

# Mass Spectra of Designer Drugs 2022

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## User Manual

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## PUBLISHER'S NOTE

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For over 45 years, John Wiley and Sons and Wiley-VCH have worked with the world's leading researchers and practitioners to deliver the spectral libraries mass spectrometrists have come to rely on as the gold standard in mass spectrometry.

*Mass Spectra of Designer Drugs 2022* features 32,855 mass spectra and 25,343 unique compounds predominantly classified as novel psychoactive substances (NPS). The rapid development of these drugs poses serious challenges to current policies, procedures, and methods for detection and identification of these substances. With the dramatic surge of fentanyl addiction, this library helps labs combat the opioid and novel psychoactives epidemics that threaten public health.

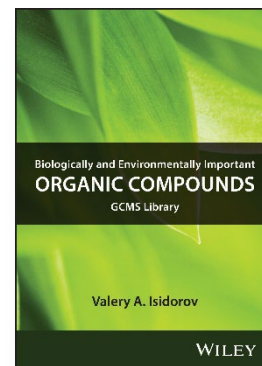
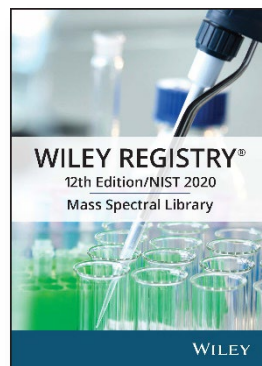
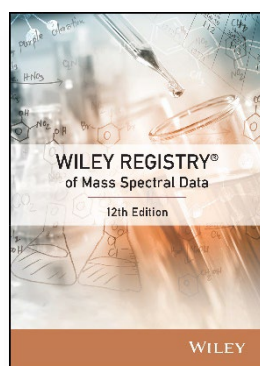
This edition features the addition of over 1,600 new mass spectra and over 1,400 new, unique compounds in over 30 different classification groups such as fentanyl, synthetic cannabinoids, and opiates. With an average quality index per spectrum of 960 and 21,335 Kovats retention indices, this spectral library provides comprehensive data on the most up-to-date list of novel psychoactive substances.

## COMPOUND SEARCH

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Address: <http://www.compoundsearch.com>

**Compound Search** is a free web-based database that provides free instant access to the latest compounds covered by Wiley spectral libraries.



# CONTACT INFORMATION

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## Editorial Correspondence

Wiley welcomes contributions of spectra for compounds, especially novel compounds not presently covered in the spectral library. Wiley can handle data in any machine-readable format. Data submissions, editorial notes, and corrections should be sent to the address below:

### **Wiley Science Solutions**

c/o John Wiley & Sons, Inc.

111 River Street

Hoboken, NJ 07030-5774 USA

Telephone: +1-201-748-6000

Fax: +1-201-748-8888

Email: [dbinquiry@wiley.com](mailto:dbinquiry@wiley.com)

Website: <https://sciencesolutions.wiley.com/>

Author correspondence: [p.roesner@t-online.de](mailto:p.roesner@t-online.de) or by fax: 0049 431/32723

## Customer Care

Customer care is available online or through correspondence at:

### **Customer Care Center – Consumer Accounts**

10475 Crosspoint Blvd.

Indianapolis, IN 46256 USA

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

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<b>Substance</b>	<b>Maximum Limit (ppm)</b>
Lead (Pb)	1000
Cadmium (Cd)	100
Mercury (Hg)	1000
Hexavalent Chromium (Cr6+)	1000
Poly Brominated Biphenyls (PBB)	1000
Poly Brominated Diphenyl ethers (PBDE)	1000

# GETTING STARTED

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## Hardware and Software Recommendations

- Operating System: Microsoft Windows (Windows 10 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

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

If you have questions about the format of the database or need to order a replacement, please contact Wiley Customer Care at <https://support.wiley.com/s/>.

## Registration Code

A registration code accompanies the packaging provided with the flash drive. This database may be installed on only one machine.

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# COMPATIBILITY

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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 Customer Support. This flash drive contains the following manufacturer formats:

- Agilent ChemStation
- Agilent MassHunter
- Agilent PCD
- NIST MS Search\*
- Shimadzu GCMSsolution
- Thermo Xcalibur™

\*Compatible with Agilent, Bruker, JEOL, LECO, PerkinElmer, Thermo, Waters, and most other manufacturer software

# DIRECTORY ASSISTANCE

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The table below lists the format, installation file, and their default target directory. If two directories are listed, the first directory is for the spectral data files, the second directory is for the structure files. If one directory is listed, all spectra and structure files are installed into that directory. All installations allow a manual override of the default directory path.

Format	Installation File	Default Directory
ChemStation	SetupDD2022Chemstation.exe	C:\Database\{libraryname}\{filename}
MassHunter	SetupDD2022MassHunter.exe	C:\MassHunter\Library\{libraryname}\{filename}
PCD	SetupDD2022PCD.exe	C:\MassHunter\PCDL\{libraryname}\{filename}
MS Search	SetupDD2022MSSearch.exe	C:\NIST20\MSSEARCH\{libraryname}\{filename}
GCMSsolution	SetupDD2022GCMS-Solution.exe	C:\GCMSsolution\Library\{libraryname}\{filename}
Xcalibur	SetupDD2022Xcalibur.exe	C:\ProgramFiles\NISTMS\MSSearch\{libraryname}\{filename}



# QUICK-START

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1. **Registration Code:** After reading the EULA, enter the Registration Code found on the Certificate of Authenticity provided and begin installation.
2. **Computer ID:** The installation program will combine the Registration Code with unique information from your computer to generate a unique Computer ID. If the computer is attached to the internet, the installer can automatically register your computer and provide a Registration Code. If the computer is not attached to the internet, follow procedure 2a or 2b below to manually register your installation.
  - a. **Computer ID – No direct internet:** Note the Computer ID and Registration Code and go to <https://www.wileyptmediareg.com/Activation> and follow the on-screen instructions. Note the resulting Activation Code and use it to complete on-screen installation prompts on the computer.
  - b. **Computer ID – No internet:** Contact Wiley Customer Support at <https://support.wiley.com/s/> or by telephone at (877) 762-2974.
3. **Installation:** Please note installation requires the Registration Code that accompanied your packaging. Install the formats you wish to use on a single computer, following the on-screen prompts to “run” the installer. N.B.: For Chrome and Firefox browsers, copy the install file onto a temporary directory. The installer requires RegistrationProcess.dll. Please copy the installer and dll into one directory and activate the installer.

## **Customer Care Center – Consumer Accounts**

10475 Crosspoint Blvd.  
Indianapolis, IN 46256 USA

# STEP-BY-STEP INSTALLATION

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\* This installation process mirrors installation on the NIST MS Search software.

1. A Registration Code will accompany the packaging provided with your flash drive. If your provided code does not work or your flash drive is not accompanied by a Registration Code, alert Wiley Customer Service at <https://support.wiley.com/s/>.

You will be unable to install this library without a Registration Code. Carefully read the End User License Agreement contained on the flash drive or the accompanying packaging before using and/or installing this product.

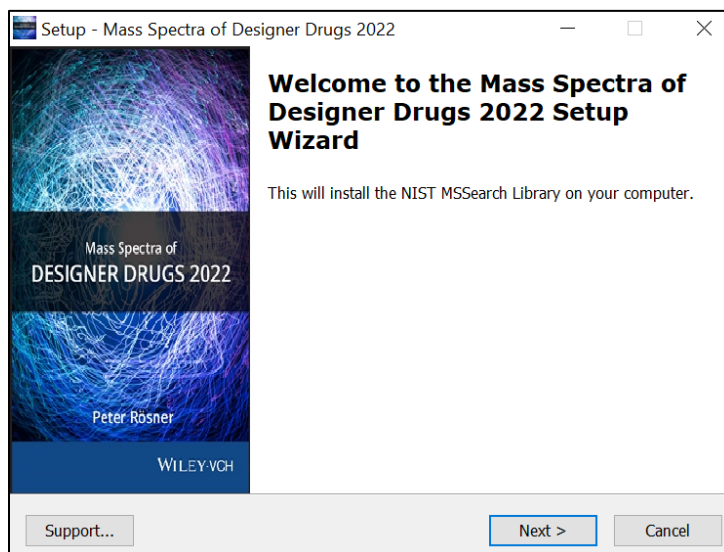
2. Insert the flash drive for installation. One file "Installation.htm" is included on the drive to simplify installation by using your web browser. Choose the format(s) you wish to install. Choosing to run the installer will bring you to a set-up wizard splash screen. Choose "Next."

N.B.: For Chrome and Firefox browsers, copy the install file onto a temporary directory. The installer requires RegistrationProcess.dll. Please copy the installer and dll into one directory and activate the installer.

Your license entitles you to install the library on one (1) machine.

Please note that the installation files are unsigned – so a warning may be displayed in Windows. Press run and proceed to the installation. Repeat this process for all of the formats you wish to install on the one computer.

**N.B.: Install your spectra/data analysis software prior to installing the format(s) you wish to install.**

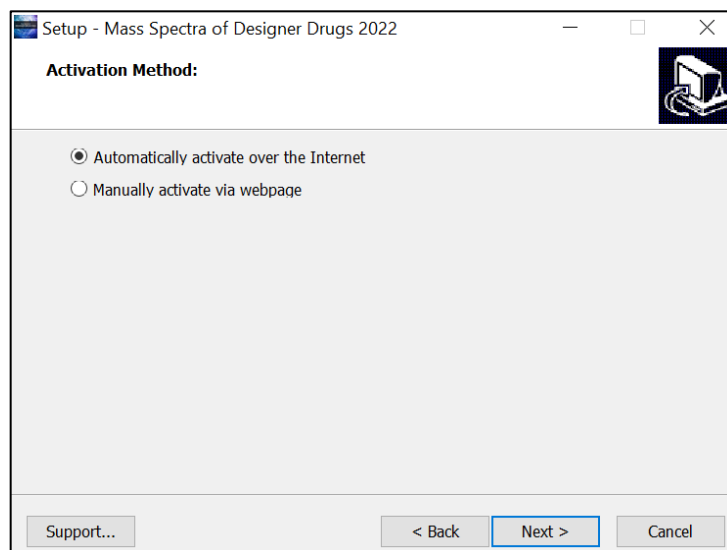
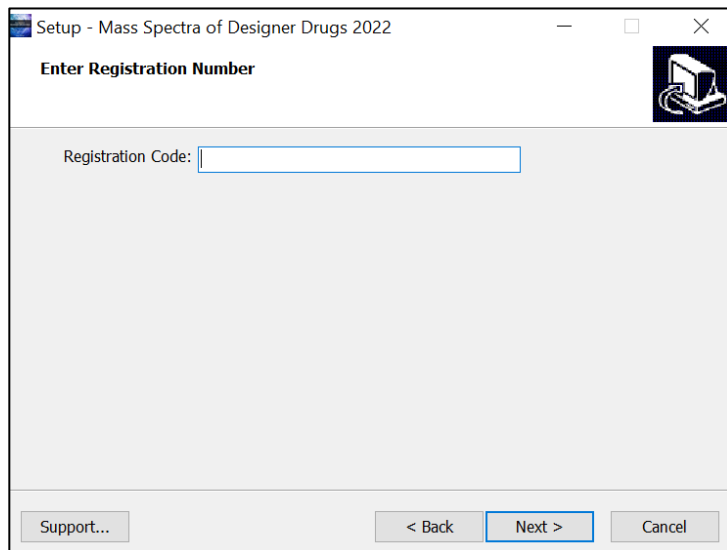


### 3. Registration Code and Machine ID

Your Registration Code appears on the Certificate of Authenticity accompanying your packaging.

Enter the Registration Code exactly as it appears to begin the installation and press "Next." If the code is incorrect, an error screen will appear.

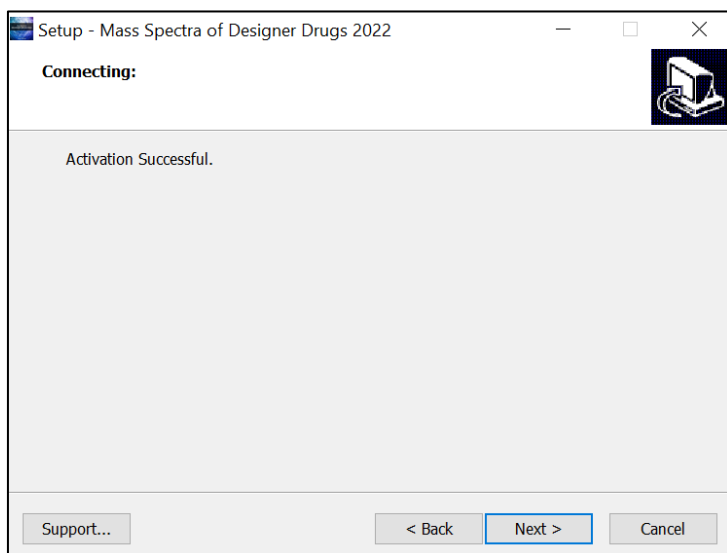
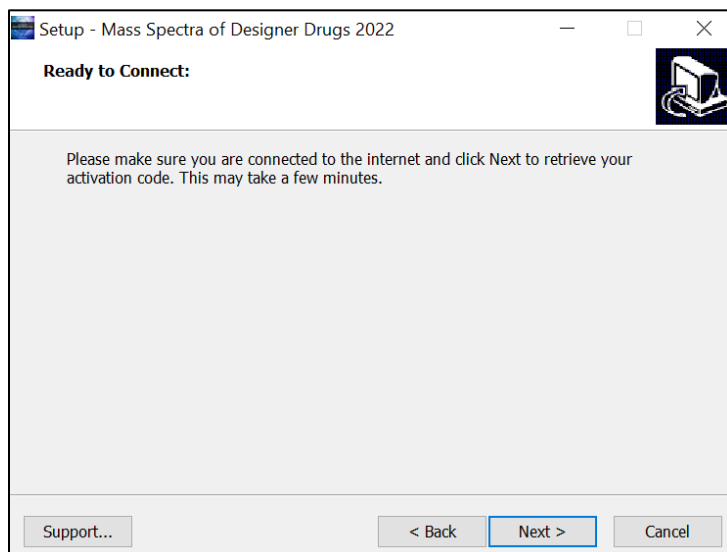
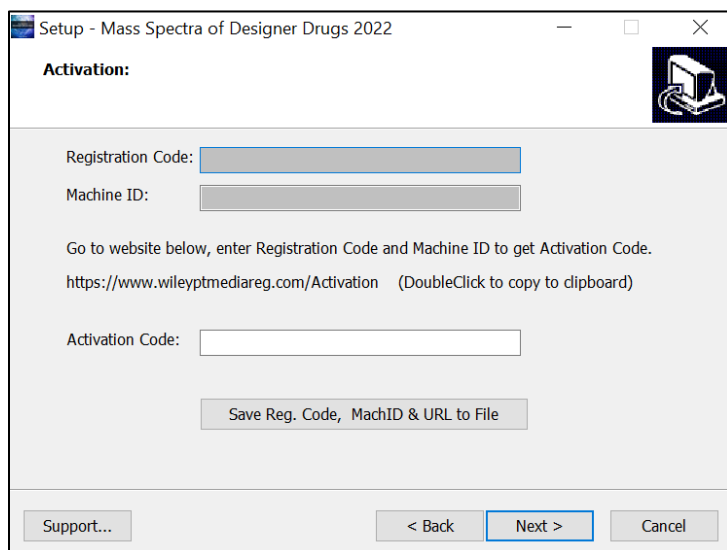
If the Registration Code is correct, you will be brought to the Activation screen. If your machine has internet connectivity, choose to "Automatically activate over the internet" and then click "Next" to begin internet activation.



- If you choose to manually activate, the Registration Code and the Machine ID will be automatically filled in. You may either double click the web address to copy it to your computer's clipboard and paste it in a web browser, or enter the URL as listed in your web browser.

Alternatively, you may save the Registration Code, Machine ID and URL to a text file that will be saved to the root directory.

In the web browser, enter the Registration Code and the Machine ID. The next screen will provide the Activation Code. Copy this code down and save it, entering it into the Activation screen on the computer that you are installing the spectral library on.

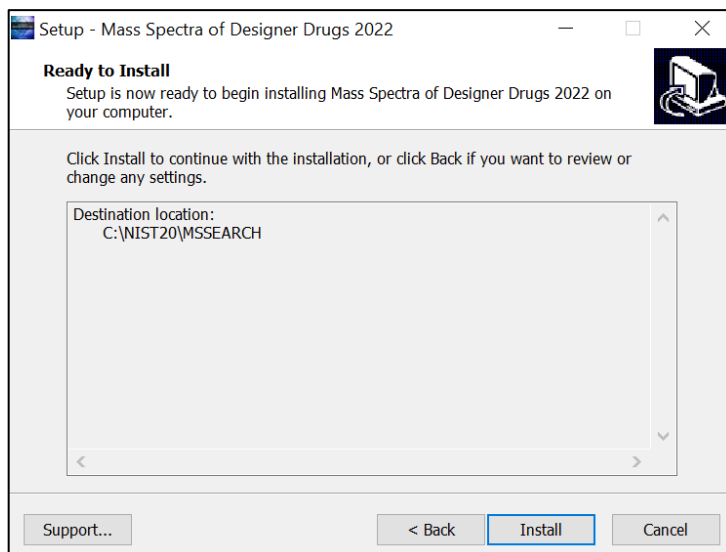
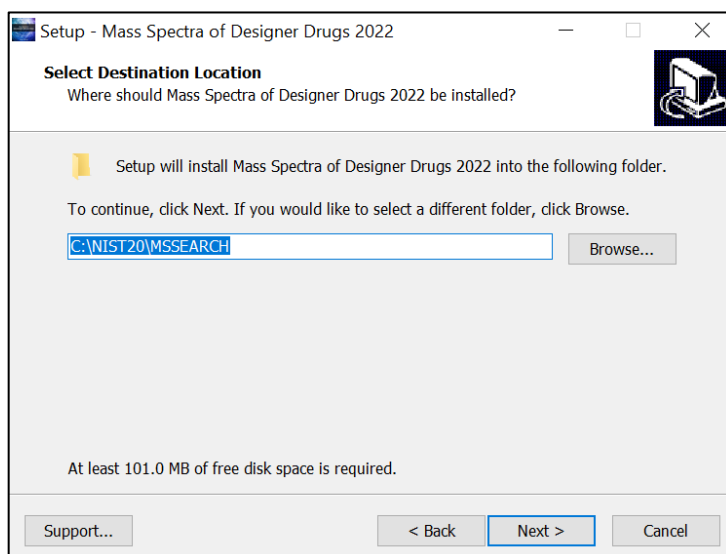
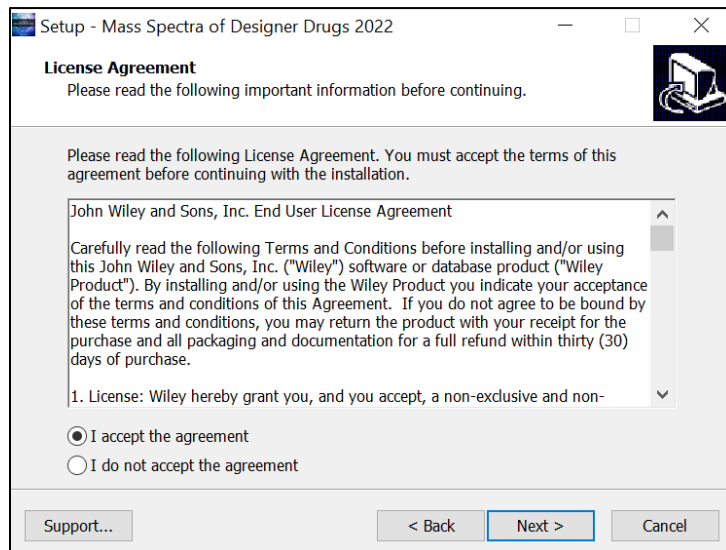


5. Once your activation is successful, proceed by pressing "Next." The next screen contains the End User License Agreement (16).

Read the agreement carefully and select the "I accept the agreement" option. Then, choose "Next" to proceed to install the library. Spectral libraries should only be used by qualified individuals who meet the requirements outlined in the agreement.

6. Press "Next" to proceed to the next step. At this point, the installer will unpack and install the library in the format you have selected. Confirm the target directory and destination location before proceeding.
7. Ready to install? After selection of the Destination Folder, choose the "Install" button to begin installation. Allow installation to finish before closing out any applications.

N.B.: For Chrome and Firefox browsers, copy the install file onto a temporary directory. The installer requires RegistrationProcess.dll. Please copy the installer and dll into one directory and activate the installer.



8. Once installation is complete, press “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 within 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.

## Getting Help

Getting Help – you can choose to go to: <https://support.wiley.com/s/>

# GENERAL DATABASE CONTENT

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Wiley mass spectrometry libraries have a wide variety of uses. Practitioners and researchers are encouraged to evaluate their own needs and decide what libraries are appropriate for them.

Mass Spectra of Designer Drugs – A specialized, high-quality library for analytical laboratories. Often used as an additive library for the targeted identification of unknown novel psychoactive substances. Updated annually, the 2022 edition covers the entire range of known novel psychoactive substances through December 31, 2021.

Wiley Registry 12th/NIST 2020 – A more comprehensive library for mission-critical tasks, including quality control, deformation, forensics, toxicology, and homeland defense applications. This library forms the basis for toxicology screening, steroid screening, and related applications.

See <https://sciencesolutions.wiley.com/> for other mass spectrometry, NMR, IR, and enterprise spectroscopy software from Wiley-VCH and John Wiley and Sons, Inc.

## Basic Functions

The enclosed library, Mass Spectra of Designer Drugs 2022, can be used as the primary search library or can be searched along with other libraries. We recommend, for mission-critical tasks, that users consult both a general library such as the Wiley Registry® of Mass Spectral Data, 12th Edition and a specialized library such as MS of Drugs, Poisons, Pesticides, Pollutants, and Their Metabolites, 5th Edition or Mass Spectra of Flavors and Fragrances of Natural and Synthetic Compounds, 3rd Edition.

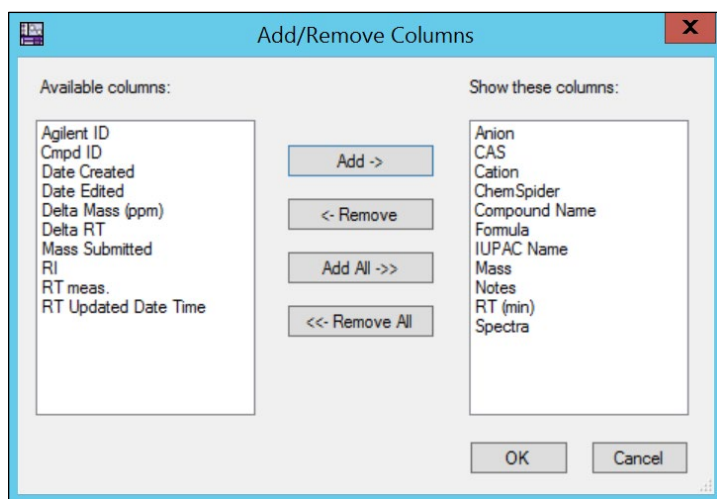
## Search Tips

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:

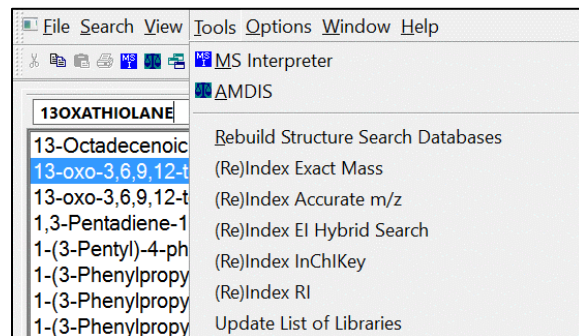
The Notes column contains WileyIDs and is not automatically visible in PCDL Manager. To make this column visible, navigate to View > Add/Remove Compound Columns... and add the Notes column:



### 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:

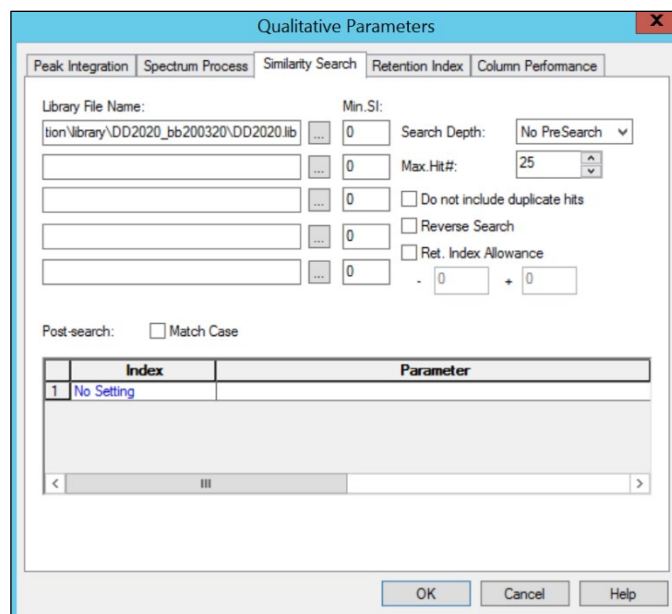
- Structure Search Databases
- Exact Mass
- EI Hybrid Search





## Shimadzu GCMSsolution:

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



Qualitative Parameters

Peak Integration | Spectrum Process | **Similarity Search** | Retention Index | Column Performance

Library File Name:  Min.SI:  Search Depth:  Max.Hit#:

Do not include duplicate hits  
 Reverse Search  
 Ret. Index Allowance

Post-search:  Match Case

	Index	Parameter
1	No Setting	

< ||| >

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.

**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.**

# DATA SUBMISSION

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Wiley welcomes submissions of new data for consideration for inclusion in forthcoming editions of the Wiley Registry, as well as other works. Wiley also accepts data in the following areas:

- Classical EI-MS
- Tandem MS (MSn)
- MS-TOF exact mass
- C-NMR, H-NMR, P-NMR, Si-NMR, X-NMR
- FT-IR, Raman, UV-Vis, Near-Infrared, Diamond-ATR

Data proposals, sample data, or inquiries are best sent to [dbinquiry@wiley.com](mailto:dbinquiry@wiley.com).

You might send the original TIC file (Xcalibur (\*.raw), ChemStation (.D data folder)) by an e-mail attachment directly to: [dbinquiry@wiley.com](mailto:dbinquiry@wiley.com). The data will be evaluated. If you have questions or if you need assistance, please contact us. We are always willing to help.

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