

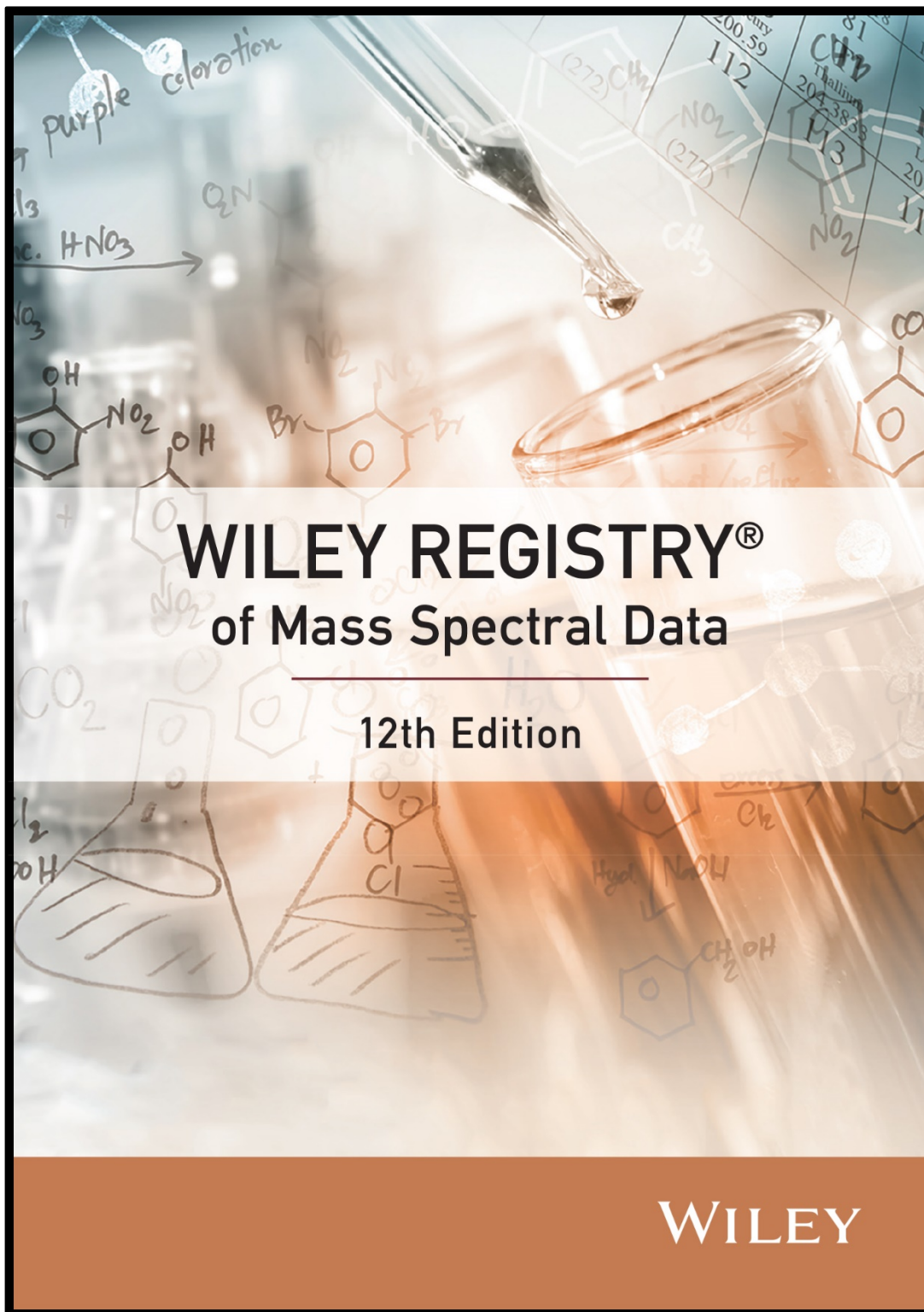
Wiley Registry® of Mass Spectral Data, 12th Ed.

USER MANUAL

VERSION 1.1

USER MANUAL

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TABLE OF CONTENTS

PUBLISHER'S NOTE	4
COMPOUND SEARCH	4
CONTACT INFORMATION.....	5
Editorial Correspondence.....	5
Customer Care.....	5
COMPLIANCE	5
GETTING STARTED	6
Hardware and Software Recommendations.....	6
Registration Code	6
License.....	6
COMPATIBILITY	7
DIRECTORY ASSISTANCE.....	7
QUICK-START	8
STEP-BY-STEP INSTALLATION.....	9
Getting Help	13
GENERAL DATABASE CONTENT	14
Basic Functions	14
Search Tips.....	15
CAS RN Field.....	16
DATA SUBMISSION	17
JOHN WILEY AND SONS, INC. PRIVACY POLICY AND TERMS OF USE.....	18
JOHN WILEY AND SONS, INC. END USER LICENSE AGREEMENT.....	18

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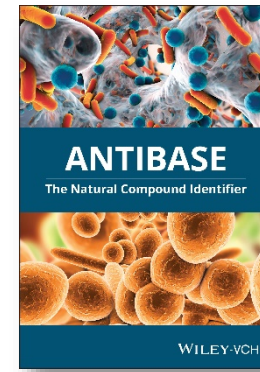
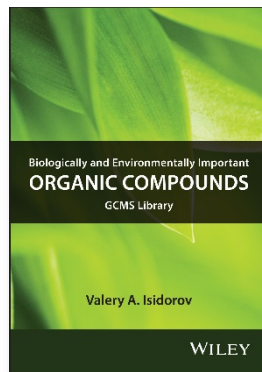
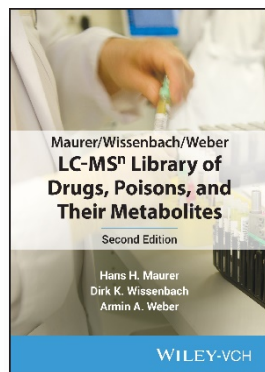
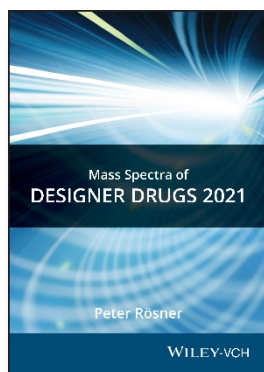
For over 45 years, John Wiley and Sons and Wiley-VCH have worked with the world's leading researchers and practitioners to deliver the spectral libraries scientists have come to rely on.

The *Wiley Registry® of Mass Spectral Data*, now in its 12th edition, is the most comprehensive mass spectral library available. Applications include untargeted GCMS screening and accurate mass workflows with MS-TOF spectra. Included in the 12th edition are over 817,250 mass spectra, 785,050 searchable chemical structures, and 668,400 unique compounds. Improvements to the Wiley Registry include removal and sequestration of suspect spectra from the main library and the addition of chemical classifications, calculated Kovats RI values, and splash IDs. The result is a main library that has increased overall breadth and improved spectral search performance.

COMPOUND SEARCH

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 and NIST spectral libraries.



CONTACT INFORMATION**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:

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c/o John Wiley & Sons, Inc.

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Telephone: +1-201-748-6000

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Email: dbinquiry@wiley.com

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

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Indianapolis, IN 46256 USA

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Substance	Maximum Limit (ppm)
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

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

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
- PerkinElmer TurboMass
- Shimadzu GCMSsolution
- Thermo Xcalibur™
- Waters MassLynx

DIRECTORY ASSISTANCE

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	SetupW12ChemStation.exe	C:\Database\{libraryname}\{filename}
MassHunter	SetupW12MassHunter.exe	C:\MassHunter\Library\{libraryname}\{filename}
PCD	SetupW12PCD.exe	C:\MassHunter\PCDL\{filename}
MS Search	SetupW12MSSearch.exe	C:\NIST17\MSSEARCH\{libraryname}\{filename}
TurboMass	SetupW12TurboMass.exe	C:\TurboMass\ldendb\{libraryname}\{filename} C:\TurboMass\ldendb\STRUCTDB\{libraryname}\{filename}
GCMSsolution	SetupW12GCMS-Solution.exe	C:\GCMSsolution\Library\{libraryname}\{filename}
Xcalibur	SetupW12Xcalibur.exe	C:\ProgramFiles\NISTMS\MSSearch\{libraryname}\{filename}
MassLynx	SetupW12MassLynx.exe	C:\MassLynx\ldendb\{libraryname}\{filename} C:\MassLynx\ldendb\STRUCTDB\{libraryname}\{filename}

*Installations will include download of a minimum of four {libraryname}: W12main, W12rep, W12leg, W12lq

QUICK-START

- 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.
 - 2a. 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 **Registration Code** and use it to complete on-screen installation prompts on the computer.
 - 2b. 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.

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STEP-BY-STEP INSTALLATION

- * **This installation process mirrors installation on a NIST MS Search program.**

Step 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.

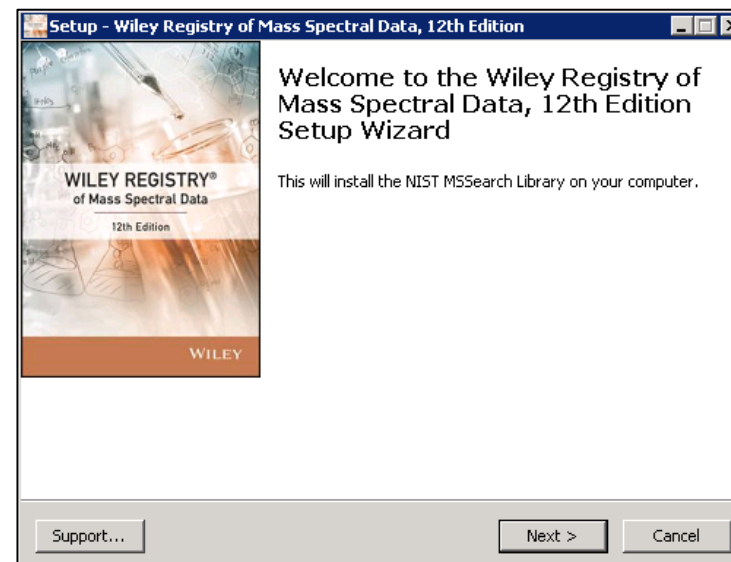
Step 2. Insert the flash drive for installation. One file "Installation.htm" is included on the drive to simplify installation by using your web browser. Choose the format(s) you wish to install. Choosing to run the installer will bring you to a set-up wizard splash screen. Choose "Next."

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.

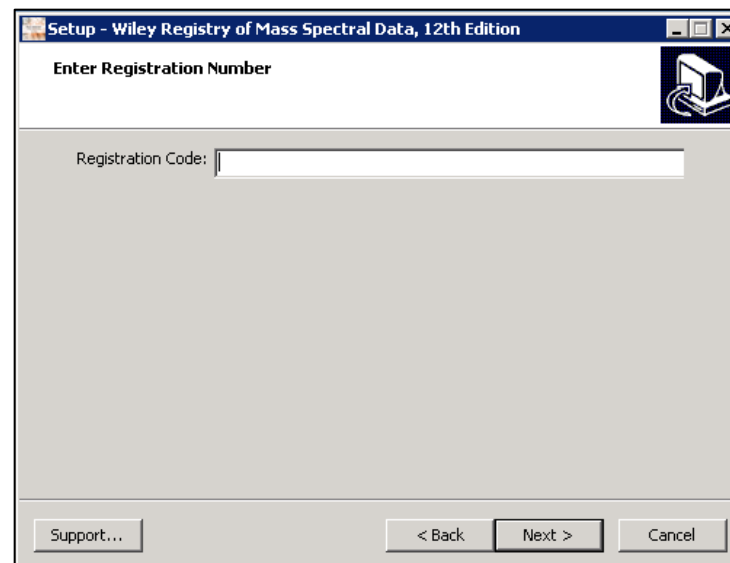
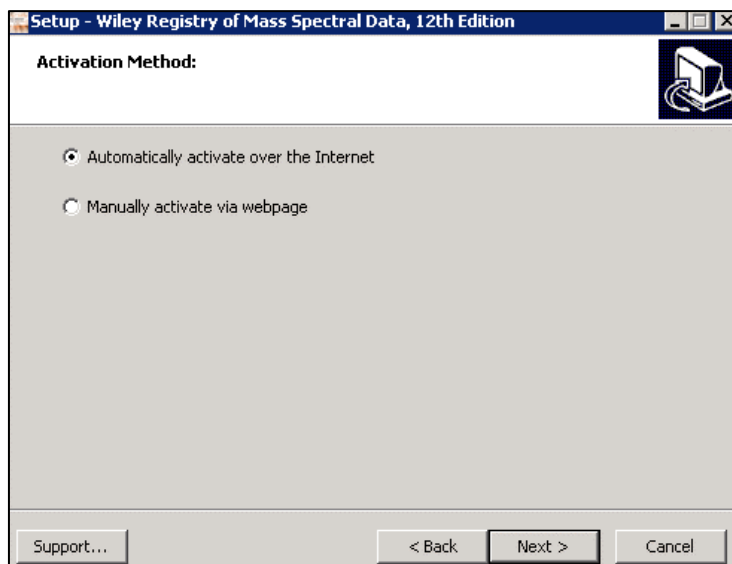


Step 3. Registration Code and Machine ID

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.

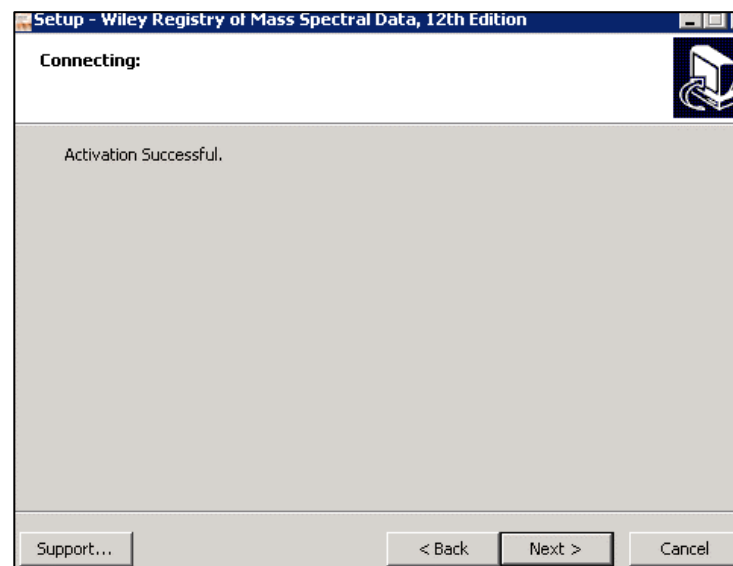
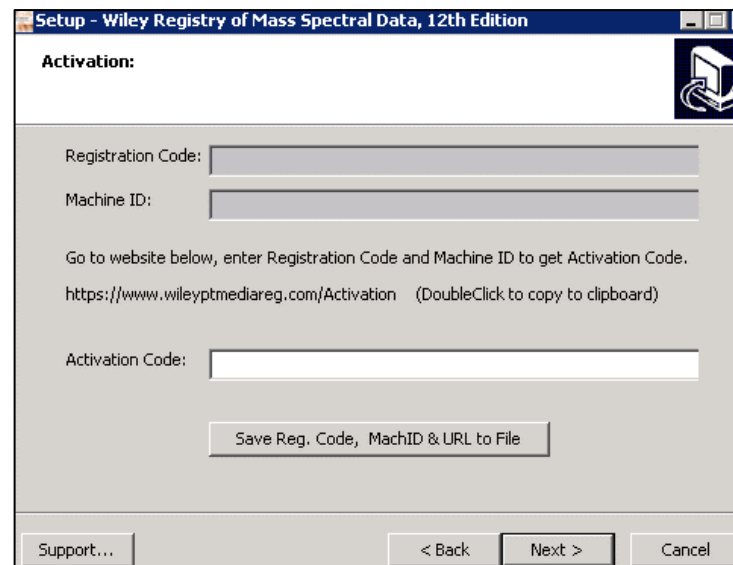
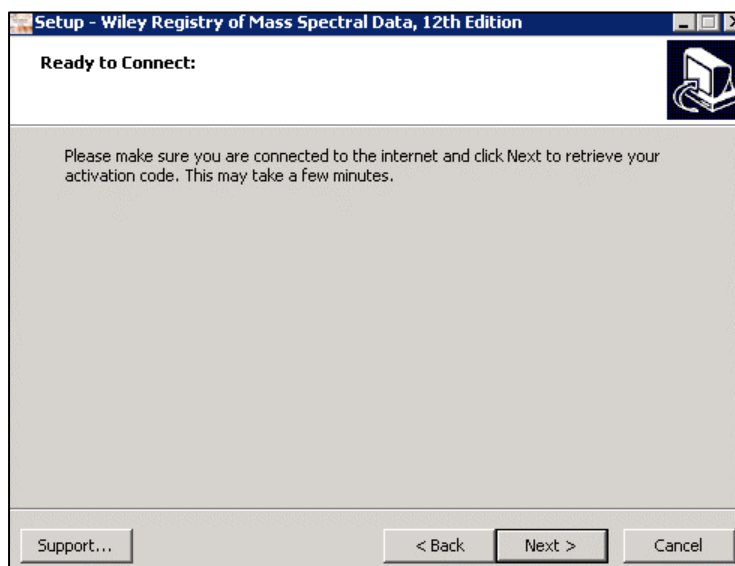
If the **Registration Code** is correct, you will be brought to the Activation screen. If your machine has internet connectivity, choose to "Automatically activate over the internet" and then click "Next" to begin internet activation.



Step 4. 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.

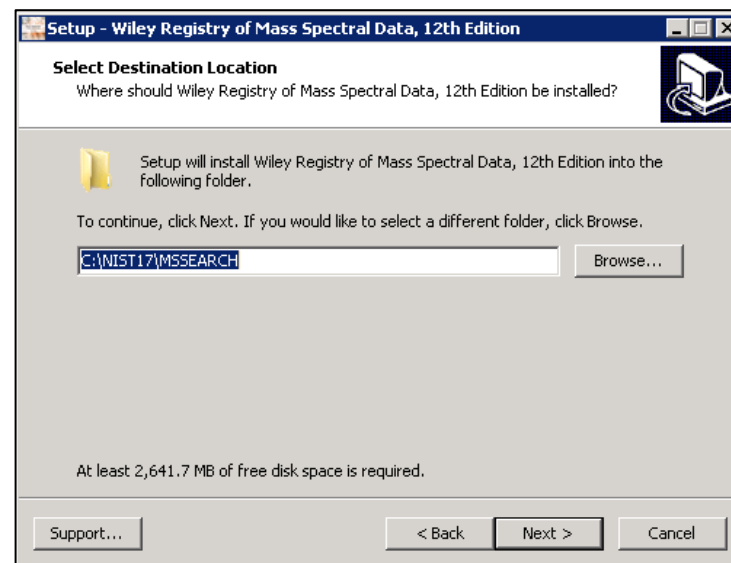
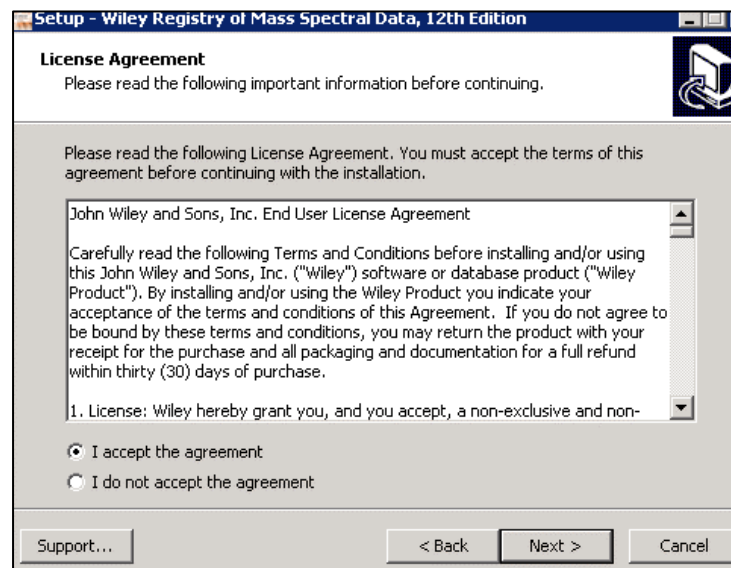
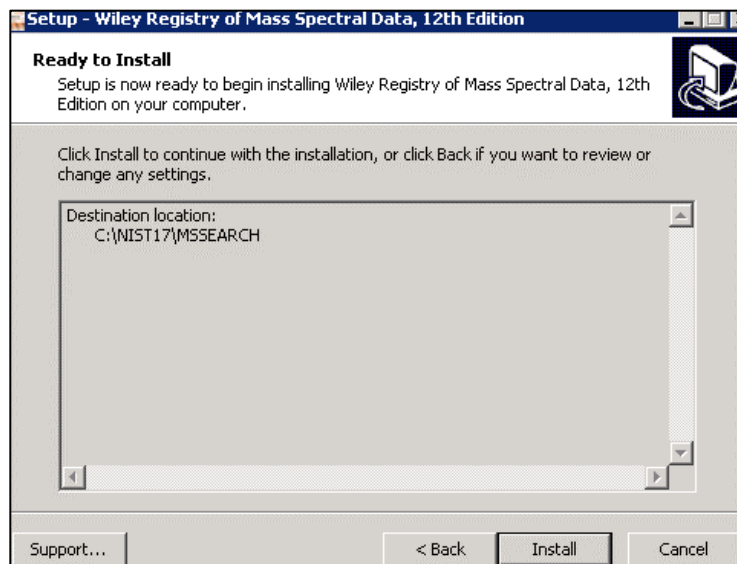


Step 5. Once your activation is successful, proceed by pressing “Next.” The next screen contains the End User License Agreement (18). Read the agreement carefully and select the “I accept the agreement” option. Then, choose “Next” to proceed to install the library. Spectral libraries should only be used by qualified individuals who meet the requirements outlined in the agreement.

Step 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.

Step 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.

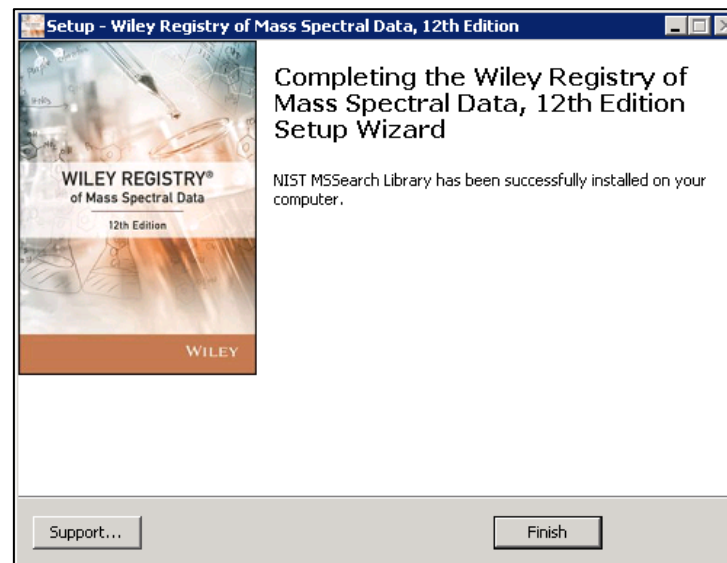
N.B.: For Chrome and Firefox browsers, copy the install file onto a temporary directory. The installer requires RegistrationProcess.dll. Please copy the installer and dll into one directory and activate the installer.



Step 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

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.

Wiley Registry 12th Edition – A complete, general-purpose high-quality library comprised of main, replicate, and deleted sections for analytical laboratories. Often used as the foundation library for research, quality control, deformation, and for forensic, toxicology, and homeland defense applications.

- W12 main: Use this library for untargeted analysis in everyday scientific work.
- W12 replicate: Use this library when further confirmation or results are required.
- W12 legacy: Use this library when searching for confirmation on past work.
- W12 low quality: Use this library when further confirmation or results are required.

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 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 *Wiley Registry of Mass Spectral Data 12th Edition* and a specialized library such as *MS and GC Data of Drugs, Poisons, Pesticides, Pollutants, and Their Metabolites* 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.

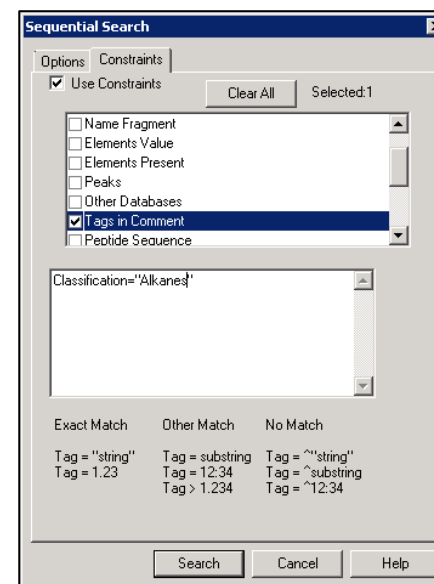
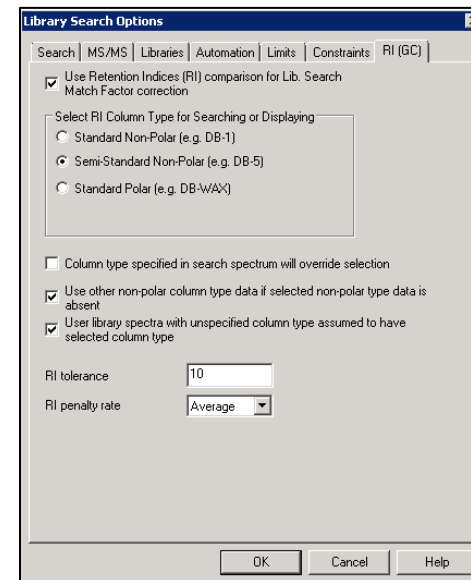
NIST MS Search: Calculated RI values are added under a built-in data field, which show up in the hit list under RI and in the record pane under Experimental RI median±deviation. Please note that these are *not* experimental RI values. Additionally, for n-alkanes, theoretical RI values were used rather than calculated ones. The RI values can be used to improving search results by navigating to Options > Library Search Options and selecting the Use Retention Indices option under the RI tab. Similarly, the Sequential Search method can be used to narrow your search by tags within the Comment field, such as classification. (See screenshots to the right.)

Agilent ChemStation/MassHunter: In this software, the User Index field is populated with calculated Kovats retention indices.

Shimadzu GCMSsolution: In this software, the W12main library is broken up into 3 parts, W12MAIN1, W12MAIN2, and W12MAIN3.

PerkinElmer Turbomass/Waters MassLynx: In this software, the Value 2 field is populated with calculated Kovats retention indices.

For training videos, visit: <https://sciencesolutions.wiley.com/WR12>



CAS RN FIELD

Some mass spectrometry software programs rely on a field labeled "CAS-RN" to link spectral records with 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 a 10-digit number prefixed by 2000, for Agilent ChemStation/MassHunter and PerkinElmer TurboMass/Waters MassLynx respectively.**

Please note that 9 or 10-digit IDs prefixed with the numbers 999 and 2000 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

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.

You might send the original TIC file (Xcalibur (*.raw), ChemStation (.D data folder)) by an e-mail attachment directly to: 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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