

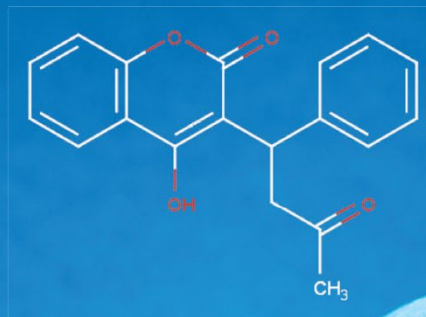
MMHW LC-HR-MS/MS Library

USER MANUAL

VERSION 1.3

USER MANUAL

VERSION 1.3



Maurer | Meyer | Helfer | Weber

LC-HR-MS/MS LIBRARY OF DRUGS, POISONS, AND THEIR METABOLITES

Hans H. Maurer, Markus R. Meyer, Andreas G. Helfer, Armin A. Weber

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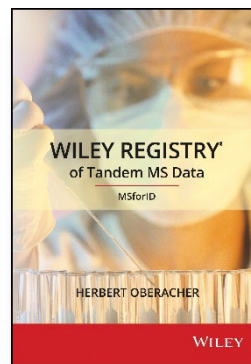
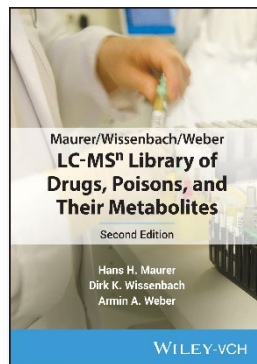
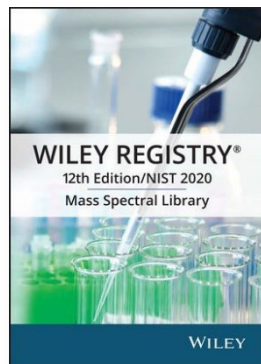
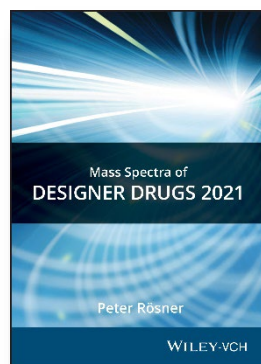
For over 45 years, John Wiley and Sons and Wiley-VCH have worked with the world's leading researchers and practitioners to deliver the spectral libraries mass spectrometrists have come to rely on as the gold standard in mass spectrometry.

A major goal in clinical, forensic, and doping laboratories is a broad screening procedure for detection of toxic compounds or drugs of abuse. LC-high-resolution-tandem mass spectrometry (LC-HR-MS/MS) provides various advantages for screening approaches such as higher versatility, sensitivity and specificity. Detection of metabolites increases selectivity, allows confirmation of the body passage, and finally, minimizes the risk of false negative LC-MS results possibly caused by ion suppression of the target analyte. The *Maurer/Meyer/Helfer/Weber: LC-HR-MS/MS Library of Drugs, Poisons, and Their Metabolites* library provides spectra for over 2,000 parent drugs or poisons and over 3,000 of their metabolites or artifacts making it the basis for metabolite-based screening procedures for various drug classes. With over 5,000 spectra and retention index values for over 125 different compound classification groups, the MMHW mass spectral library is an invaluable tool for clinical and forensic research.

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 of compounds, especially novel compounds not presently covered in the spectral library. Wiley can handle data in any machine-readable format. Data submissions, editorial notes, 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

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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 anyformat.

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 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 flash drive contains the following manufacturer formats:

- Bruker DataAnalysis 5.3
- Bruker MetaboScape®
- NIST MS Search
- Shimadzu LabSolutions
- Thermo Scientific™ TraceFinder™
- Waters UNIFI

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
Bruker DataAnalysis 5.3	SetupMMHWBruker-DataAnalysis.exe	D:\Data\Libraries\{libraryname}
Bruker MetaboScape	SetupMMHWBruker-MetaboScape.exe	D:\Data\Libraries\{libraryname}
NIST MS Search	SetupMMHWMSSearch.exe	C:\NIST17\MSSearch\{libraryname}
Shimadzu LabSolutions	SetupMMHWShimadzu-LS.exe	C:\LabSolutions\MSLibrary\{libraryname}
Thermo TraceFinder	SetupMMHWTraceFinder.exe	C:\Thermo\Shared\Spectral Libraries\{libraryname}
Waters UNIFI	SetupMMHWWaters-Unifi.exe	C:\Wiley Databases\{libraryname}

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 Installation Key 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 contact them by telephone at (877) 762-2974.
- 3. Warning:** Please note installation consists of setup*.exe and registrationprocess.dll. Attempting to install from a hard drive using the *setup.exe will require the presence of the registrationprocess.dll

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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.

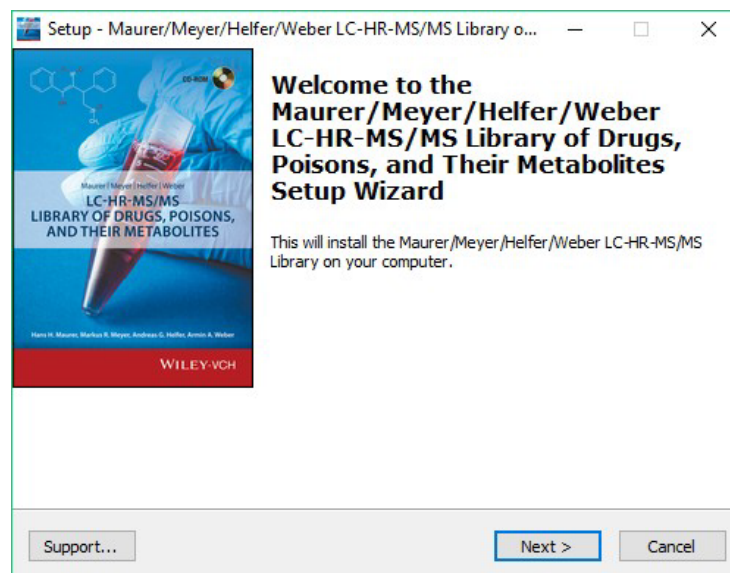
Step 2. Insert the flash drive for installation. One file "Installation.htm" is included on the flash drive to simplify installation by using your web browser. Choose the format(s) you wish to install. Choosing to run the installer will bring you to a set-up wizard splash screen. Choose "Next."

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.

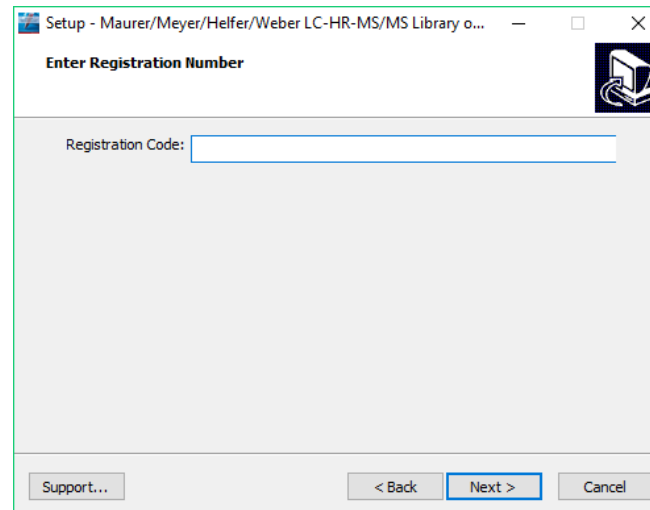
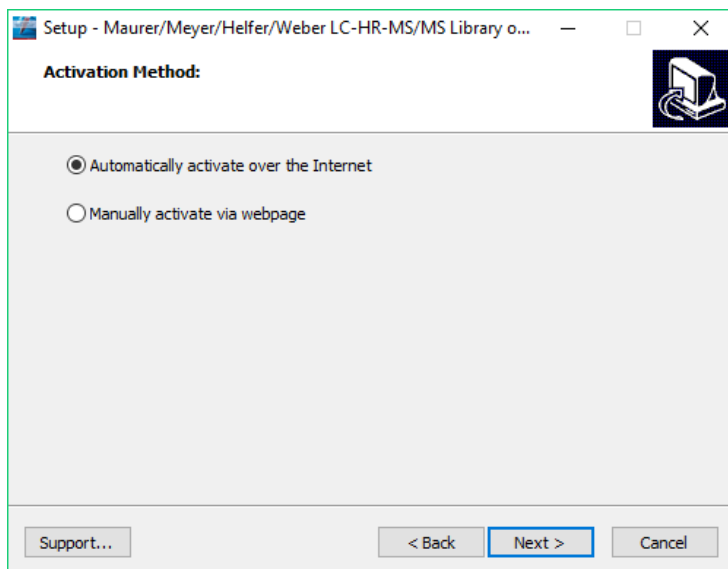


Step 3. Registration Code and Machine ID

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.



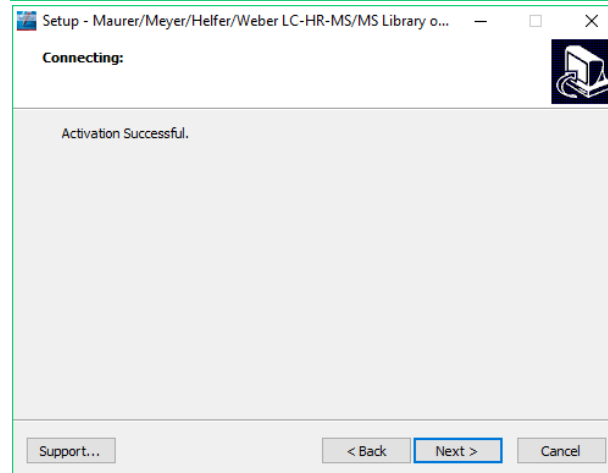
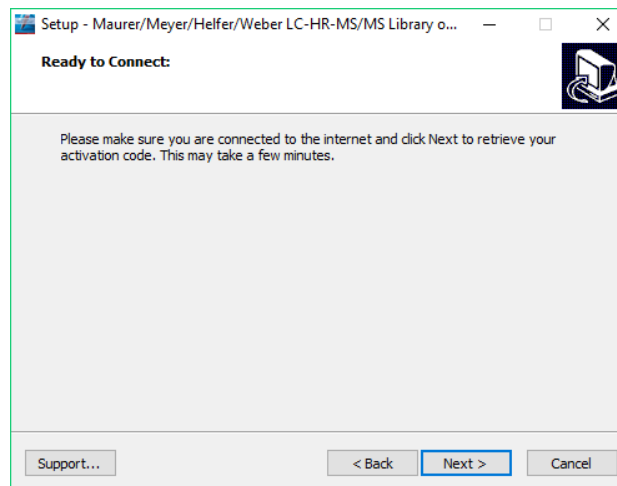
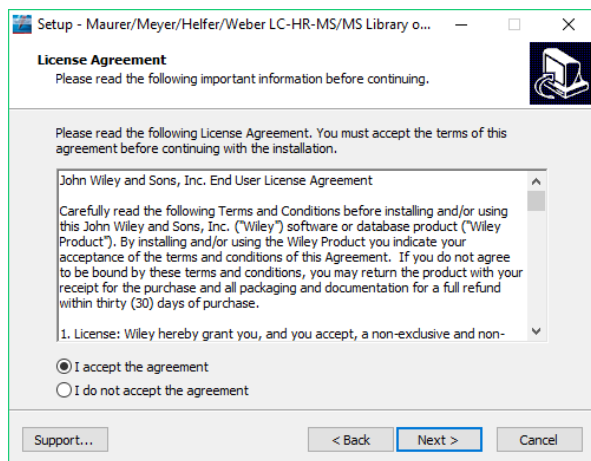
Step 4. If you choose to manually activate, the **Registration Code** and the Machine ID will be automatically filled in. You may either double click the web address to copy it to your computer's clipboard and paste it in a web browser, or enter the URL as listed in your web browser.

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 (17).

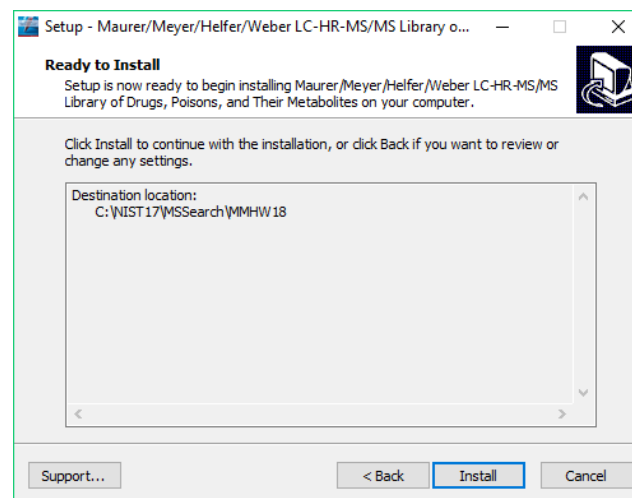
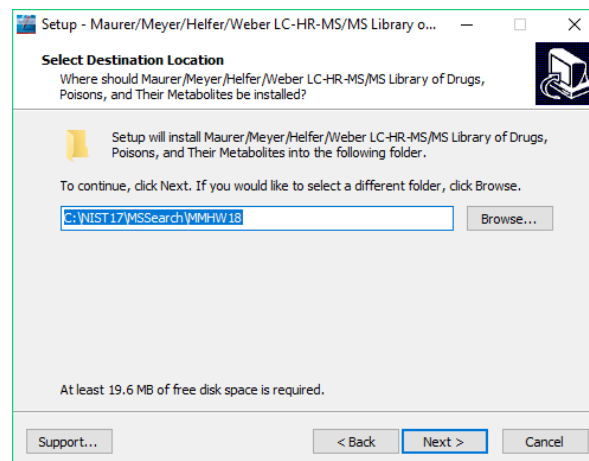
Read the agreement carefully and select the "I accept the agreement" option. Then, choose "Next" to proceed to install the library. Spectral libraries should only be used by qualified individuals who meet the requirements outlined in the agreement.



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.

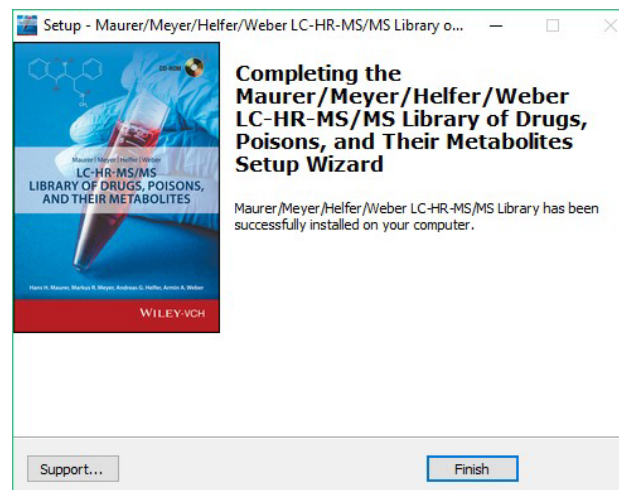
N.B.: For Chrome and Firefox browsers, copy the install file onto a temporary directory. The installer requires RegistrationProcess.dll. Please copy the installer and dll into one directory and activate the installer.



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/>

DATABASE SPECIFICATIONS

For further information on Sample Preparation, Quality Assurance Procedures, ApparatusParameters and more for the Maurer/Meyer/Helfer/Weber LC-HR-MS/MS Library of Drugs, Poisons, and Their Metabolites, please consult the below documentation:

[MMHW LC-HR-MS/MS LIBRARY PRODUCT INFORMATION](#)

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.

MMHW LC-HR-MS/MS Library of Poisons, Pesticides, and Their Metabolites – With over 5,000 spectra and retention index values for over 125 different compound classification groups, theMMHW mass spectral library is an invaluable tool for clinical and forensic research.

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, Raman, UV-Vis, and enterprise spectroscopy software from Wiley-VCH and John Wiley and Sons, Inc.

BASIC FUNCTIONS

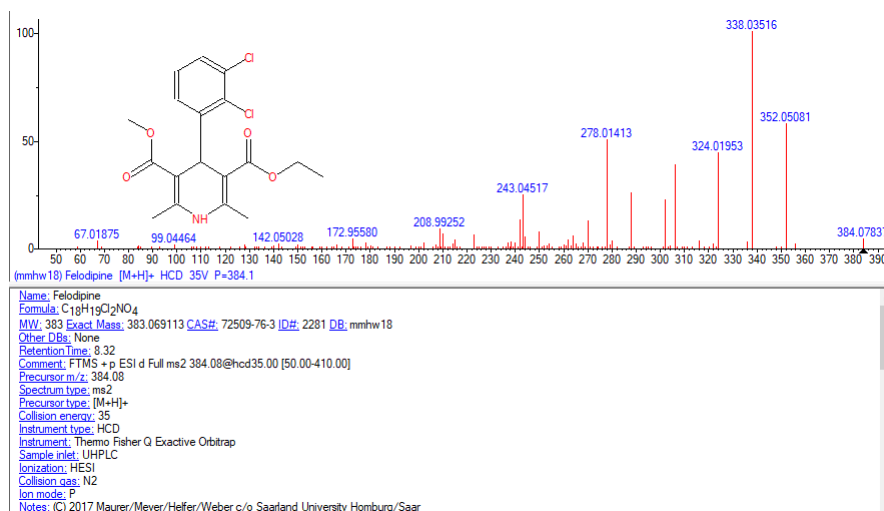
The enclosed library, *MMHW LC-HR-MS/MS Library of Poisons, Pesticides, and Their Metabolites* can be used as the primary search library or can be searched along with other libraries. We recommend, for mission-critical tasks, that users consult both a general library such as *Wiley Registry of Mass Spectral Data 12th Edition* and a specialized library such as *Mass Spectra of Designer Drugs 2021* or *Mass Spectral Library of Drugs, Poisons, Pesticides, Pollutants, and Their Metabolites 5th Edition*.

SEARCH TIPS

To pull out fields from the Comment section found under each spectrum in the NIST MS Search format, access 'Comment fields options' from the **View** Tab. For displaying the data as separate data fields, enter each tag as a separate line and select OK. Estimated non-polar retention index (n-alkane scale) values were not measured by the Maurer/Meyer/Helfer/Weber group and are generated by the NIST MS Search program.

Available 'special' fields for the MMHW library are:

- Retention Time



Display comment field options ✕

To show tag=value from Comments as separate line in spectrum text, enter tag as a separate line.

RetentionTime

For example, if RI=132.1 is embedded in Comments, it can be displayed as a separate line in the text by entering the line:

RI

in the above field. Multiple lines will display multiple tag=value pairs in the order entered.

Show tag=value on plot

OK
Cancel
Help

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.**

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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