

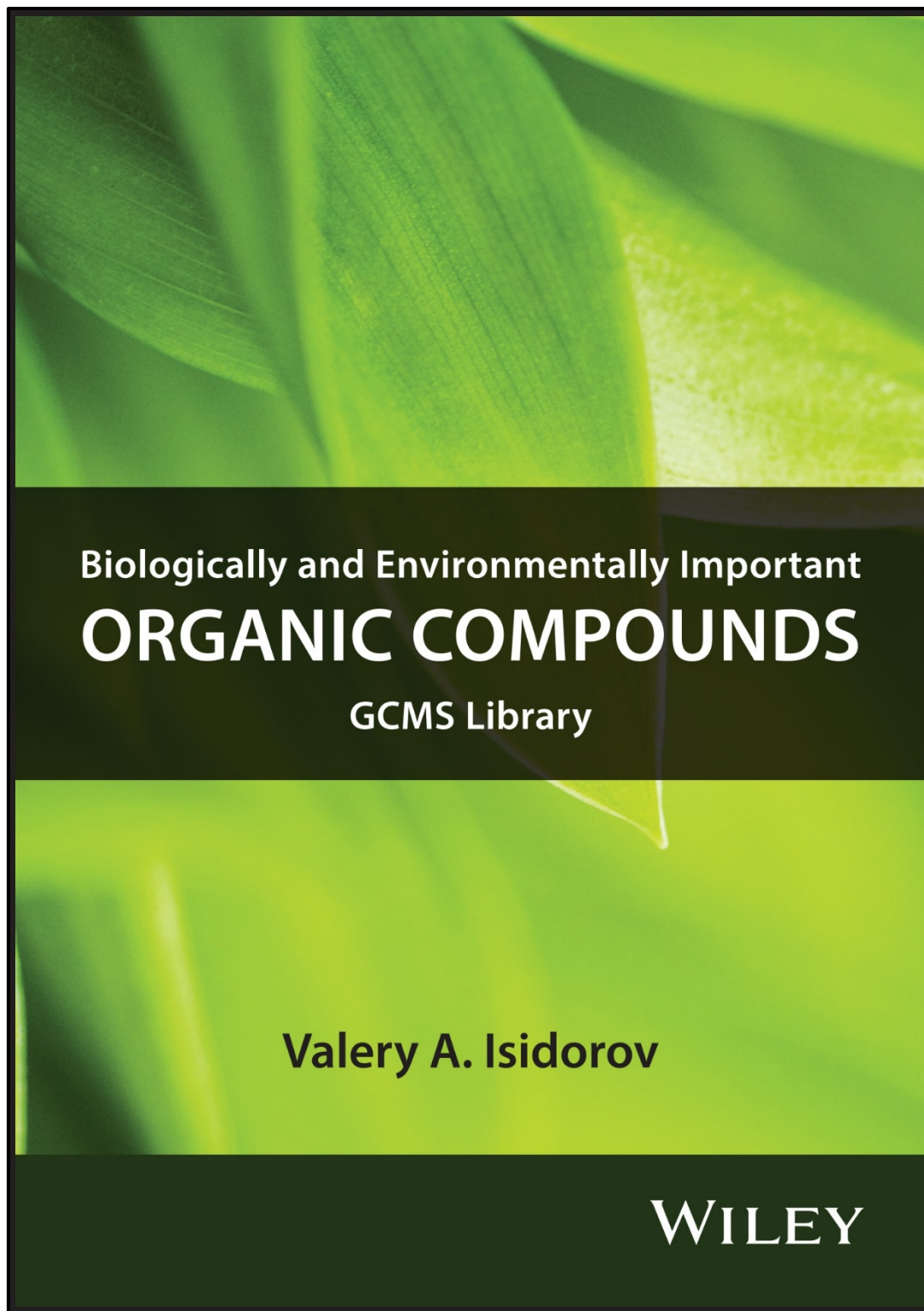
Biologically and Environmentally Important
Organic Compounds: GCMS Library

USER MANUAL

VERSION 1.1

USER MANUAL

VERSION 1.1



Biologically and Environmentally Important
ORGANIC COMPOUNDS
GCMS Library

Valery A. Isidorov

WILEY

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Biologically and Environmentally Important Organic Compounds: GCMS Library

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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.

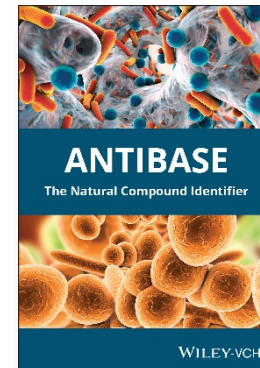
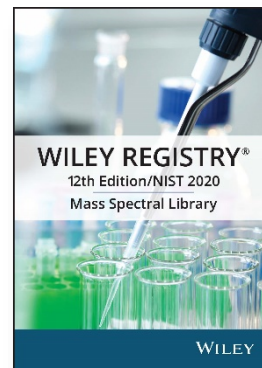
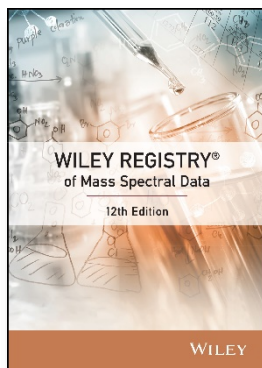
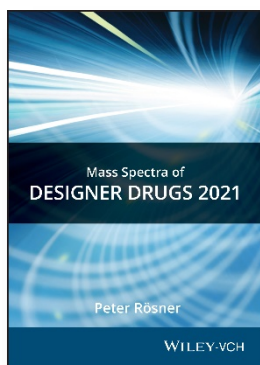
The Biologically and Environmentally Important Organic Compounds: GCMS Library contains mass spectra and retention indices for over 1,900 biologically and environmentally important organic compounds, in the form of their trimethylsilyl (TMS) derivatives. This database contains a number of compounds detected by the author's team in plant tissues, some of which have never before been analyzed by mass spectrometry and gas chromatography. Additionally, more than 60% of the presented compounds have not been previously characterized by their mass spectra and more than 70% have not been previously characterized by their RI values.

This database is a supplement to the following book: *GC-MS of Biologically and Environmentally Significant Organic Compounds: TMS Derivatives* by Valery A. Isidorov
ISBN: 978-1-119-61134-9

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.



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c/o John Wiley & Sons, Inc.

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

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Indianapolis, IN 46256 USA

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

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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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Help keep the cost of libraries down by reporting all copyright and license violations to the publisher at dbinquiry@wiley.com.

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
- NIST MS Search
- PerkinElmer TurboMass
- Shimadzu GCMSsolution
- 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	SetupSIChemStation.exe	C:\Database\{libraryname}\{filename}
MassHunter	SetupSIMassHunter.exe	C:\MassHunter\Library\{libraryname}\{filename}
MS Search	SetupSIMSSearch.exe	C:\NIST20\MSSEARCH\{libraryname}\{filename}
TurboMass	SetupSITurboMass.exe	C:\TurboMass\ldendb\{filename} C:\TurboMass\ldendb\STRUCTDB\{libraryname}\{filename}
GCMSsolution	SetupSIGCMS_Solution.exe	C:\GCMSsolution\Library\{libraryname}\{filename}
MassLynx	SetupSIMassLynx.exe	C:\MassLynx\ldendb\{filename} C:\MassLynx\ldendb\STRUCTDB\{libraryname}\{filename}

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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46256 USA

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.

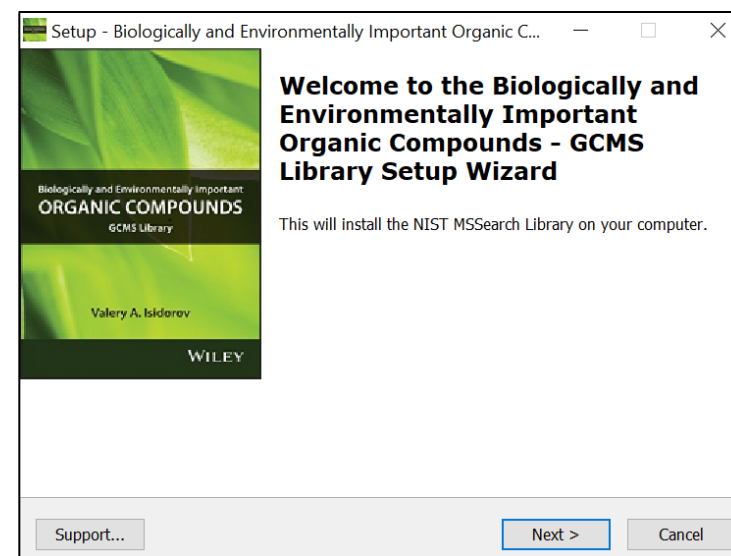
Step 2. Insert the flash drive for installation. One file "Installation.htm" is included on the flash drive to simplify installation by using your web browser. Choose the format(s) you wish to install. Choosing to run the installer will bring you to a set-up wizard splash screen. Choose "Next."

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.

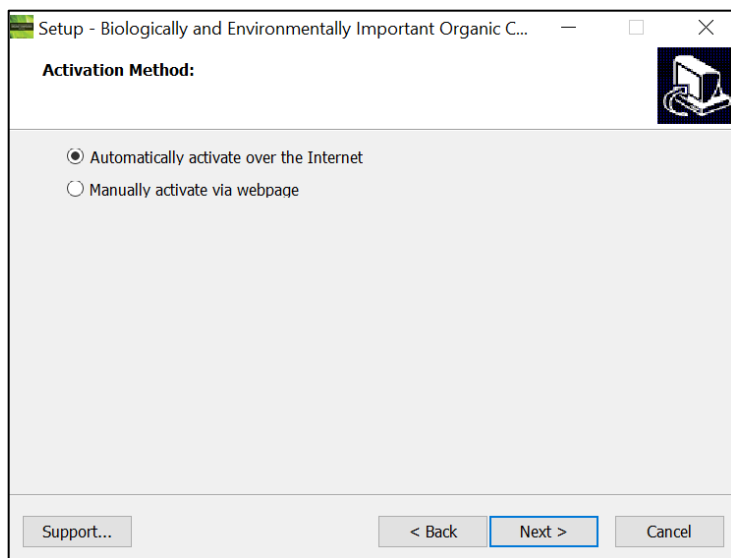
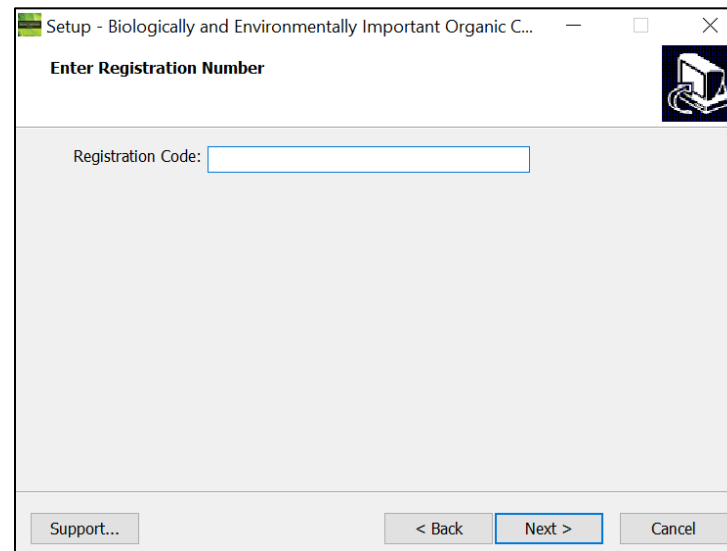


Step 3. Registration Code and Machine ID

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.

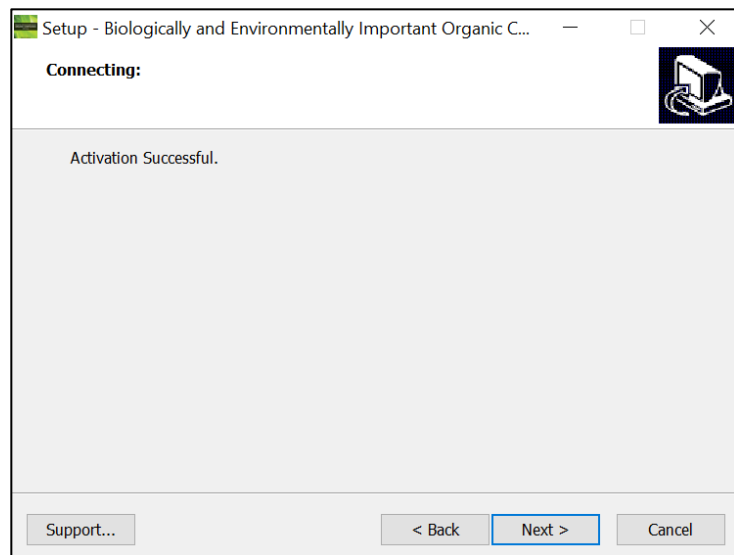
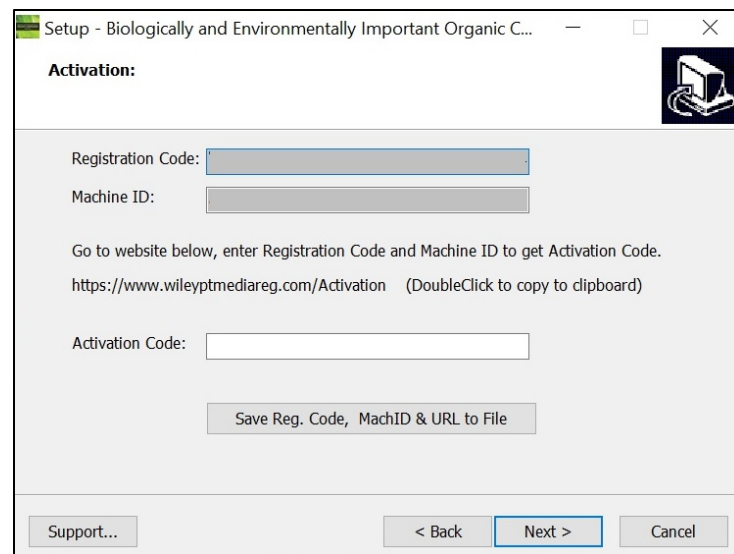
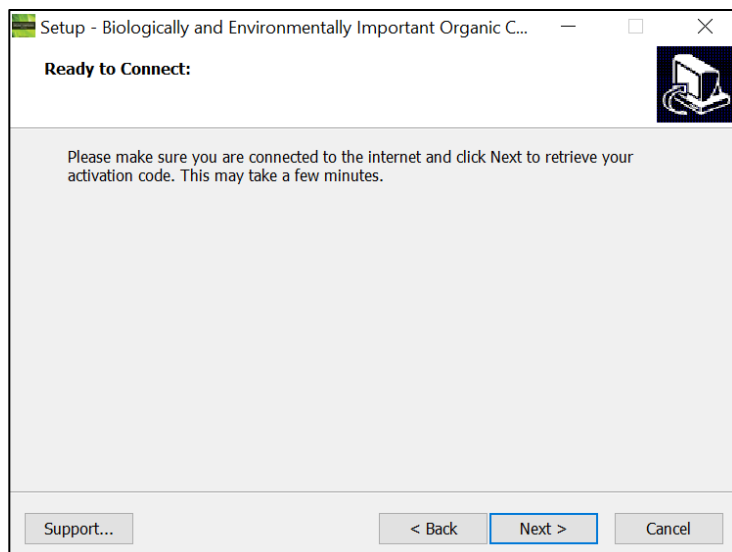
If the **Registration Code** is correct, you will be brought to the Activation screen. If your machine has internet connectivity, choose to "Automatically activate over the internet" and then click "Next" to begin internet activation.



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.

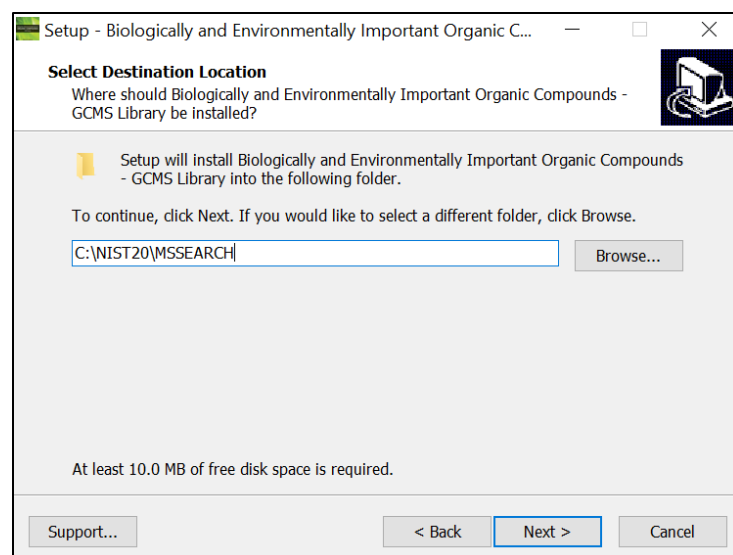
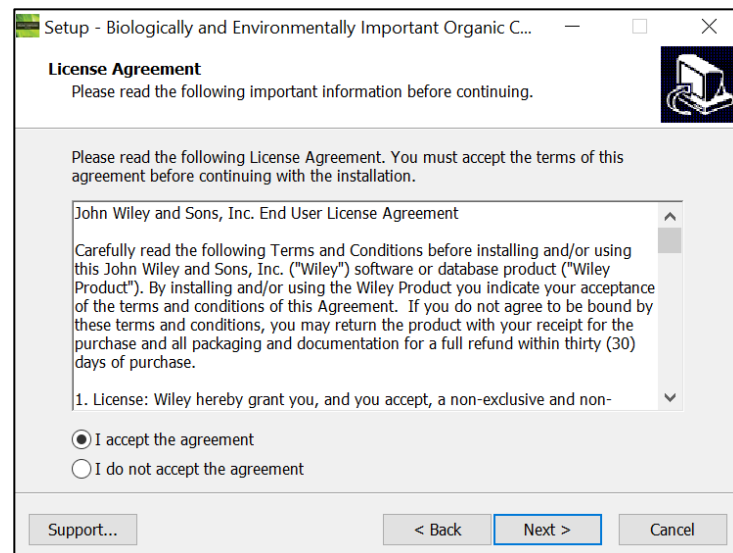
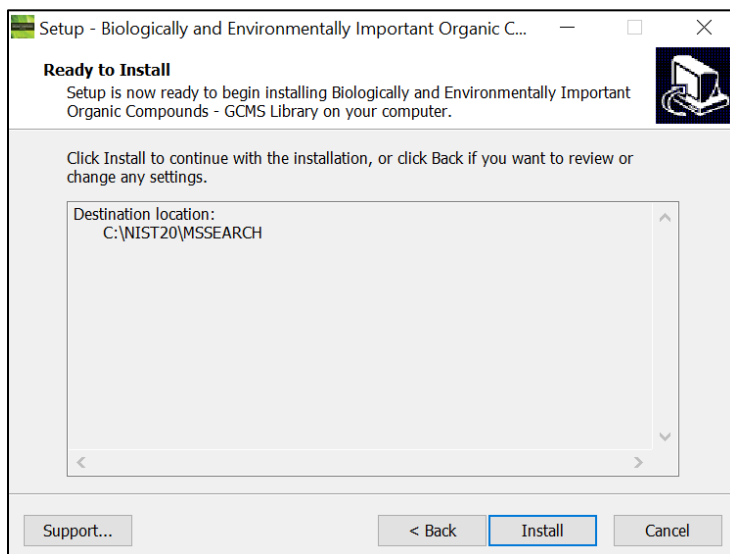


Step 5. Once your activation is successful, proceed by pressing “Next.” The next screen contains the End User License Agreement (19). Read the agreement carefully and select the “I accept the agreement” option. Then, choose “Next” to proceed to install the library. Spectral libraries should only be used 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.

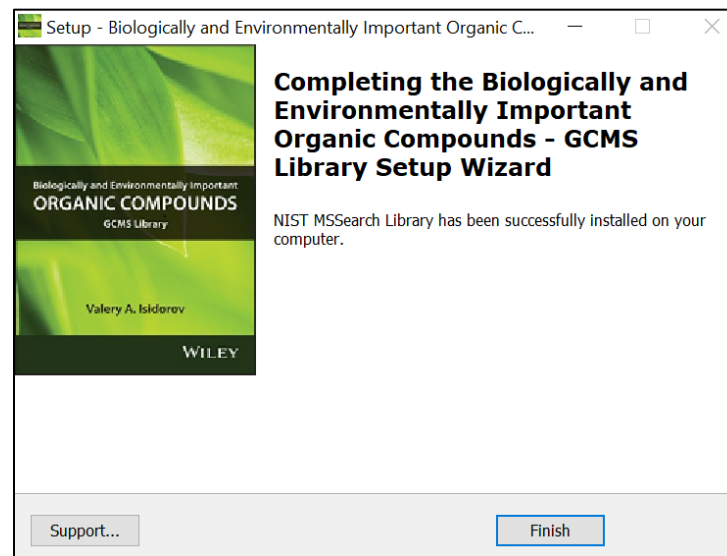
N.B.: For Chrome and Firefox browsers, copy the install file onto a temporary directory. The installer requires RegistrationProcess.dll. Please copy the installer and dll into one directory and activate the installer.



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.

Spectra in this database are accompanied by an RI value, CAS number (if available), molecular and structural formula, formula weight, chemical name and list of synonyms, as well the source of compounds used for registration of spectrum and RI value. Compounds studied include essential oils and extracts from plant tissues, food products, environmental and industrial samples, etc.

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 the *Wiley Registry 12th Edition/NIST 2020 Mass Spectral Library* and a specialized library such as the *Biologically and Environmentally Important Organic Compounds: GCMS Library*.

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:

The 'Comment' line contains the following items (which could be made to appear on separate lines via the 'Tags in Comments' functionality):

- WileyID
- RI_HP5 – Retention Index values (measured on 'HP5' columns)
 - These are also indexed as 'Semi-Standard Non-Polar' and appear therefore in the 'Experimental RI' section (and could be used when spectrum searching).
- RI_aver – Averaged RI values
- Source – Source of spectrum

To the Synonyms field, the PCN and PCN Synonyms are added (PCN = Parent Compound Name).

Agilent ChemStation/MassHunter:

Comment field contains:

- WileyID
- RI_HP5 and RI_aver values
 - RI_HP5 values given in Retention Index field.
 - RI_aver values given in the User Index field.
- Source information
- Indication if a pseudo CASRN is used.
 - Pseudo CASRN are of form '999xxx-xx-x' (i.e. 9-digit CASRN starting with '999'). Pseudo CASRN also used for (replacing) four 10-digit CASNOs.

Shimadzu GCMSsolution:

Names and synonym names added to the name field, separated by ' \$\$ '.

RI values given in 'Ret Index:' field are 'HP5' Retention Index values.

- These are Semi-Standard Non-Polar Retention Index values.

PerkinElmer TurboMass/Waters MassLynx:

RI_HP5 and RI_aver values

- RI_HP5 values given in 'Value 1' field.
- RI_aver values given in the 'Value 2' field.

Indication if a pseudo CASRN is used.

- Pseudo CASRNs are of form '999xxx-xx-x' (i.e. 9-digit CASRNs starting with '999').
- Pseudo CASRN also used for (replacing) four 10-digit CASNOs.

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 a 9-digit number prefixed by 999 for Agilent ChemStation/MassHunter and PerkinElmer TurboMass/Waters MassLynx.**

Please note that 9-digit IDs prefixed with the numbers 999 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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