, and other methods of identification.

A foundational tool for any laboratory engaged in MS analysis, this spectral library remains a lab standard, consistently evolving to meet the ever-growing research demands of today in Wiley's continued commitment to delivering relevant, quality data resources.



## LIBRARY SPECIFICATIONS

Data Type	GC-MS	MS/MS
	Wiley Registry/ NIST 2023*	NIST MS/MS 2023
<b>Spectra</b>	1,180,800	2.3M+
<b>Structures</b>	1,148,600	1.4M+
<b>Unique Compounds</b>	950,200	51,500
<b>Ions</b>	—	399,200

\*Wiley Registry/NIST EI database counts = Wiley Registry and NIST, minus any overlap.



## 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 of this combined powerful database:**

- Addition of over 74,000 unique compounds and over 91,900 spectra
- Now also available as a KnowItAll subscription for continued access to new data added to the Wiley Registry between major releases

### **Wiley Registry of Mass Spectral Data - New Features:**

- Expanded coverage of world patents and peer reviewed literature, including DOIs of source articles
- Spectra have been assigned a quality index where possible, enabling searches to be tuned to exclude spectra below a quality index threshold

### **NIST/EPA/NIH - New Features:**

- AI-RI values have been added 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.



## 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, defense/homeland security**, and many more.

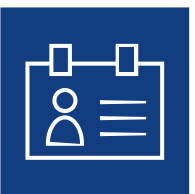


## ADDITIONAL INFORMATION

When it comes to spectral analysis, the more data you have the better. Wiley spectral databases provide 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
- Calculated Kovats RI values
- Splash IDs
- Formula
- InChI/InChIKey
- Molecular Weight
- Experimental RI Values
- AI RI Values

And because it's searchable, you can use this information to narrow your results even further.



## ABOUT THE AUTHORS

### Wiley Registry of Mass Spectral Data

Originating through a collaboration by Drs. Einar August Stenhagen, Fred McLafferty, and Sixten Abrahamsson, the Wiley Registry pioneered the use of spectral data in mass spectrometry.

- Sixten Abrahamsson, a member of the Royal Swedish Academy of Sciences, was an x-ray crystallographer whose group studied structure and function of biologically active molecules.
- Fred McLafferty, a member of the National Academy of Sciences, was a leading light in mass spectrometry, known for top-down analysis and the McLafferty rearrangement.
- Einar Stenhagen, a member of the Royal Swedish Academy of Sciences, invented, with his wife, Stina Stållberg-Stenhagen, the jet separator, enabling the combination of gas and liquid chromatography with mass spectrometry.

Since 2009, the Wiley Registry has been maintained and updated by the Wiley Science Solutions data team.

### NIST/EPA/NIH Mass Spectral Library

The NIST/EPA/NIH Mass Spectral Library 2023, developed by the experienced mass spectrometry team at the National Institute of Standards and Technology (NIST). 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.

The Wiley Registry/NIST combined library is produced by the Wiley Science Solutions data team.



## STAY ON TOP OF THE LATEST DATA WITH OUR NEW SUBSCRIPTION OPTIONS

Be sure to ask us about our KnowItAll MS Identification Pro + NIST bundles.

- **No need to wait until the next release for new Wiley Registry data!** Get access to spectral data as it's added to the Wiley Registry between releases.
- **By adding a subscription to the KnowItAll software, you will also have access to one of the most powerful tools** for automated non-targeted GC-MS analysis (deconvolution + library search), MS Adaptive Search for novel compounds, and more.

### El Product Version Comparison Chart

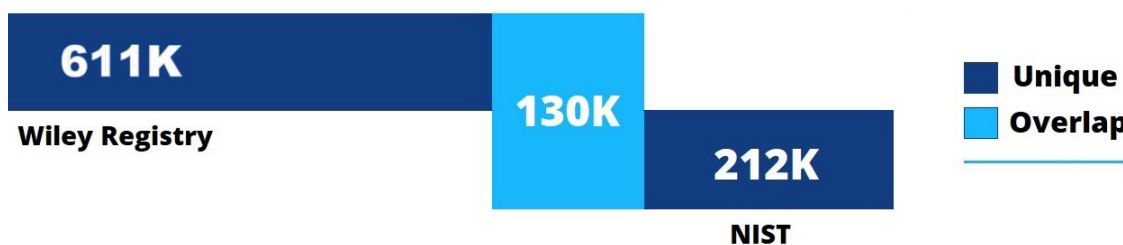
Data Type	WR23 (2023)	WR Subscription	WR12 (2020)	WR11 (2017)	NIST23* (EI Spectra)	NIST20* (EI Spectra)	NIST17* (EI Spectra)	WR23/NIST23* (EI Spectra)
Mass Spectra	873,300	913,300	817,200	775,800	394,000	350,000	306,600	1,180,00
Searchable Structures	841,100	881,100	785,000	741,200	347,100	350,000	306,600	1,148,600
Unique Compounds	741,000	771,400	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.

WR = Wiley Registry

Wiley Registry/NIST EI database counts = Wiley Registry and NIST, minus any overlap.

### Unique EI Spectra Comparison - Wiley Registry 2023 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

### 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.

[\*\*www.sciencesolutions.wiley.com\*\*](https://sciencesolutions.wiley.com)

Quality Data. Results You Can Rely On.