

WILEY



Mass Spectra of Designer Drugs 2025

User Manual

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Wiley-VCH GmbH, Weinheim, Germany

 Please do not print this manual.

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CONTACT INFORMATION

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

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

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

Physical products manufactured by Flashbay Electronics comply with the limits as set by the RoHS Directive (EU) 2015/863 amending Annex II to Directive 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment:

Substance	Limit (mg/kg)
Lead (Pb)	1000
Cadmium (Cd)	100
Mercury (Hg)	1000
Hexavalent Chromium (Cr(VI))	1000
Polybrominated Biphenyls (PBBs)	1000
Polybrominated, Diphenyl Ethers (PBDEs)	1000
Bis-(2-ethylhexyl) Phthalate (DEHP)	1000
Benzyl butyl Phthalate (BBP)	1000
Dibutyl Phthalate (DBP)	1000
Diisobutyl Phthalate (DIBP)	1000

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*
- Shimadzu LabSolutions/GCMSsolution
- Thermo Xcalibur

*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	SetupDD2025Chemstation.exe	C:\Database\{libraryname}\{filename}
MassHunter	SetupDD2025MassHunter.exe	C:\MassHunter\Library\{libraryname}\{filename}
PCD	SetupDD2025PCD.exe	C:\MassHunter\PCDL\{filename}
MS Search	SetupDD2025MSSearch.exe	C:\NIST23\MSSEARCH\{libraryname}\{filename}
GCMSSolution	SetupDD2025LabSolutions-GCMSSolution.exe	C:\GCMSSolution\Library\{libraryname}\{filename}
LabSolutions	SetupDD2025LabSolutions-GCMSSolution.exe	C:\LabSolutions\MSLibrary\{libraryname}\{filename}
Xcalibur	SetupDD2025Xcalibur.exe	C:\ProgramFiles\NISTMS\MSSearch\{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



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/s/>.

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.

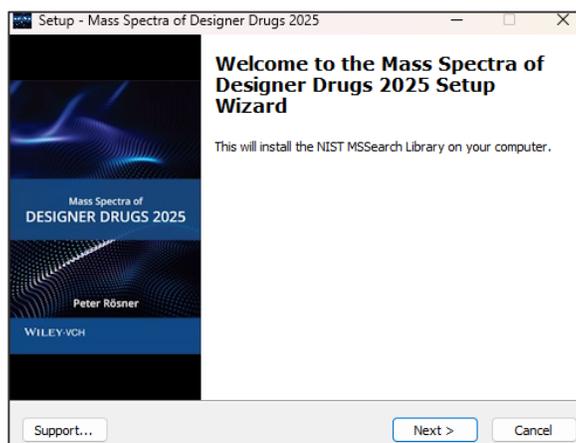
- Click on the **Installation.htm** file included to simplify installation by using your web browser.
- Choose the format(s) you wish to install and copy the installer (setup *.exe file) **and** the **RegistrationProcess.dll** into the same directory.

Step 2 – Run the installer

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

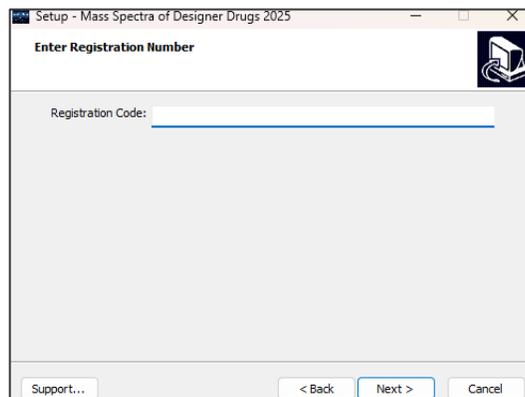


Please note that the installation files are digitally unsigned, so a warning may appear in Windows. Press **Run** and proceed to the installation to continue. Repeat this process for all the formats you wish to install on the one computer.



Step 3 – Enter your Registration Code

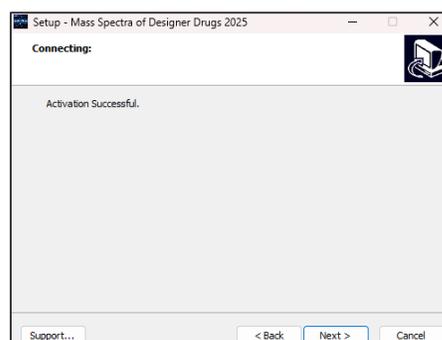
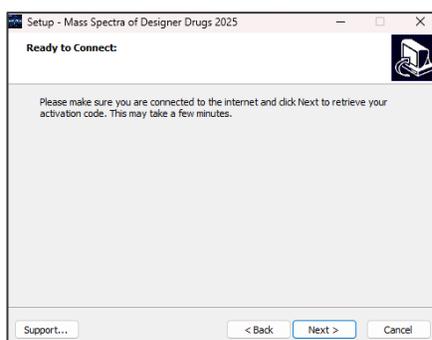
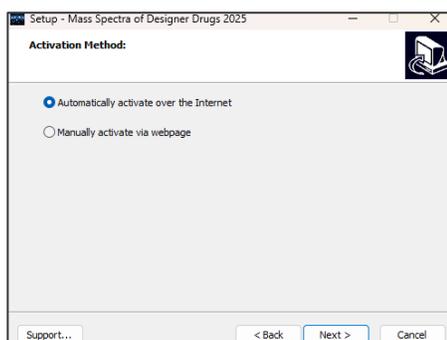
Enter the Registration Code exactly as it appears, including dashes, and click **Next**.



Step 4 – Activate the installer

If your computer is connected to the internet:

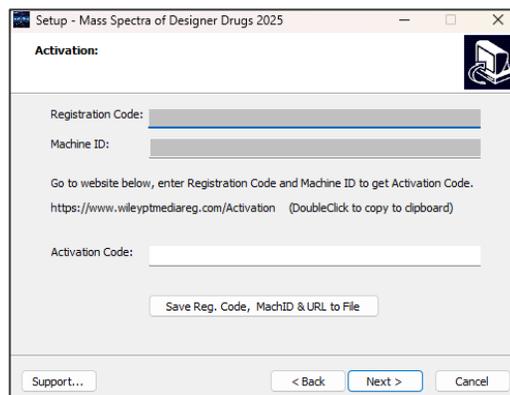
- Select **Automatically activate over the internet** and click **Next** to begin internet activation.
- Click **Next** a second time to complete the activation.
- Once your activation is successful, proceed by clicking **Next**.



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.

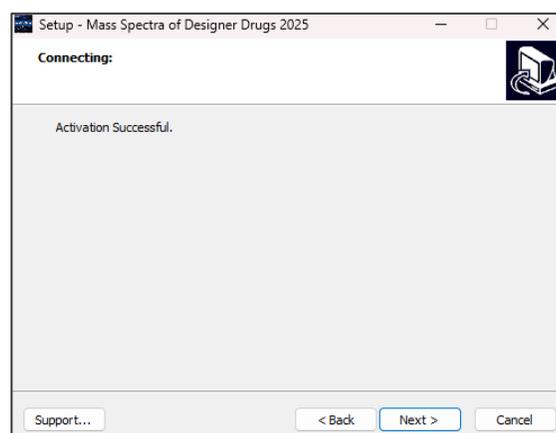


- Next, go to a device that is connected to the internet and navigate to this web page: <https://www.wileyptmediareg.com/Activation>

- 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"/>
<input type="button" value="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**.

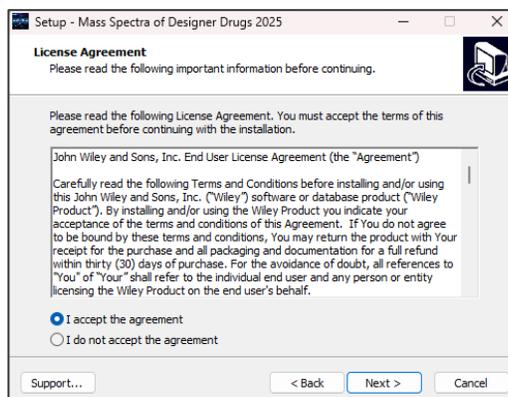


Step 5 – Accept EULA

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.

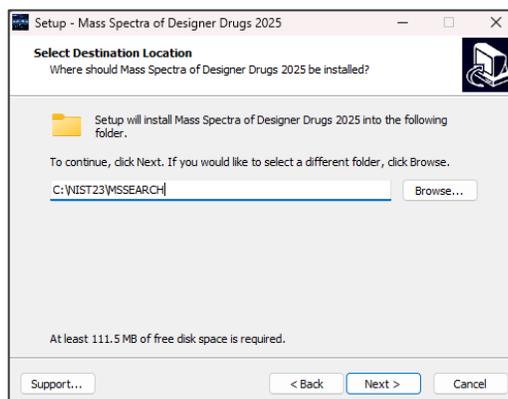


Spectral libraries should only be used by qualified individuals who meet the requirements outlined in the agreement.



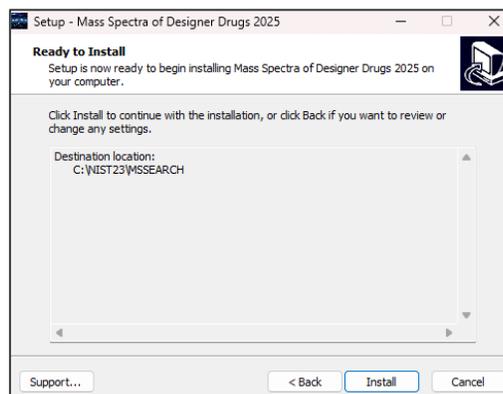
Step 6 – Confirm installation directory

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



Step 7 – Installation of library files

Click **Install** to begin installation.

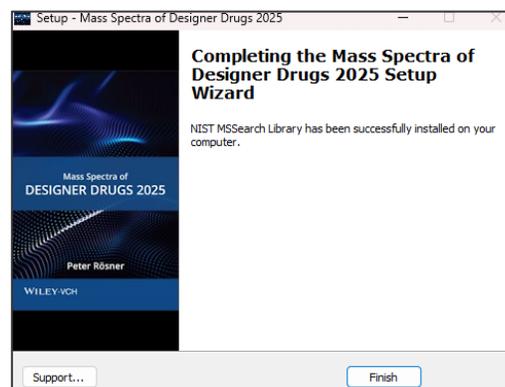


Step 8 - Complete installation

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.

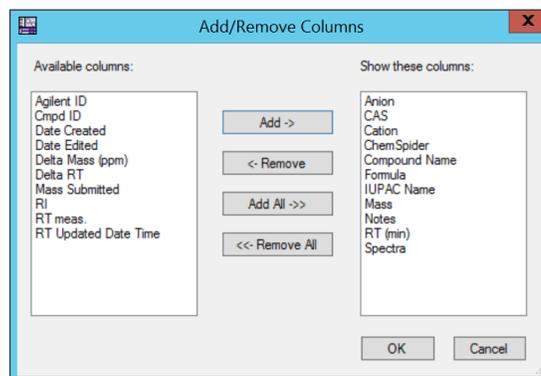
Search tips

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.

Agilent PCD:

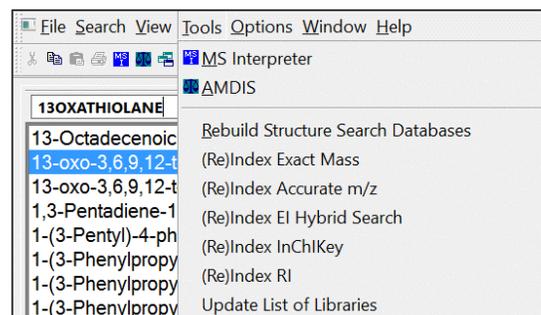
The Notes column contains WileyIDs and is not automatically visible in PCDL Manager. To make this column visible, navigate to **View > Add/Remove Compound Columns...** and add the **Notes** column.



NIST MS Search:

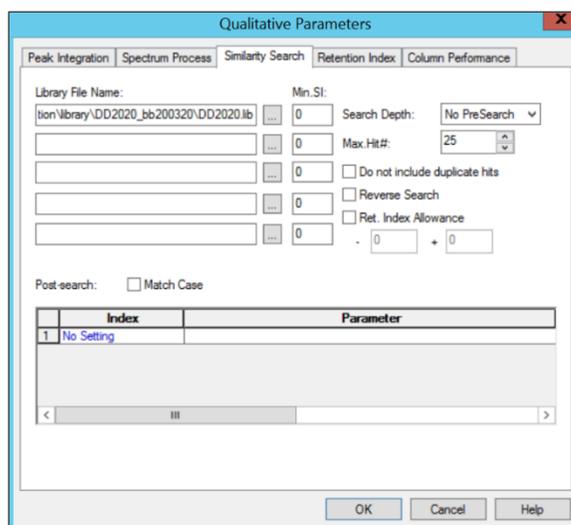
Please note that this library has not been indexed in NIST MS Search. To do this, please navigate to **Tools** and reindex the following:

- Structure Search Databases
- Exact Mass
- EI Hybrid Search



Shimadzu GCMSsolution:

For more accurate search results, navigate to **Qualitative > Qualitative Parameters** and under the **Similarity Search** tab, set **Search Depth** to **No PreSearch**:



CAS-RN field

Some mass spectrometry software programs rely on a field labeled "CAS-RN" to link spectral records with their corresponding structure record. As many of the compounds found within the Wiley Registry and other libraries do not have an assigned CAS-RN, this engineering decision would result in those spectra not being linked to their unique structure. To solve this problem, Wiley has created unique identifiers for the sole purpose of linking the spectrum and its structure using this field. To differentiate these numbers from actual CAS RNs, each is either a 9-digit number prefixed by 999 or 998, for Agilent ChemStation/MassHunter and PerkinElmer TurboMass/Waters MassLynx.

Please note that 9-digit IDs prefixed with the numbers 910 respectively do not in any way represent CAS Registry Numbers, nor are they used for anything other than referring to the structure record in the separate structure database as a workaround to accommodate engineering decisions made by other software publishers.

PRIVACY POLICY AND TERMS OF USE

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