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Wiley Registry of Mass Spectral Data 2026

The essential GC-MS database. Trusted data, faster answers.

Where accuracy has real consequences, you need data you can trust. The ***Wiley Registry of Mass Spectral Data*** is one of the world's largest and most trusted GC-MS libraries — relied on by laboratories worldwide where fast, accurate results are critical, including environmental science, forensics, pharmaceutical R&D, food safety, defense, QA/QC, and many more.

The 2026 release is the strongest yet with **over 915,500* expertly curated, high-quality GC-MS spectra**, including over 42,000 new spectra — giving analysts the spectral intelligence to move from unknown to identified faster, with greater confidence.

Comprehensive analyses

Broad compound coverage for targeted and non-targeted analyses across a range of applications.

Superior data quality

Data curated and reviewed by experts, with searchable metadata included.

Seamless integration

Supports major MS instruments to fit in your existing workflow.

Not just a database. The GC-MS intelligence your workflow needs.

Foundational | Proven | Trusted by labs worldwide

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Highlights in this release

- **Expanded compound coverage:** This release adds over 42,000 spectra covering more than 34,100 newly included unique compounds.
- **Authoritative data:** Expanded content from labs, world patents, and peer-reviewed literature, including DOIs to source articles.
- **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.

Product version & comparison chart:

Data Type	Mass spectra	Searchable structures	Unique compounds
WR26/NIST 2026 (EI spectra)*	1,259,900	1,227,700	1,016,700
WR23/NIST23* (EI spectra)	1,180,000	1,148,600	950,200
WR subscription	915,500	883,300	775,300
WR26 (2026)	915,500	883,300	775,300
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

Laboratories face increasingly complex analytical challenges—from detecting emerging environmental contaminants to identifying novel substances in forensic investigations. As a result, having access to a comprehensive, rigorously validated spectral database has become foundational to getting results right.

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:

Forensics & Toxicology | Pharmaceuticals & Biotech | Automotive & Aerospace | QA & QC | Environmental | Food & Cosmetics | Metabolomics | Defense & Security | Many others

Library specifications

Data Type	Wiley Registry 2026
GC-MS spectra	915,500
Searchable structures	883,300
Unique compounds	775,300
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.

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** (Digital download)	Download
9781394439904	**Wiley Registry of Mass Spectral Data 2026,** Upgrade	USB
978EALDB07509	**Wiley Registry of Mass Spectral Data 2026, Upgrade** (Digital download)	Download

Need more coverage?

Be sure to ask about our Wiley Registry/NIST and KnowItAll GC-MS Library packages with powerful tools to optimize and automate your workflow.

**Subscription is subject to change as data may be added or deleted from collections periodically.*

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.

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

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