

USER MANUAL

VERSION 1.1



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 Please do not print this manual.

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PUBLISHER'S NOTE

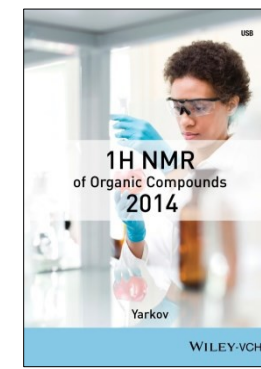
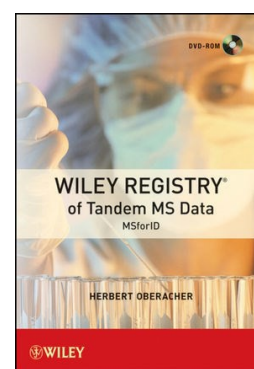
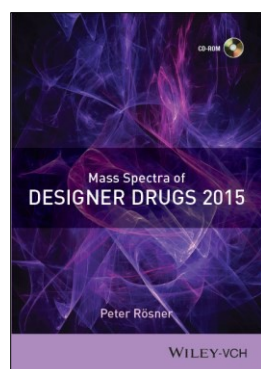
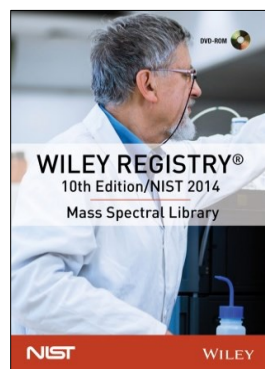
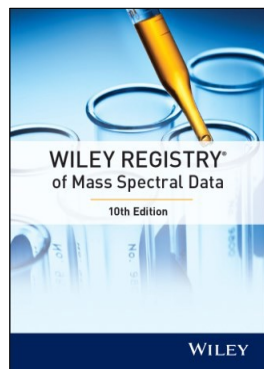
For over 45 years, John Wiley and Sons has worked with the world's leading researchers and practitioners to deliver the spectral libraries mass spectrometrists have come to rely on as the gold standard in mass spectrometry. Dr. Luigi Mondello continues this tradition with a highly controlled measurement of flavors and fragrances on a variety of columns, with a variety of linear retention index.

This latest edition contains:

- 3,462 Spectra of compounds of interest for fragrance and flavors research
- 3,462 Searchable Chemical Structures
- Multiple LRI measurements and calculated Kovats RI values per compound

ACKNOWLEDGEMENTS

Edited and compiled by Dr. Luigi Mondello



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.

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

E-mail: dbinquiry@wiley.com

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

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<https://hub.wiley.com/community/support>

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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 (Windows7 or later)
- CPU: AMD or Intel processor, preferably multiple core
- Memory: 2GB
- Disk Space: At least 2GB free discspace
- Software: 32-bit or 64-bit software

The library is provided in multiple native manufacturer 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 disc, please contact Wiley Customer Care at <https://hub.wiley.com/community/support>. Shimadzu format for this database is available exclusively through Shimadzu Instruments.

REGISTRATION CODE

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

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COMPATIBILITY

Wiley has provided you with a broad 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 DVD contains the following manufacturer formats:

- ACD/Labs MS Manager
- Agilent ChemStation
- AgilentMassHunter
- Bruker
- Cromatoplus
- JEOL
- Leco
- NIST MS Search
- Thermo Xcalibur
- PerkinElmer TurboMass
- Waters MassLynx

MS Search (NIST) is compatible with most manufacturer software systems. Consult your software manufacturer's manual to determine compatibility.

DIRECTORY ASSISTANCE

The table below lists the formats, installation files, and their default target directories. 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	SetupFFNSC3ChemStation.exe	C:\DATABASE\FFNSC3.L\ C:\DATABASE\FFNSC3.L\STRUCTDB\
MassHunter	SetupFFNSC3MassHunter.exe	C:\MassHunter\Libraries\FFNSC3.L C:\MassHunter\Libraries\FFNSC3.L\STRUCTDB\
MassLynx	SetupFFNSC3MassLynx.exe	C:\MassLynx\Idendb\ C:\MassLynx\Idendb\StructDB\FFNSC3\
MS Manager	SetupFFNSC3SpecManager.exe	C:\Program Files\ACD2015\DATABASE\
MS Search	SetupFFNSC3MSSearch.exe	C:\NIST14\MSSEARCH\FFNSC3\
TurboMass	SetupFFNSC3TurboMass.exe	C:\TurboMass\Idendb\ C:\TurboMass\Idendb\Structdb\FFNSC3\
Thermo Xcalibur	SetupFFNSC3XCalibur.exe	C:\Program Files\NISTMS\MSSEARCH\FFNSC3

QUICK-START

1. Registration Code: After reading the EULA contained in the DVD packaging, note 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://hub.wiley.com/community/support> or by telephone at (877) 762-2974.

3. INSTALLATION: Please note installation requires the **Registration Code** that accompanied your disc 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.
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46256 US

STEP-BY-STEP INSTALLATION



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

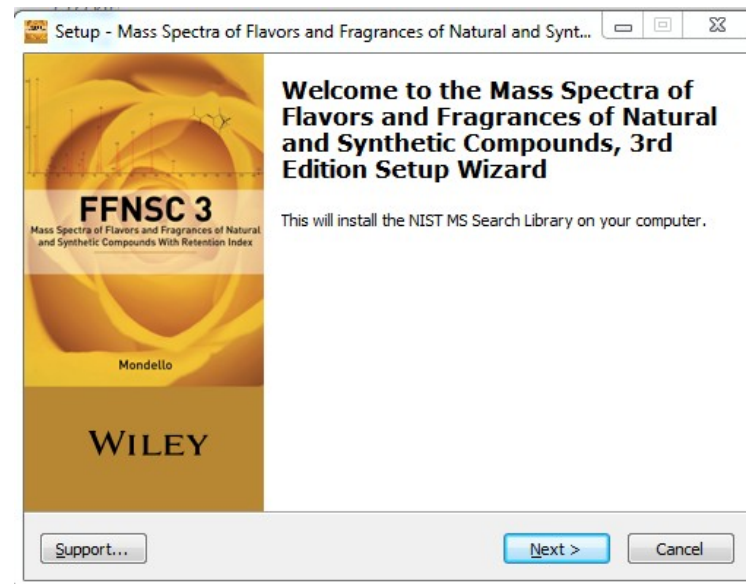
You will be unable to install this library without a **Registration Code**. Carefully read the End User License Agreement contained on the disc or the accompanying packaging before using and/or installing this product.

Step 2. Enter the disc for installation. One file "installation.htm" is included on the disc 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 setup 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 chromatography data software prior to installing the format(s) you wish to install.

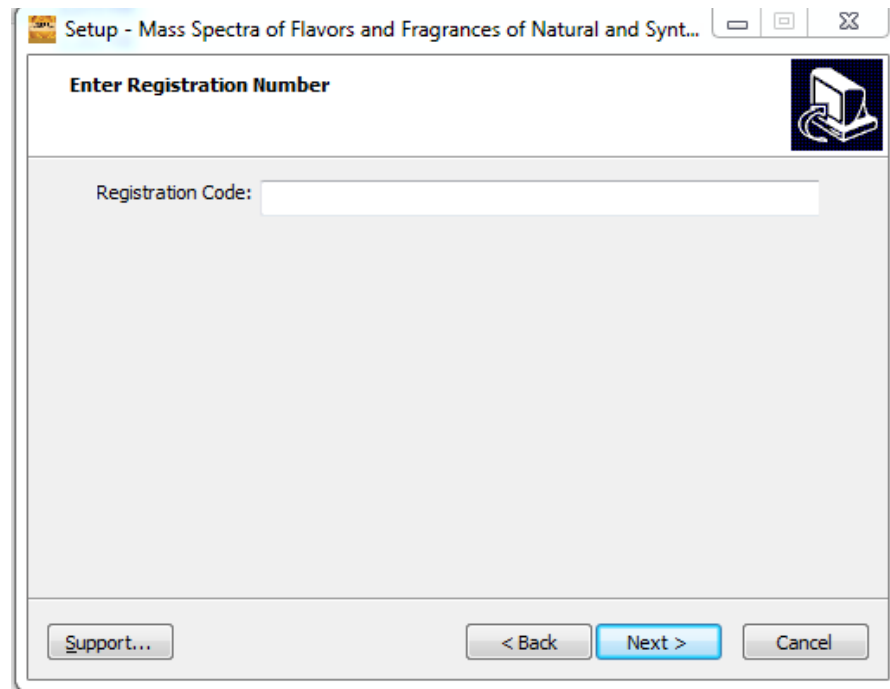
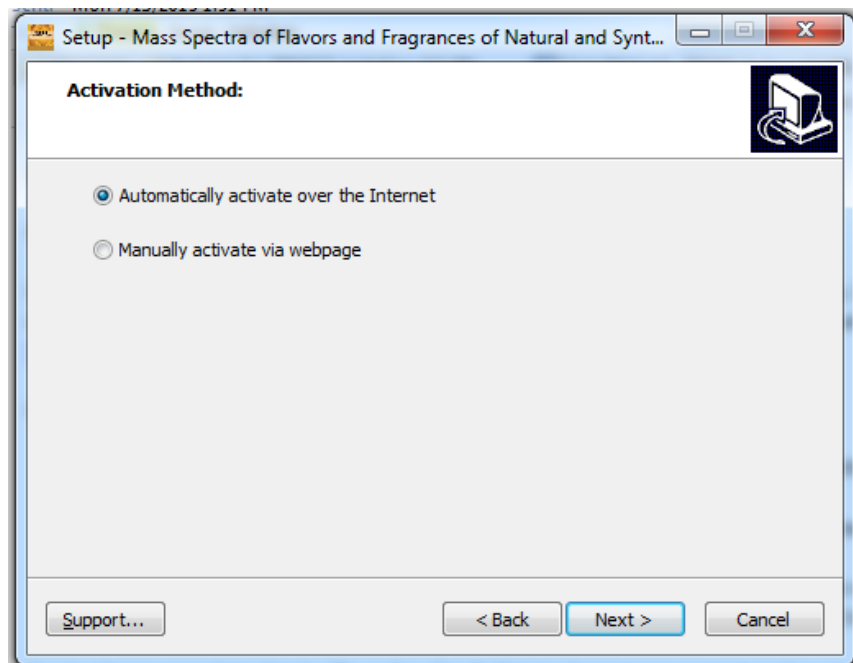


Step 3. Registration Code and Machine ID

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.

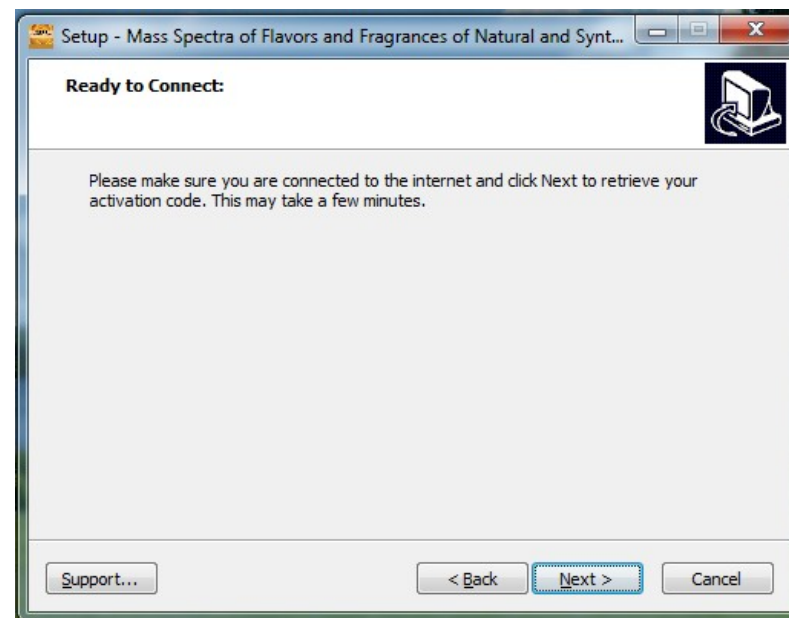
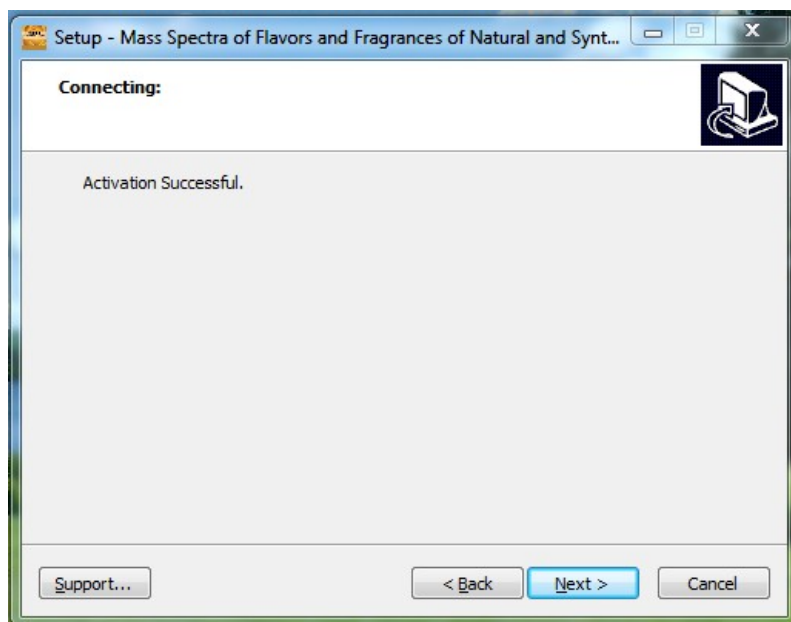
If the **Registration Code** is correct, you will be brought to the Activation screen. If your machine has internet connectivity, choose to “Automatically activate over the Internet” and then click “Next.”



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.

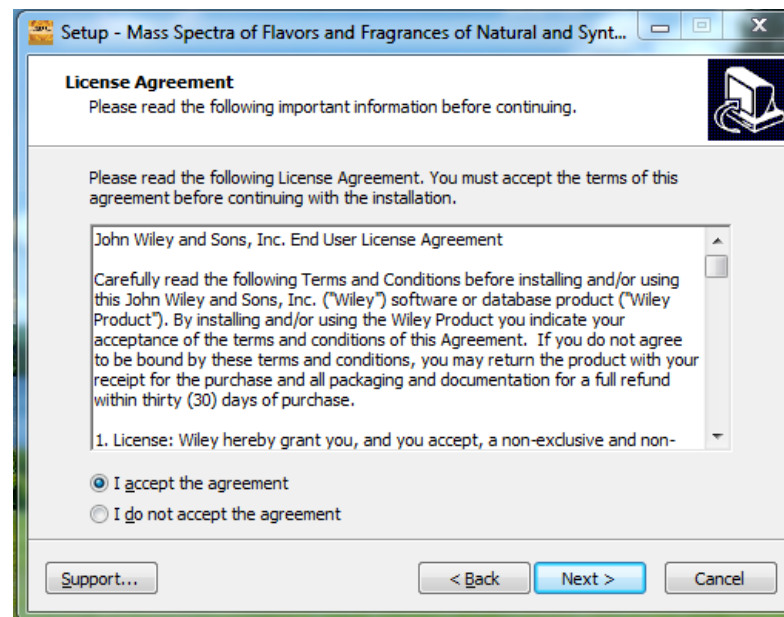
Alternatively, you may save the **Registration Code**, Machine ID, and URL to a text file that will be saved to the root directory.

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 Activation screen on the computer that you are installing the spectral library on.



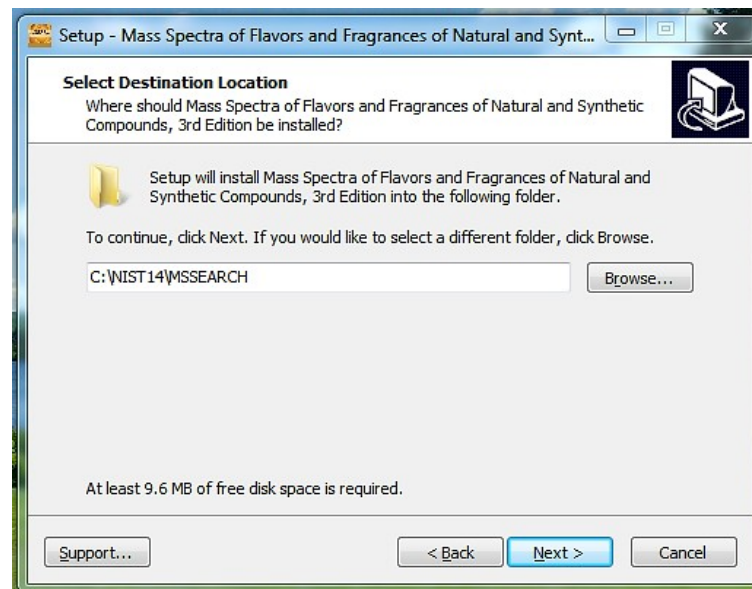
Step 5. Once your activation is successful, proceed by pressing “Next.” The next screen contains the End User License Agreement (18).

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.



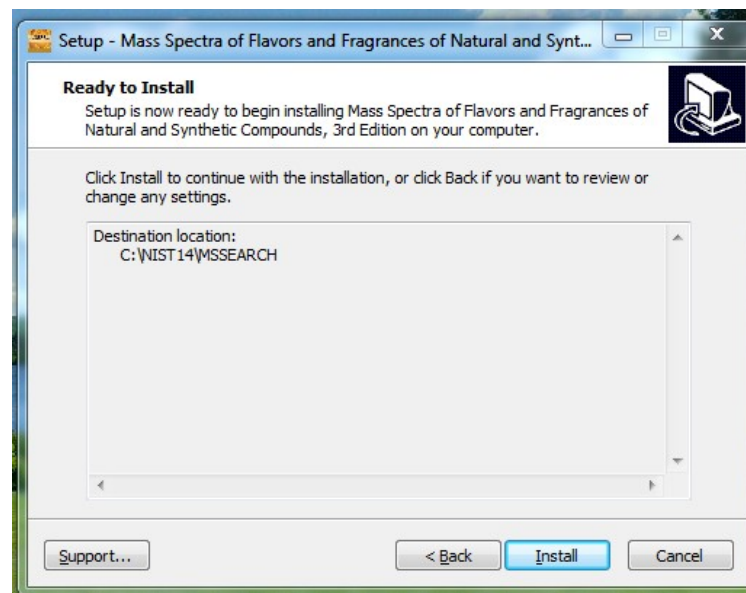
Step 6. At this point, the installer will unpack and install the library in the format you have selected.

Confirm the target directory and destination location and choose “Next.”



Step 7. Ready to install? After selection of the destination folder, click the “Install” button to begin installation. Allow installation to finish before closing out any applications.

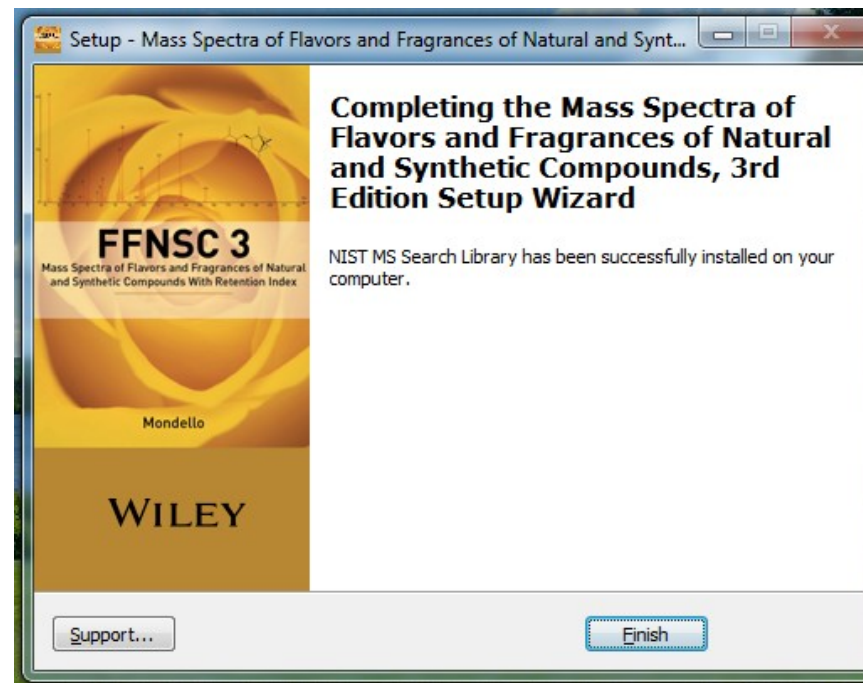
N.B.: For Chrome and Firefox browsers, copy the install file onto a temporary directory. The installer requires RegistrationProcess.dll. Please copy the installer and dll into one directory and activate the installer.



Step 8. Once installation is complete, press “Finish.” Be sure to consult your mass spectrometry 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://hub.wiley.com/community/support>

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 10th Edition – A complete, general-purpose high-quality library for analytical laboratories. Often used as the foundation library for research, quality control, deformation, and for forensic, toxicology, and homeland defense applications.

Wiley Registry 10th/NIST 2014 – 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/> or 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 10e/NIST 2014 Mass Spectral Library and a specialized library such as FAMEs.

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 MSSearch, this approach will not work.

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, NIST/EPA/NIH, and other mass spectral libraries are not in the CAS Registry or 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 number is prefixed with the number 999000.

Please note that IDs prefixed with the number 999000 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.

To read more about more modern methods of compound identification, please go to <http://www.inchitrust.org/>.

DATA SUBMISSIONS

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:

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- Tandem MS (MS^n)
- 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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