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Wiley Registry of Mass Spectral Data 2026



When a missed identification carries consequences, you need data you can defend.

In every field where identification accuracy has real consequences — from forensics to environmental science, to pharmaceutical R&D, quality control, and beyond, laboratories worldwide rely on the **Wiley Registry of Mass Spectral Data**.

The 2026 release delivers **over 915,500* expertly curated GC-MS spectra**, expanding coverage by more than 42,000 spectra to accelerate your workflow and strengthen every identification.

- **Identify more compounds, more often.** Broad coverage for both targeted and non-targeted analyses.
- **Each record includes** searchable metadata (chemical structure, exact mass, computed retention index) to narrow results beyond the spectrum alone.
- **Data is rigorously reviewed** by Wiley's internal and external experts to meet quality standards for results you can rely on.
- **Spectra are segmented into separate libraries**, including replicate spectra, to ensure robust results regardless of instrument or laboratory settings.
- **Available in all major instrument manufacturer formats.** KnowItAll subscription access adds software integration for automated GC-MS workflows.

A foundational tool for laboratories engaged in GC-MS analysis, the Wiley Registry remains the **lab standard**, consistently evolving to meet the growing research demands of modern analytical science.



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Highlights in this release

- **Expanded compound coverage:** Over 42,000 spectra for over 34,100 unique compounds added to the collection.
- **Authoritative data:** Expanded content derived from labs, world patents, and peer-reviewed literature, including DOIs of source articles.
- **Quality-indexed spectra:** Spectra are assigned a Quality Index (QI) where possible, enabling searches to be tuned to exclude spectra below a quality index threshold.
- **Broader spectra coverage:** With chemical structures assigned to most GC-MS spectra, users can apply structure- and class-based search filters (including Markush-style queries) to target specific chemistries during identification.

Now available as a KnowItAll subscription for continuous access to new spectra as they are added. No waiting for the next release.

Product version & comparison chart:

Data Type	Mass spectra	Searchable structures	Unique compounds
WR/NIST23* (EI spectra)	1,180,000	1,148,600	950,200
WR subscription	915,500	883,300	743,100
WR26 (2026)	915,500	883,300	743,100
WR23 (2023)	873,300	841,100	741,000
WR12 (2020)	817,200	785,000	668,400
WR11 (2017)	775,800	741,200	632,500
NIST23* (EI spectra)	394,000	347,100	341,600
NIST20* (EI spectra)	350,000	350,000	306,000
NIST17* (EI spectra)	306,600	306,600	262,100

*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

Be sure to ask about KnowItAll Wiley MS Identification Pro + NIST bundles for access to even more data, plus powerful analysis tools.



Applications

Used across environmental, forensics/toxicology, metabolomics, pharmaceutical, biotech, food/cosmetics, defense/homeland security applications, and many more.



Library specifications

Data Type	Wiley Registry
GC-MS spectra	915,500
Searchable structures	883,300
Unique compounds	743,100
Computed retention indices	772,600



Additional information

Every Wiley Registry record includes rich, searchable metadata to support more precise identification, including (where available):

- Chemical structure
- Chemical name
- Exact mass
- Computed retention index
- SPLASH IDs
- Wiley ID
- Formula
- InChI/InChIKey
- Molecular weight
- Quality Index (QI)
- Digital Object Identifier (DOI)



Wiley Registry — the history

The Wiley Registry was pioneered by members of the National Academy of Sciences and the Royal Swedish Academy of Sciences, and has been maintained by Wiley's data science team since 2009.

- Dr. Sixten Abrahamsson, a member of the Royal Swedish Academy of Sciences, was an X-ray crystallographer whose group studied the structure and function of biologically active molecules.
- Dr. 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.
- Dr. 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.



Stay current: continuous access with a KnowItAll subscription

The Wiley Registry is available as a KnowItAll subscription, giving you access to new spectra as they're added. No waiting for the next release.

- By subscribing to KnowItAll, you gain access to one of the most powerful tools for automated GC-MS analysis (deconvolution + library search), MS Adaptive Search for novel compounds, and more.



Ordering information

Product Code	Product	Format
978EALDB05482	Wiley Registry of Mass Spectral Data (Annual subscription)	KnowItAll subscription
978EALDB05499	Wiley Registry of Mass Spectral Data (Annual subscription renewal)	KnowItAll subscription
9781394439898	Wiley Registry of Mass Spectral Data 2026	USB
978EALDB07493	Wiley Registry of Mass Spectral Data 2026	Download
9781394439904	Wiley Registry of Mass Spectral Data 2026, Upgrade	USB
978EALDB07509	Wiley Registry of Mass Spectral Data 2026, Upgrade	Download



Compatibility

- Compatible with most common instrumentation manufacturer formats
- Also available as a subscription for use with the KnowItAll software, which supports [multiple instrument vendor formats](#)

For full compatibility information, visit sciencesolutions.wiley.com/compatibility



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.

For more information:

www.sciencesolutions.wiley.com