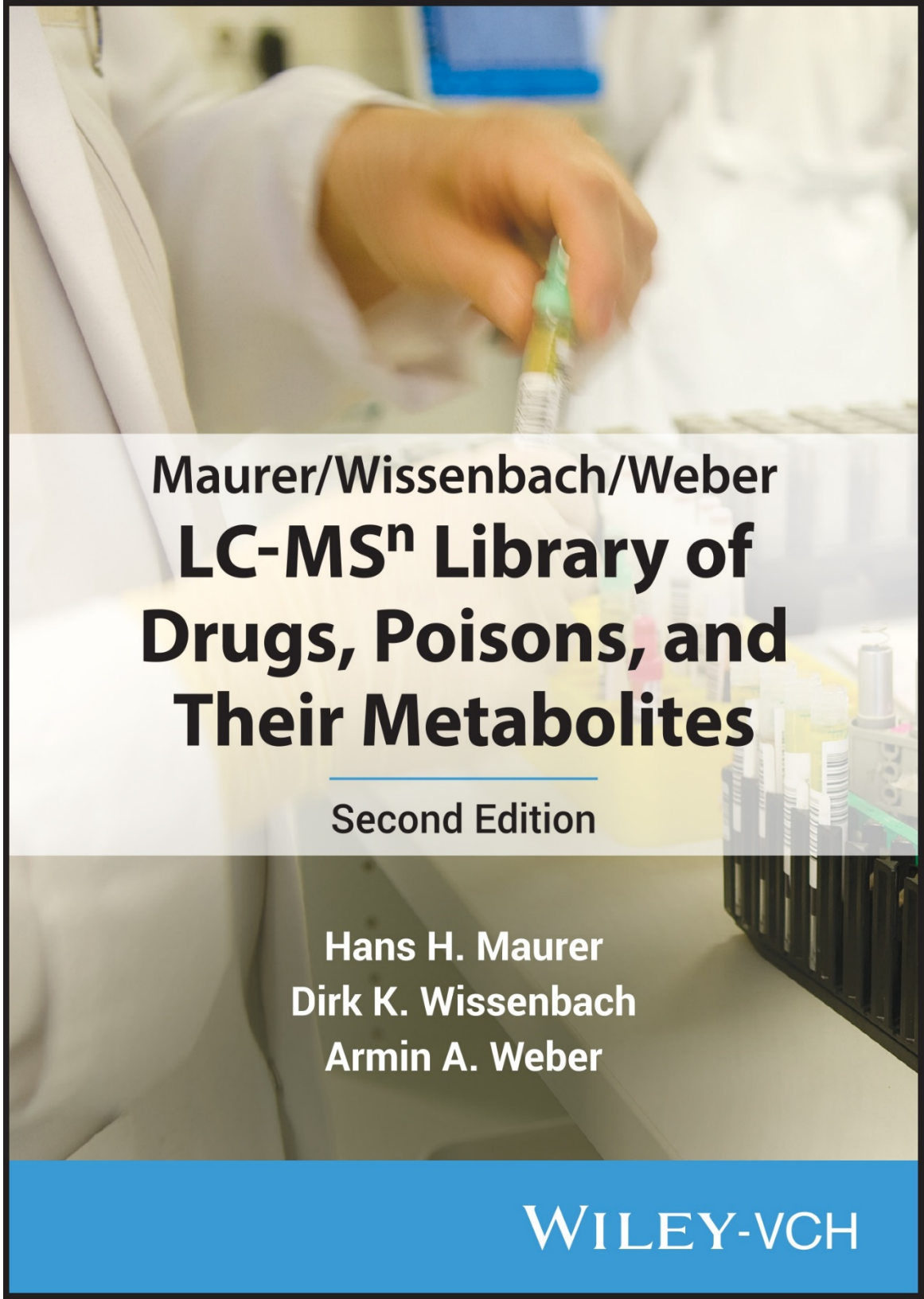
USER MANUAL

VERSION 1.0



Wiley-VCH, Weinheim, Germany

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Please do not print this manual.

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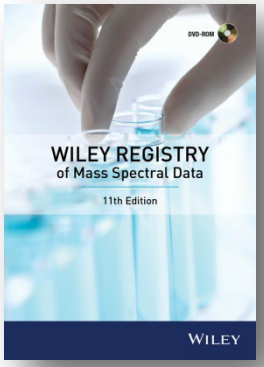
For over 45 years, John Wiley and Sons and Wiley-VCH have worked with the world's leading researchers and practitioners to deliver the spectral libraries mass spectrometrists have come to rely on as the gold standard in mass spectrometry.

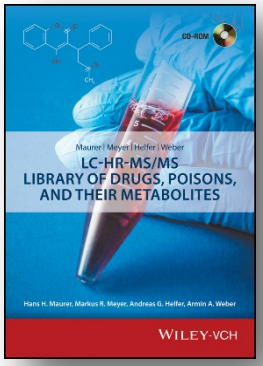
The ***Maurer/Wissenbach/Weber LCMS^n Library of Drugs, Poisons, and Their Metabolites, Second Edition*** provides a proven metabolite-based LCMS^n screening method and MS^2 and MS^3 spectra of over 2,270 parent compounds and over 3,600 of their metabolites. Detection of metabolites increases the sensitivity, detection window and selectivity, allows confirmation of the body passage, and minimizes the risk of false negative LC-MS results possibly caused by ion suppression of the target analyte. Even the risk of false positive results can be reduced considering the metabolite patterns.

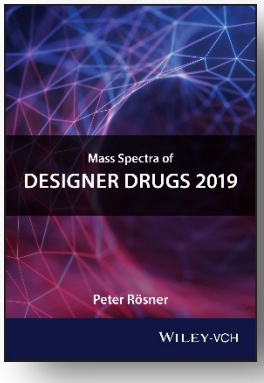
COMPOUND SEARCH

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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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 7, Windows 8, Windows 10)
* 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 disc, please contact Wiley Customer Care at https://hub.wiley.com/community/support.

REGISTRATION CODE

A registration code accompanies the packaging provided with the DVD. 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:

- Bruker Toxtyper™ 2.0
- NIST MS Search
- Thermo Scientific™ Xcalibur

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 and 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
Bruker	SetupMWWtox2019Bruker.exe	D:\Data\Libraries\{MWWtox2019.mlb}
NIST MS Search	SetupMWWtox2019NISTMSSearch.exe	C:\NIST17\MSSEARCH\{MWWtox2019}
Thermo	SetupMWWtox2019Thermo.exe	C:\Program Files (x86)\NistMS\MSSearch\{MWWtox2019}

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://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.
Indianapolis, IN 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 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**.

Step 2. Carefully read the End User License Agreement contained on the disc or the accompanying packaging before using and/or installing this product.

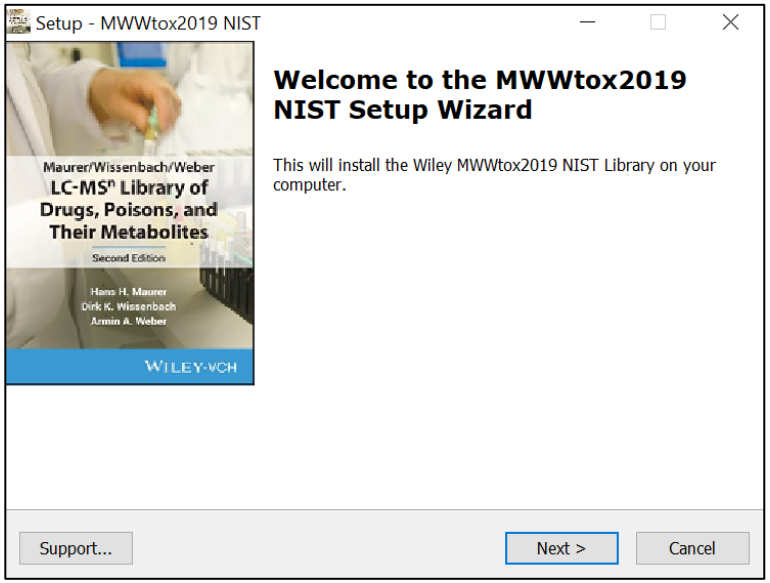
Step 3. Enter the disc for installation. One file "Installation.htm" is included on the disc to simplify installation by using your web browser. Choose the format(s) you wish to install. Choosing to run the installer will bring you to a setup wizard splash screen. Choose "Next."

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 mass spectrometry software prior to installing the format(s) you wish to install.

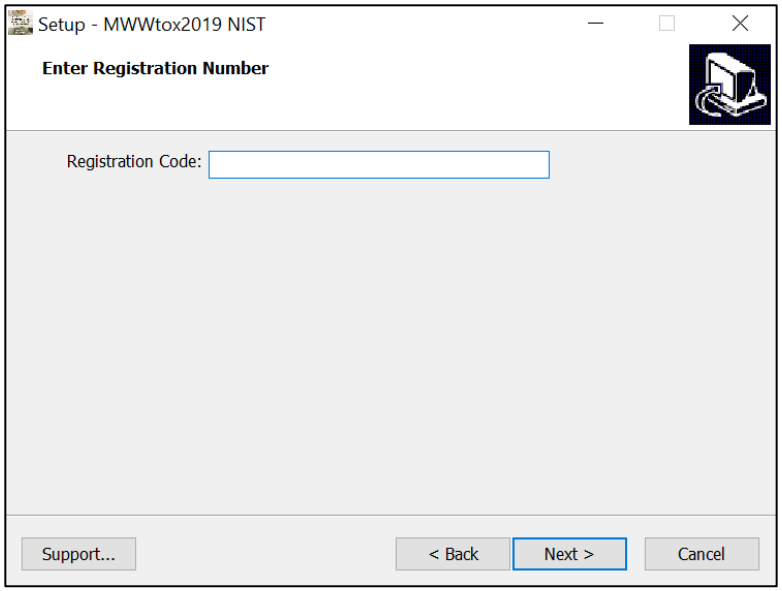


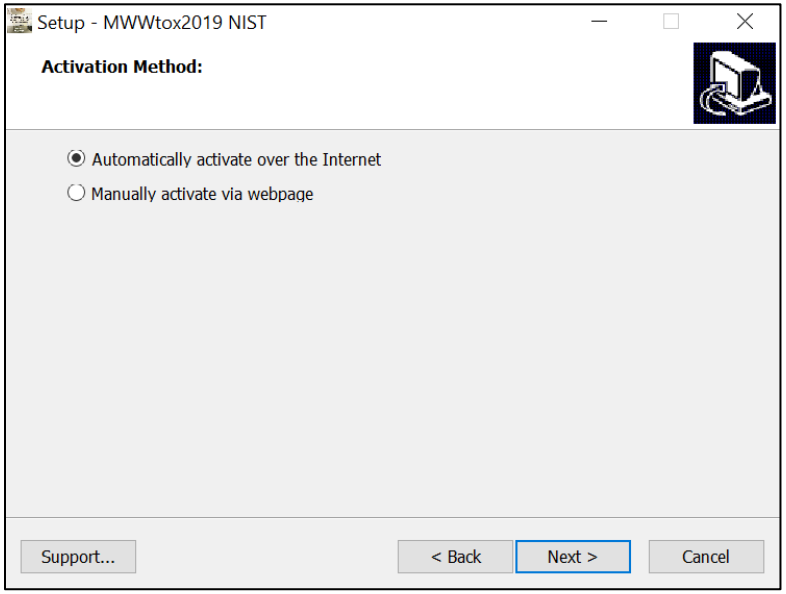
Step 4. Registration Code and Machine ID

Choosing to run the installer will bring you to a splash screen. Choose "Next." Your **Registration Code** appears on the instructions 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.

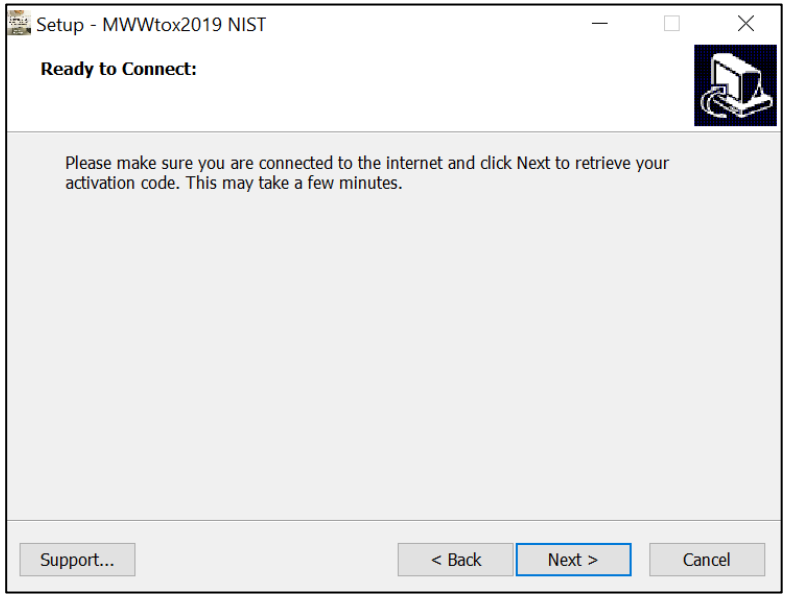
If the **Registration Code** is correct, you will be brought to the Activation screen. If your machine has internet connectivity, choose to "Automatically activate over the internet" and then click "Next" to begin internet activation.



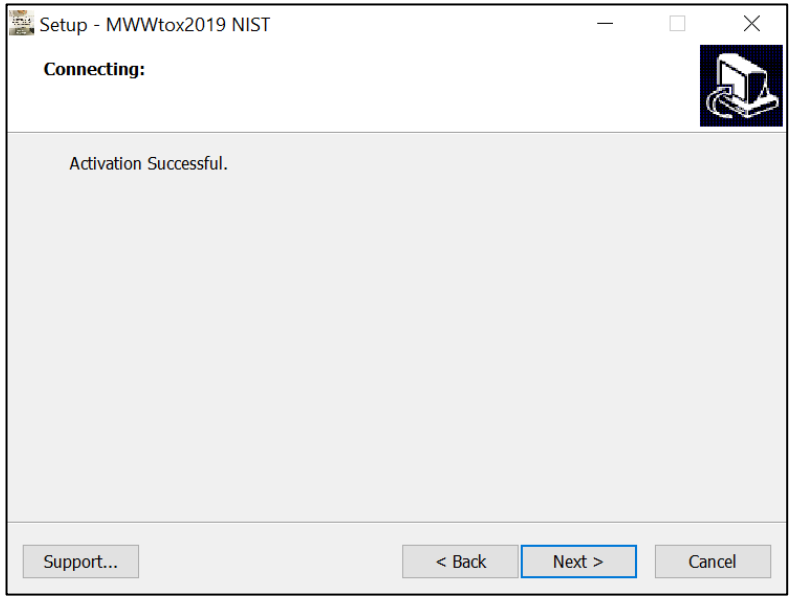


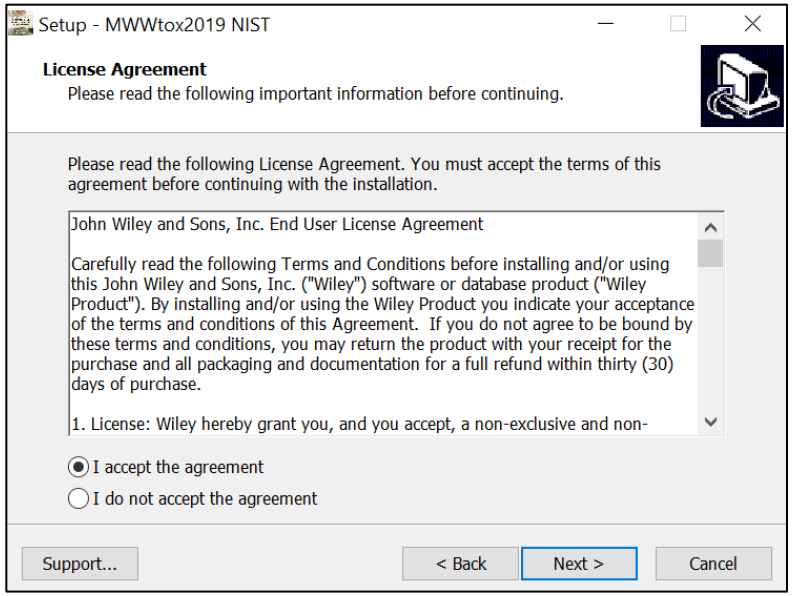
Step 5. If you choose to manually activate, the **Registration Code** and the Machine ID will be automatically filled in. You may either double click the web address to copy it to your computer's clipboard and paste it in a web browser, or enter the URL as listed in your web browser.

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 6. 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.



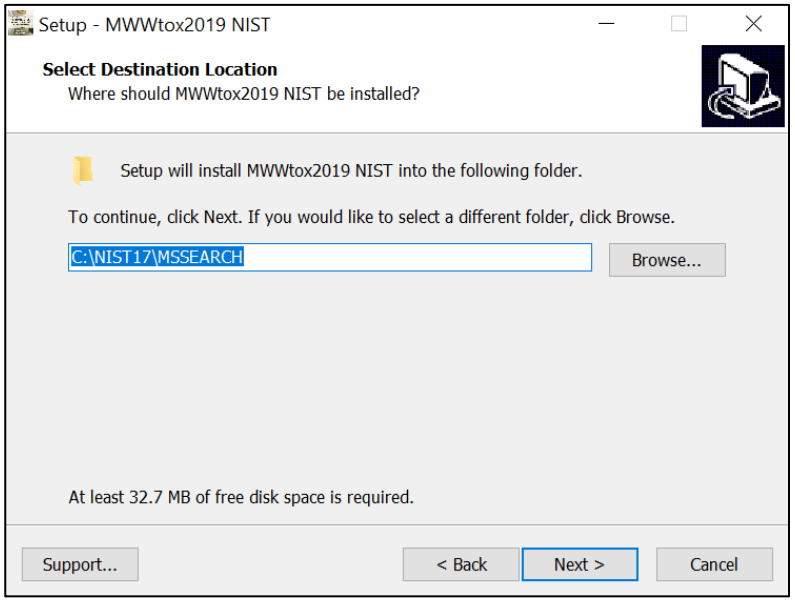


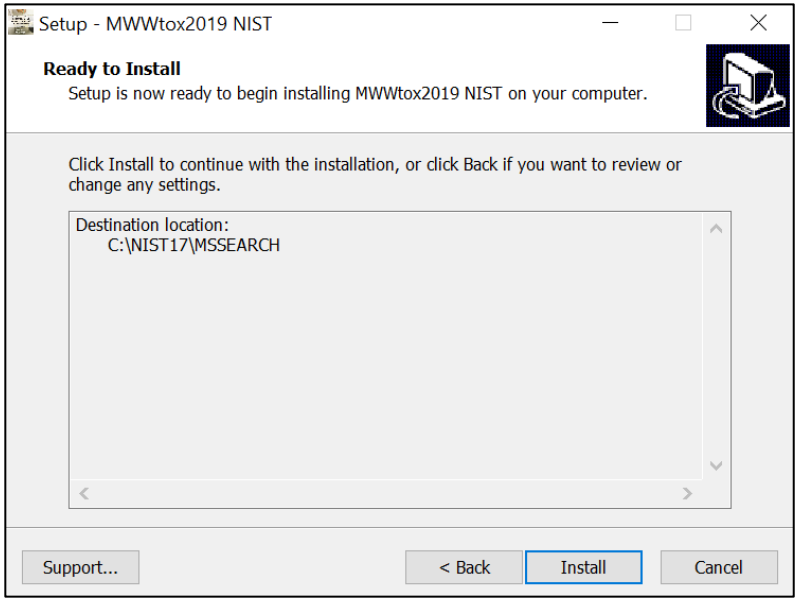
Step 7. Press "Next" to proceed to the next step. At this point, the installer will unpack and install the library in the format you have selected.

Confirm the target directory and destination location before proceeding.

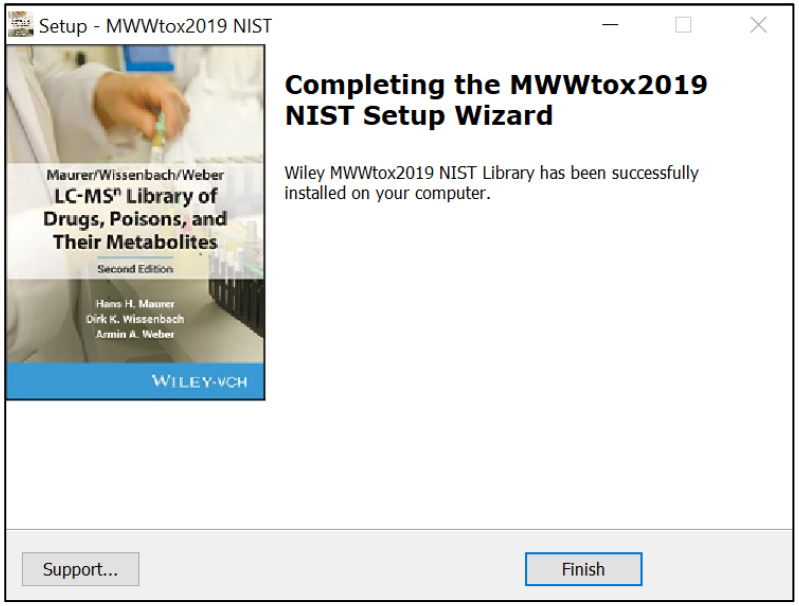
Step 8. Ready to install? After selection of the Destination Folder, choose the "Install" button to begin installation. Allow installation to finish before closing out any applications.

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 9. 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

GENERAL DATABASE CONTENT

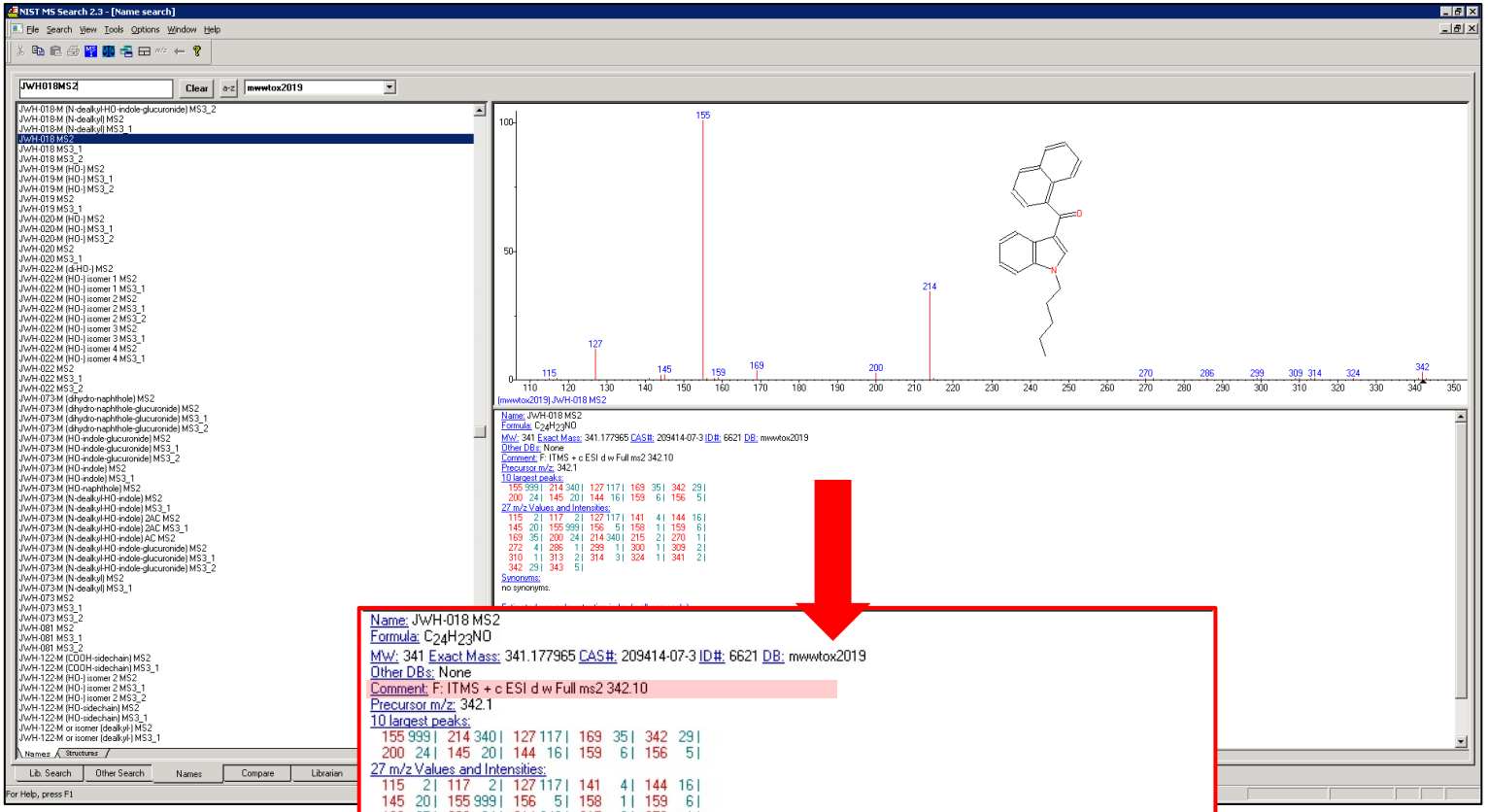
Wiley mass spectrometry libraries have a wide variety of uses. Practitioners and researchers are encouraged to evaluate their own needs and decide what libraries are appropriate for them.

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 11th/NIST 2017 Mass Spectral Library* and a specialized library such as this library or *MS and GC Data of Drugs, Poisons, Pesticides, Pollutants, and Their Metabolites.*

SEARCH TIPS


NIST MS Search 2.3 - [Name search]
File Search View Tools Options Window Help
JWH018MS2
Clear
mwwtox2019
JWH-018 MS2
Lib. Search
Other Search
Names
Compare
Librarian
For Help, press F1
Name: JWH-018 MS2
Formula: C24H23NO
MW: 341 Exact Mass: 341.177965 CAS#: 209414-07-3 ID#: 6621 DB: mwwtox2019
Other DBs: None
Comment: F: ITMS + c ESI d w Full ms2 342.10
Precursor m/z: 342.1
10 largest peaks:
155 999 | 214 340 | 127 117 | 169 35 | 342 29 |
200 24 | 145 20 | 144 16 | 159 6 | 156 5 |
27 m/z Values and Intensities:
115 2 | 117 2 | 127 117 | 141 4 | 144 16 |
145 20 | 155 999 | 156 5 | 158 1 | 159 6 |
169 35 | 200 24 | 214 340 | 215 2 | 270 1 |
272 4 | 286 1 | 299 1 | 300 1 | 309 2 |
310 1 | 313 2 | 314 3 | 324 1 | 341 2 |
342 29 | 343 5 |
Synonyms:
no synonyms.
Estimated non-polar retention index (n-alkane scale):
Value: 2989 iu
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu
Retention index.
1. Value: 3253.9 iu
Column Type: Capillary
Column Class: Semi-standard non-polar
Active Phase: VF-5MS
Column Length: 35 m
Carrier Gas: He
Column Diameter: 0.25 mm
Phase Thickness: 0.25 um
Data Type: Linear RI
Program Type: Complex
Description: 60C(1min)[20C/min]200C[5C/min]300C(12min)
Source: Tretyakov, K.V., Retention Data. NIST Mass Spectrometry Data Center., 2015.

SEARCH TIPS

The comment row provides additional information. This is summarized by “ITMS + c ESI d w Full ms2 342.10”. An ion trap MS (ITMS) working with electrospray ionization (ESI) in positive ionization mode (+) was used to provide a centroid (c) data dependent (d) full scan (Full) MS/MS (MS2) product ion spectrum on the measured M+H mass of the compound (here m/z 342.10) by wideband activation (w) collision-induced dissociation fragmentation using 35% normalized collision energy. Precursor information of the MS/MS spectrum is extracted by the software based on information given by the comment row and is stored in the corresponding field.

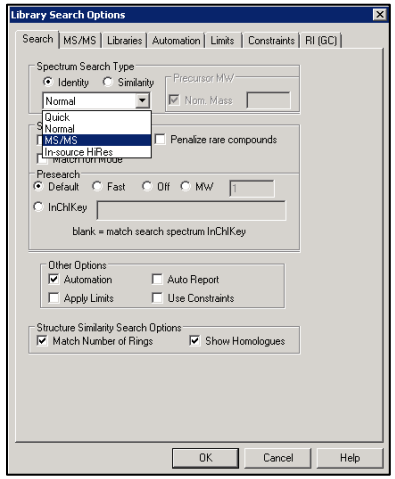
When using parametric searching, many text search programs provide better results when names are begun and ended with wild cards (e.g., “*”). However, in NIST MS Search, this approach will not work.

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.

LC-MS^n libraries should be searched using specialized MSMS search algorithms, which generally provide superior results.

Operating on NIST instrumentation software? This library contains LC-MS^n data. For best results in NIST software, **ensure that search settings are set to MS/MS.**

Operating on Bruker or Thermo instrumentation software? Please consult the documentation that accompanied your software.



DATABASE DATA DESCRIPTION

In general, one MS^2 and two MS^3 spectra (most and second most abundant MS^2 fragment) were stored in the library for each compound. Based on the compound structure some compounds (e.g. trimipramine) do not provide a second reproducible MS^3 spectrum under the used MS conditions. The library entries for those compounds consist of one MS^2 and one MS^3 spectrum. As according to instrument variations (36) and the CID fragmentation properties of each compound, a third MS^3 was stored for some compounds (e.g. morphine). Consequently, one MS^2 and three MS^3 spectra are stored in the database for those compounds.

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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 (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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