

WILEY REGISTRY[®]
of Mass Spectral Data

2026

WILEY

Wiley Registry of Mass Spectral Data 2026

User Manual

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Contact information

Contact information: <https://sciencesolutions.wiley.com/contact-us/>

Support: <https://support.wiley.com/>

Submitting data

Wiley welcomes contributions of spectra for compounds, especially novel compounds not presently covered in this spectral library. Wiley can handle data in any machine-readable format. Please contact us if you are interested in submitting data: <https://sciencesolutions.wiley.com/contact-us/>

Compliance

Flashbay Inc. certifies that all products are RoHS Compliant and fulfill the requirements defined in EU Directive 2015/863 (RoHS 3) – Restriction of Hazardous Substances in Electrical and Electronic Equipment and do not contain any of the below mentioned 10 hazardous substances above the specified limits.

Substance	MCV
Lead (Pb)	0.1% by weight (1000 ppm)
Mercury (Hg)	0.1% by weight (1000 ppm)
Cadmium (Cd)	0.01% by weight (100 ppm)
Hexavalent Chromium (Cr(VI))	0.1% by weight (1000 ppm)
Polybrominated Biphenyls (PBBs)	0.1% by weight (1000 ppm)
Polybrominated Diphenyl Ethers (PBDEs)	0.1% by weight (1000 ppm)
Bis-(2-ethylhexyl) phthalate (DEHP)	0.1% by weight (1000 ppm)
Benzyl butyl phthalate (BBP)	0.1% by weight (1000 ppm)
Dibutyl phthalate (DBP)	0.1% by weight (1000 ppm)
Diisobutyl phthalate (DIBP)	0.1% by weight (1000 ppm)

License

Unless specified otherwise in writing, this product is sold as a **single computer license**. It can only be installed on **one** machine, not networked. Multiple license and network licenses are available. For additional licenses, please contact your sales representative. Please read the End User License Agreement (EULA) for further details.

Compatibility

Wiley has provided you with a selection of native manufacturer formats to aid you in your installation. Please consult your software manufacturer's documentation and customer support before contacting Wiley Support. This product includes the following manufacturer formats:

- Agilent ChemStation
- Agilent MassHunter
- Agilent PCD
- NIST MS Search*
- PerkinElmer TurboMass
- Shimadzu LabSolutions/GCMSsolution
- Thermo Xcalibur
- Waters MassLynx

*The NIST format is compatible with Agilent, Bruker, JEOL, LECO, PerkinElmer, Thermo, Waters, and most other manufacturer software.

Compatibility information for the latest version can always be found at <https://sciencesolutions.wiley.com/compatibility/>.

Installation

NOTE: If you have purchased this database in KnowItAll format, you will need to install KnowItAll and follow installation instructions found here instead: <https://sciencesolutions.wiley.com/training/>

Installation directory

The table below lists the format, installation file name, and the default target directory to which it will be installed. All installations allow manual override of the default directory path.

Format	Installation File	Default Directory
ChemStation	SetupW26ChemStation.exe	C:\Database\{libraryname}\{filename}
MassHunter	SetupW26MassHunter.exe	C:\MassHunter\Library\{libraryname}\{filename}
PCD	SetupW26PCD.exe	C:\MassHunter\PCDL\{filename}
MS Search	SetupW26MSSearch.exe	C:\NIST23\MSSEARCH\{libraryname}\{filename}
TurboMass	SetupW26TurboMass.exe	C:\TurboMass\ldendb\{libraryname}\{filename}

LabSolutions/ GCMSsolution*	SetupW26LabSolutions- GCMSsolution .exe	C:\LabSolutions\MSLibrary\{libraryname}\{filename}
Xcalibur	SetupW26Xcalibur.exe	C:\Program Files\NistMS\MSSearch\{libraryname}\{filename}
MassLynx	SetupW26MassLynx.exe	C:\MassLynx\ldendb\{libraryname}\{filename}

*If you are installing for use with GCMSsolution, change default directory to: C:\GCMSsolution\Library\{libraryname}\{filename}.

Hardware and software recommendations

- **Operating System:** Microsoft Windows (Windows 10 or 11 recommended)
- **CPU:** AMD or Intel processor, preferably multiple core
- **Software:** 32-bit or 64-bit software
- **Memory:** At least 2GB
- **Disk Space:** At least 2GB free space

For KnowItAll system requirements, please visit: [KnowItAll System Recommendations - Wiley Science Solutions](#).



This library is provided in multiple formats but is not supplied with the manufacturer software. Mass spectrometry software should be installed **prior** to installing the mass spectrometry library in any format.

Registration code

Ensure you have your **registration code** handy. This is required for installation. If you cannot locate your code, please contact us at <https://support.wiley.com/>.

Step-by-step guide

Step 1 – Choose your format(s)



Ensure your spectra/data analysis software is installed prior to installing the library format(s). The installer (setup *.exe file) also requires the **RegistrationProcess.dll** file to run.

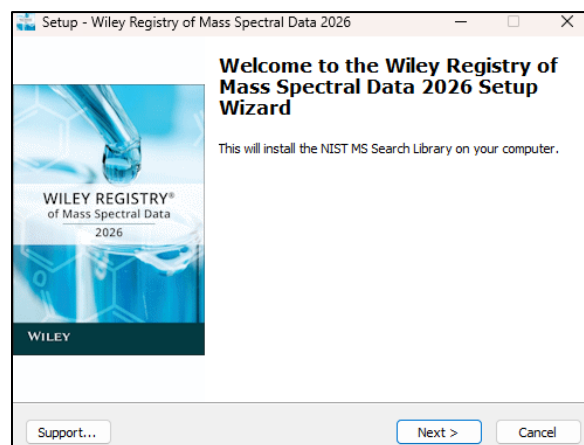
- Click on the **InstallationWizard.html** file included to simplify installation by using your web browser.
- Choose the format(s) you wish to install and download the installer(s) (setup *.exe file) **and** the **RegistrationProcess.dll** into the same directory.

Step 2 – Run the installer

Running the installer will start up the setup wizard. Click **Next** to proceed.

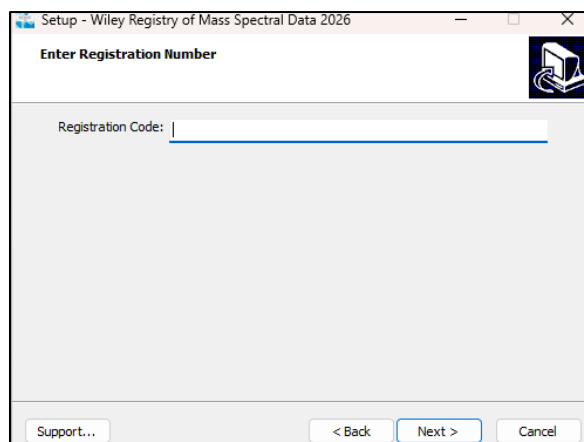


Please note that the installation files are digitally unsigned, so a warning may appear in Windows. Press **Run** and proceed to the installation to continue. Repeat this process for all the formats you wish to install on the one computer.



Step 3 – Enter your Registration Code

Enter the Registration Code exactly as it appears, including dashes, and click **Next**.

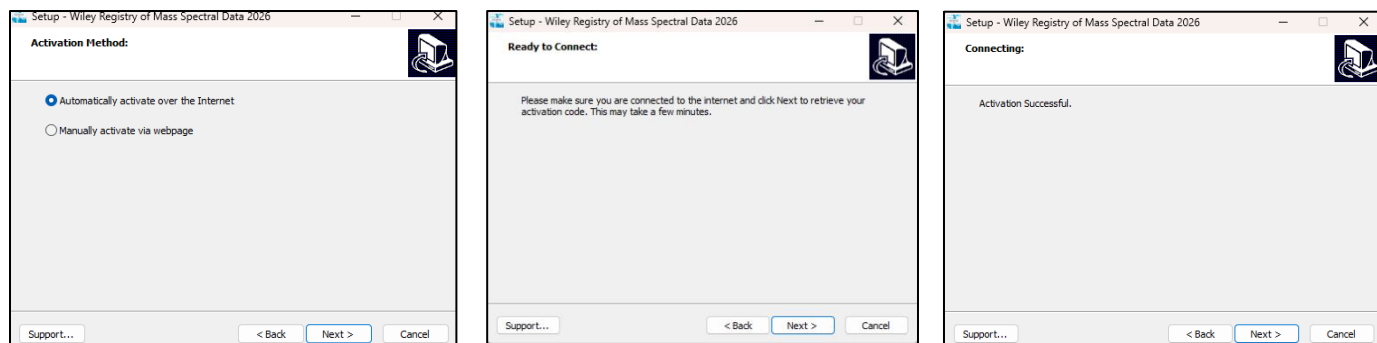


Step 4 – Activate the installer

If your computer is connected to the internet:

- Select **Automatically activate over the internet** and click **Next** to begin internet activation.
- Click **Next** a second time to complete the activation.

- Once your activation is successful, proceed by clicking **Next**.

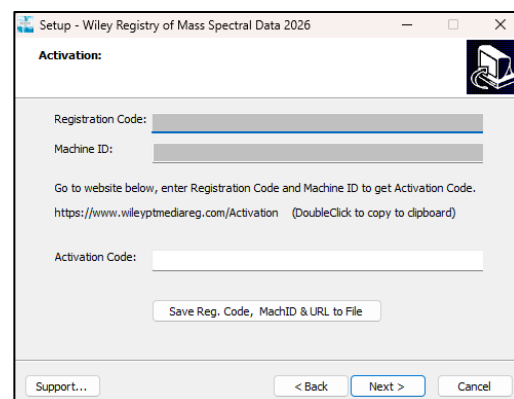


If your computer is “offline” and NOT connected to the internet:

Select **Manually activate via webpage** and click **Next**.

- The **Registration Code** and the **Machine ID** will be automatically populated into the **Setup** dialog box. You will need this information along with the web address in the next steps.

You can click the button to save the Registration Code, Machine ID and URL to a text file that will be saved to the root directory and/or double click the web address to copy it to your computer’s clipboard.



- Next, go to a device that is connected to the internet and navigate to this web page: <https://www.wileyptmediareg.com/Activation>

- Enter the **Registration Code** and **Machine ID** into the activation website exactly as you copied it from the **Setup** dialog box of the “offline” computer.

Enter the Registration Code that came with the software followed by the Machine ID:	
Registration Code	<input type="text"/>
Machine ID	<input type="text"/>
GET ACTIVATION CODE	

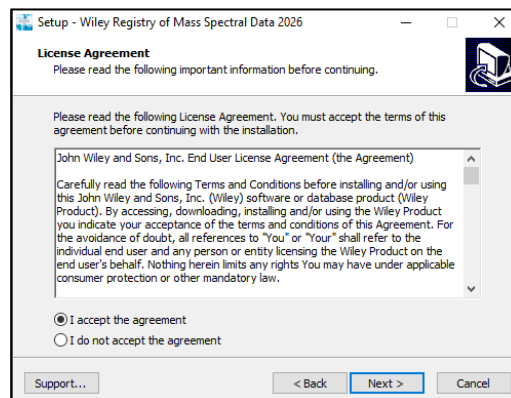
- Click **GET ACTIVATION CODE** to generate an activation code.
- You will need this Activation Code to complete the installation on your “offline” computer.
- Now, return to the “offline” computer you are installing the spectral library on and enter the Activation Code you generated in the **Setup** dialog box **Activation** screen.
- Click **Next** to activate.
- Once your activation is successful, proceed by clicking **Next**.

Step 5 – Accept the EULA

Read the EULA carefully, select **I accept the agreement**, and click **Next** to proceed with the installation of the library. If you do not accept, the installation cannot proceed.

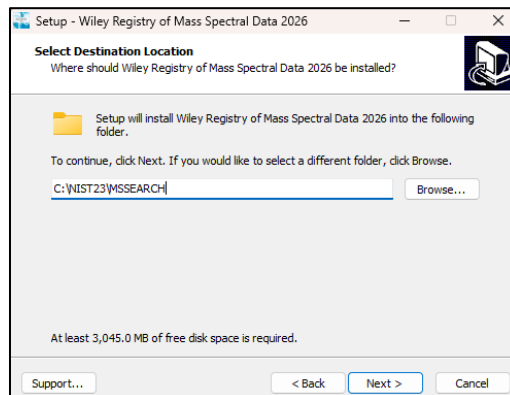


Spectral libraries should only be used by qualified individuals who meet the requirements outlined in the agreement.



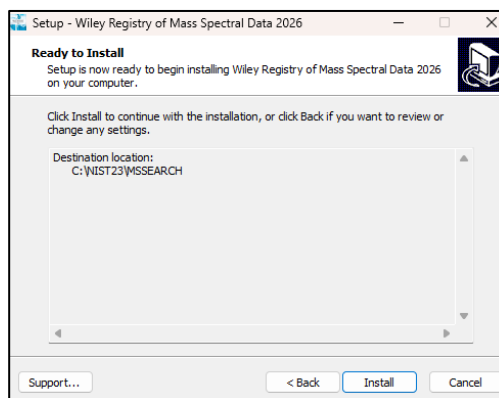
Step 6 – Confirm installation directory

Confirm the target directory before proceeding and then click **Next**.



Step 7 – Installation of library files

Click **Install** to begin installation.

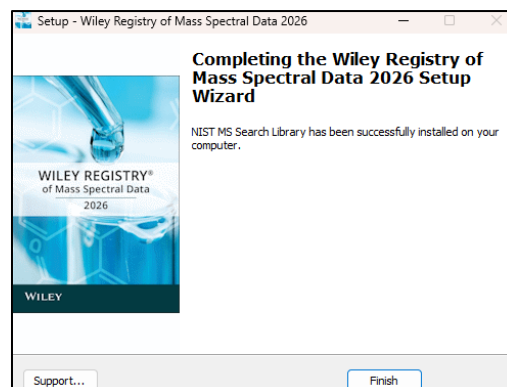


Step 8 – Complete installation

Once installation is complete, click **Finish**.



Be sure to consult your spectra/data analysis software's instructions for connecting to new libraries: some are automatic, but some require manual connection in the software.



Repairing or uninstalling

Repairing or uninstalling the library should be managed using the **Add/Remove Programs** utility in Windows. If the library is manually moved, removed, or installed using overwrite mode, the Windows utility may not work.

Appendix

See <https://sciencesolutions.wiley.com/> to explore other mass spectrometry, NMR, IR, Raman, and UV-Vis databases and KnowItAll software solutions from Wiley.

Search tips

When using parametric searching, many text search programs provide better results when names are begun and ended with wild cards (e.g., "*"). However, in NIST MS Search, this approach will not work.

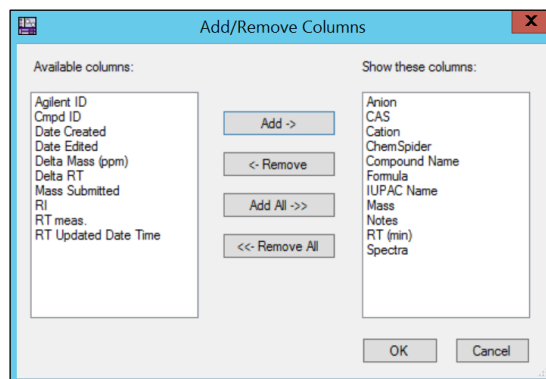
While every effort has been made to include a broad spectrum of compounds, when trying to match an unknown against the database, bear in mind that some unknowns, especially new variants of designer drugs and steroids established after publication may only be available in our specialized collections.

The Wiley Registry is segmented into 4 libraries:

- W26 main: Use this library for untargeted analysis in everyday scientific work.
- W26 replicate: Use this library when further confirmation or results are required.
- W26 lq: Use this library when further confirmation or results are required.
- W26 legacy: Use this library when searching for confirmation on past work.

Agilent PCD:

The Notes column contains WileyIDs and is not automatically visible in PCDL Manager. To make this column visible, navigate to **View > Add/Remove Compound Columns...** and add the **Notes** column.

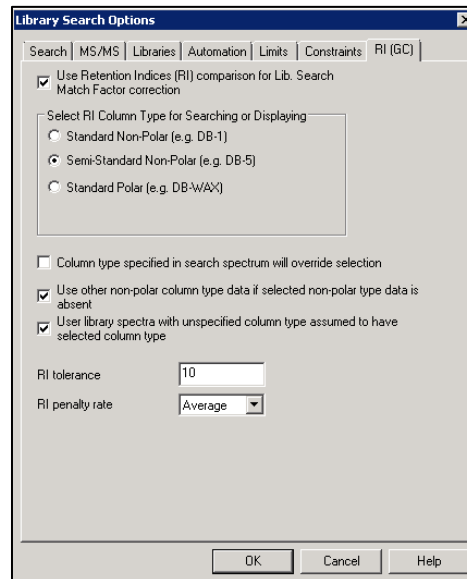


Agilent ChemStation/MassHunter:

In this software, the User Index field is populated with computed retention indices.

NIST MS Search:

Computed RI values are added under a built-in data field, which show up in the hit list under RI and in the record pane under Experimental RI median \pm deviation. Please note that these are not experimental RI values. The RI values can be used to improve search results by navigating to Options > Library Search Options and selecting the Use Retention Indices option under the RI tab.



PerkinElmer TurboMass/Waters MassLynx:

In this software, the Value 2 field is populated with computed retention indices.

Shimadzu LabSolutions/GCMSsolution:

In this software, the W26main library is broken up into 3 parts, W26MAIN1, W26MAIN2, and W26MAIN3.

CAS-RN field

Several mass spectrometry software suites - Agilent ChemStation/MassHunter, PerkinElmer TurboMass, and Waters MassLynx - link a spectrum to its associated chemical structure by using the "CAS-RN" (CAS Registry Number) field. Unique identifiers are provided by Wiley for compounds that lack a CAS RN to ensure each spectrum links correctly to its structure or to replace 10-digit CAS RNs. To keep these CAS-RN-like IDs clearly separate from genuine CAS numbers, Wiley uses unique 9-digit identifiers that start with "999" or "998". These numbers are simply a practical way to connect the spectrum to the right structure record.

Please note: Any of these 9-digit identifiers beginning with "999" or "998" are not genuine CAS Registry Numbers. These numbers are only used by Wiley to link a spectrum with its structure and have no meaning outside this purpose.

The following list details the 'CAS Registry Numbers'-like IDs used in the W26 collection created to point to the chemical structure records or to replace 10-digit CAS Registry Numbers, including a list of the 'real' 10-digit CAS Registry Numbers and the corresponding pseudo CASRN (as well as the WileyID and the main chemical name) used to replace them in the library:

CASRN_ChemStation_TurboMass_readme.txt

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- Wiley Terms of Use: <https://www.wiley.com/terms-of-use>

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