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Wiley Registry of Mass Spectral Data 2023

From the Leader in Spectral Data

The essential GC-MS library for confident spectral analysis

The field-tested and proven *Wiley Registry of Mass Spectral Data* continues to empower laboratories worldwide. The 2023 release of this vital MS database provides access to over **873,000 spectra** with expanded coverage to expedite your workflow even further.

Designed for use across multiple applications, from untargeted GC-MS screening to accurate mass workflows with MS-TOF instruments, this collection ensures confidence in your lab's spectral search results, even in the most demanding applications.

- **Broad range of compounds** for targeted and non-targeted analyses—increase both the speed and likelihood of identification with a comprehensive dataset.
- **Expanded coverage of world patents**, including USA, China, Japan, and Europe to ensure your lab is current.
- **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.



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

A foundational tool for any laboratory engaged in GC-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.

Available in the most common instrumentation manufacturer formats, this spectral library is a necessity for any laboratory engaged in GC-MS analysis.



LIBRARY SPECIFICATIONS

Data Type	Counts	Addition over prior edition
GC-MS Spectra	873,300	+56,000
Searchable Structures	841,100	+56,000
Unique Compounds	741,000	+50,000
Replicate Spectra	201,000	+35,000
Estimated Kovats Retention Indices	738,400	+50,000



WHAT'S NEW IN THIS RELEASE

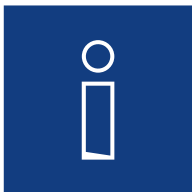
Be sure your lab is up to date with the latest release of this evolving collection. Take advantage of all the benefits in the 2023 release:

- **Addition of over 50,000 unique compounds** with over 56,000 spectra.
- **Expanded coverage of world patents and peer reviewed literature**, including DOIs of source articles. Data is also sourced from partner labs.
- **All spectra have been assigned a quality index**, enabling searches to be tuned to exclude spectra below a quality index threshold.
- **The Wiley Registry is now also available as a KnowItAll subscription** for continued access to new data between major releases.



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
- Wiley ID
- Formula
- InChI/InChIKey
- Molecular Weight
- Quality Index (QI)
- Digital Object Identifier (DOI)

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



ABOUT THE AUTHORS

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 Ställberg-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.



STAY ON TOP OF THE LATEST DATA WITH A WILEY REGISTRY SUBSCRIPTION

The Wiley Registry is also now available as a KnowItAll subscription. Get early access to new data for continual impact on your laboratory workflow.

- **No need to wait until the next release for new data.** Stay on the cutting edge by having continuous access to new data—with a subscription you get access to thousands of spectra added to the Wiley Registry annually.
- **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.
- **Combine spectrum searches with powerful structure searching** to limit searches to specific chemical classes, such as our PFAS class query.
- **Plus, you have options to increase your coverage even further** with packages that include access to even more databases, including our NIST bundles.



ACCELERATE YOUR WORKFLOW WITH THESE OPTIONS

- **More data with the Wiley Registry/NIST 2023 combined library.**
Comprehensive coverage with over 3 million spectra (includes EI & MS-MS data)
- **More data and powerful analysis tools with KnowItAll - 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

* Per license to be used on the same computer as KnowItAll license.

PRODUCT & VERSION COMPARISON CHART

Data Type	WR23 (2023)	WR12 (2020)	WR11 (2017)	WR10 (2014)	NIST23* (EI Spectra)	NIST20* (EI Spectra)	NIST17* (EI Spectra)	NIST14* (EI Spectra)	WR23/NIST23* (EI 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

* 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



COMPATIBILITY

Compatible with most current and legacy mass spectrometry data systems. For full compatibility information please visit sciencesolutions.wiley.com/compatibility



ORDERING INFORMATION

- **Wiley Registry of Mass Spectral Data 2023**
USB: 9781119736325
DOWNLOAD: 978EALDB05697
- **Wiley Registry of Mass Spectral Data 2023 (Upgrade)**
USB: 9781394198740
DOWNLOAD: 978EALDB05703

Also available as a subscription for use with Wiley's KnowItAll Software with access to new data as it is added to the collection:

- **Wiley Registry of Mass Spectral Data (Annual Subscription)**
978EALDB05482
- **Wiley Registry of Mass Spectral Data (Annual Subscription Renewal)**
978EALDB05499



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.