

## Mass Spectra of Designer Drugs 2025

User Manual

Flash Drive Compilation Copyright  $\ensuremath{\mathbb{C}}$  2025 Wiley-VCH GmbH. All Rights Reserved.

User Manual Copyright  $\ensuremath{\mathbb{C}}$  2025 Wiley-VCH GmbH. All Rights Reserved.

Mass Spectra of Designer Drugs 2025 Copyright © 2025 DigiLab Software GmbH. All Rights Reserved. The unauthorized reproduction or distribution of copyrighted work is illegal. Criminal copyright infringement, including infringement without monetary gain, is investigated by the FBI and is punishable by fines and federal imprisonment.

This document may not be reproduced by any method, translated, transmitted, or stored in a retrieval system without prior written permission of John Wiley and Sons, Inc. Although every effort is made to ensure accuracy, John Wiley and Sons, Inc. cannot be held responsible for errors or omissions and reserves the right to revise this document without notice. The software described in this document is furnished under license and may be used and copied only in accordance with the terms of such license.

All the trademarks used in this documentation are acknowledged. KnowItAll and Wiley Registry are registered trademarks of John Wiley and Sons, Inc. in the United States, the European Union, and other countries. Xcalibur is a trademark of Thermo Fisher Scientific. All other trademarks are property of their respective owners.

No part of this database may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, recording, or otherwise, without prior written permission from John Wiley and Sons, Inc. The database contained on this flash drive is protected under the European Database Directive (Directive 96/9EC).

Wiley-VCH GmbH, Weinheim, Germany

A Please do not print this manual.

### Contents

CONTACT INFORMATION	4
Submitting data	4
COMPLIANCE	4
LICENSE	5
COMPATIBILITY	5
INSTALLATION	6
Installation directory	6
Hardware and software recommendations	6
Registration code	7
Step-by-step guide	7
Repairing or uninstalling	11
APPENDIX	12
Search tips	12
CAS-RN field	13
PRIVACY POLICY AND TERMS OF USE	13

## **CONTACT INFORMATION**

**Contact information:** <u>https://sciencesolutions.wiley.com/contact-us/</u> **Support:** <u>https://support.wiley.com/s/</u>

### 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: <a href="https://sciencesolutions.wiley.com/contact-us/">https://sciencesolutions.wiley.com/contact-us/</a>.

### 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:

	III (III9/K9)
Lead (Pb) 100	00
Cadmium (Cd) 100	)
Mercury (Hg) 100	00
Hexavalent Chromium (Cr(VI)) 100	00
Polybrominated Biphenyls (PBBs) 100	00
Polybrominated, Diphenyl Ethers (PBDEs) 100	00
Bis-(2-ethylhexyl) Phthalate (DEHP) 100	00
Benzyl butyl Phthalate (BBP) 100	00
Dibutyl Phthalate (DBP) 100	00
Diisobutyl Phthalate (DIBP) 100	00

## 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 <a href="https://sciencesolutions.wiley.com/compatibility/">https://sciencesolutions.wiley.com/compatibility/</a>.

## INSTALLATION

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

### **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}\{file
		name}
PCD	SetupDD2025PCD.exe	C:\MassHunter\PCDL\{filename}
MS Search	SetupDD2025MSSearch.exe	C:\NIST23\MSSEARCH\{libraryname}\{filen
		ame}
GCMSsolution	SetupDD2025LabSolutions-	C:\GCMSsolution\Library\{libraryname}\{fil
	GCMSsolution .exe	ename}
LabSolutions	SetupDD2025LabSolutions-	C:\LabSolutions\MSLibrary\{libraryname}\
	GCMSsolution .exe	{filename}
Xcalibur	SetupDD2025Xcalibur.exe	C:\ProgramFiles\NISTMS\MSSearch\{librar
		yname}\{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

ĥ

• 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 <u>https://support.wiley.com/s/</u>.

### 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.

Ô

0

Г

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**.

Setup - Mass Spectra	of Designer Drugs 20	25	-	X
Enter Registration N	umber			Ð
Registration Code:				
Support		< Back	Next >	Cancel

#### 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**.

🔤 Setup - Mass Spectra of Designer Drugs 2025 — 🗌	×	Setup - Mass Spectra of Designer Drugs 2025	- 🗆 X	Setup - Mass Spectra of Designer Drugs 20	25 — 🗆 X
Activation Method:		Ready to Connect:		Connecting:	
• Automatically activate over the Internet		Please make sure you are connected to the internet and click Ne activation code. This may take a few minutes.	ext to retrieve your	Activation Successful.	
O Manualiy activate via webpage					
Support <back next=""> C</back>	ancel	Support < Back	Next > Cancel	Support	< Back Next > Cancel

#### 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



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: <a href="https://www.wileyptmediareg.com/Activation">https://www.wileyptmediareg.com/Activation</a>
- 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.
- Click **GET ACTIVATION CODE** to generate an activation code.

Enter the Registration Code that came with the softwar	e followed by the Machine ID:
Registration Code	
Machine ID	
	GET 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**.

Setup - Mass Spectra of Designer Dr	ugs 2025		-		×
Connecting:				¢	
Activation Successful.					
Support	< Bad	k Next	>	Can	cel

#### 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.

Ô

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

Setup - Mass Spectra of Designer Drugs 2025	-		×
License Agreement Please read the following important information before continuing.		(	
Please read the following License Agreement. You must accept the te agreement before continuing with the installation.	erms of t	his	
John Wiley and Sons, Inc. End User License Agreement (the "Agreen Carefully read the following Terms and Conditors before installing a this John Wiley and Sons, Inc. (Wiley Joshware or database produ Product?). By installing and/or using the Wiley Product you indicate y acceptance of the terms and conditions of this Agreement. If You to be bound by these terms and conditions, You may return the proor receipt for the purchase and all packaging and documentation for a within thirty (30) days of purchase. For the avoidance of doubt, all 'You' of Your' shall refer to be individual end user and any person licensing the Wiley Product on the end user's behalf.	nent") nd/or us ict ("Wile rour o not ag duct with full refur referenc or entity	ing :y ree in Your ind es to /	
• I accept the agreement			
1 do not accept the agreement			
Support < Back Next	>	Car	cel

#### Step 6 – Confirm installation directory

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

Setup - Mass Spectra of Designer Drugs 2025	-		×
Select Destination Location Where should Mass Spectra of Designer Drugs 2025 be installed?		6	
Setup will install Mass Spectra of Designer Drugs 2025 into the folder.	ne follov	ving	
To continue, click Next. If you would like to select a different folder, o	lick Bro	wse.	
C: WIST23 WSSEARCH	Bro	owse	
At least 111.5 MB of free disk space is required.			
Support < Back Next	>	Can	cel

#### Step 7 – Installation of library files

Click **Install** to begin installation.

Ready to Install Setup is now rea your computer.	dy to begin installing Mas	s Spectra of Desig	ner Drugs 2025	on (	
Click Install to co change any setti	ntinue with the installation	n, or click Back if y	ou want to revie	ew or	
Destination loca C:\VIST23\V	tion: ISSEARCH			A	
4				•	

0

Π

#### 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 <u>https://sciencesolutions.wiley.com/</u> 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.

	Add/Remove Colum	ns
Available columns: Agilent ID Cmpd ID Date Created Date Edited Deta Mass (ppm) Deta RT Mass Submitted RI RT meas. RT Updated Date Time	Add -> <- Remove Add All ->> <<- Remove All	Show these columns: Anion CAS Cation ChemSpider Compound Name Formula IUPAC Name Mass Notes RT (min) Spectra

#### 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

Eile <u>S</u> earch <u>V</u> iew	<u>T</u> ools <u>Options</u> <u>W</u> indow <u>H</u> elp
i 🖪 🖻 🗇 🎦 🚛 君	Interpreter MS Interpreter
	MDIS
13OXATHIOLANE	
13-Octadecenoic	Rebuild Structure Search Databases
13-oxo-3,6,9,12-t	(Re)Index Exact Mass
13-oxo-3,6,9,12-t	(Re)Index Accurate m/z
1,3-Pentadiene-1	(Re)Index El Hybrid Search
1-(3-Pentyl)-4-ph	(Bo)Index InChIKey
1-(3-Phenylpropy	(Ne)ITIGEN ITCHINEY
1-(3-Phenylpropy	(Re)Index RI
1-(3-Phenylpropy	Update List of Libraries



#### Shimadzu GCMSsolution:

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

Qualitative Parameters		
Peak Integration   Spectrum Process	Similarity Search	Retention Index Column Performance
Library File Name: ison \ibrary\DD2020_bb200320\DD	Mir 2020.16 0 0 0 0 0	SI:       No PreSearch ▼         Max Hit#:       25 ▼         □ Do not include duplicate hits       □         □ Reverse Search       □         □ Ret. Index Allowance       □         • 0 + 0       •
Index Index INo Setting		Parameter
c III		Þ
		OK Cancel Help

### **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**

Wiley Privacy Policy: <a href="https://www.wiley.com/privacy">https://www.wiley.com/privacy</a>

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

## sciencesolutions.wiley.com