

USER MANUAL
VERSION 1.0

CD-ROM



Mass Spectral Library of
**DRUGS, POISONS,
PESTICIDES, POLLUTANTS,
AND THEIR METABOLITES**

5th Edition

Hans H. Maurer, Karl Pflieger, Armin A. Weber

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PUBLISHER'S NOTE

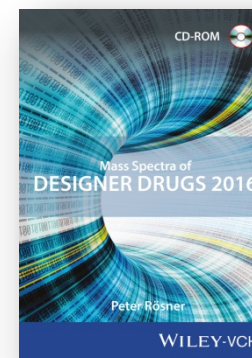
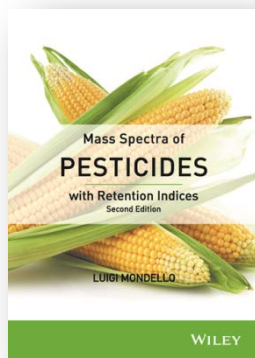
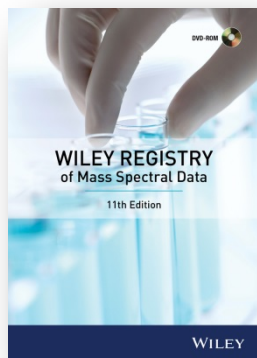
For over 45 years, John Wiley and Sons and Wiley-VCH have worked with the world's leading researchers and practitioners to deliver the spectral libraries mass spectrometrists have come to rely on as the gold standard in mass spectrometry.

This innovative MS reference library for clinical and forensic toxicologists has once more been extensively updated. The **5th Edition of Mass Spectral Library of Drugs, Poisons, Pesticides, Pollutants and their Metabolites** sees the addition of 1,780 data sets, bringing the total to 10,430 mass spectra and GC retention indices. Featured compounds of 175 categories include older and new psychoactive substances, almost all relevant therapeutic drugs as well as 7,800 of their metabolites. Available in the most common instrumentation manufacturer formats, this spectral library is a must have for any research laboratory.

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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Customer Care Center – Consumer Accounts

10475 Crosspoint Blvd.

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<http://support.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 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 <http://support.wiley.com>.

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 CD operates on the following manufacturer formats:

- Agilent Chemstation
- Agilent MassHunter
- ACD Labs
- NIST MSSearch (Bruker, LECO, JEOL)
- Waters MassLynx
- Perkin Elmer TurboMass
- Thermo Xcalibur
- Shimadzu GCMS Solutions

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	SetupMPW5e_Chemstation.exe	C:\Database\{libraryname}\{filename}
MassHunter	SetupMPW5e_MassHunter.exe	C:\MassHunter\Libraries\{libraryname}\{filename}
NIST MS Search	SetupMPW5e_MSSearch.exe	C:\NIST14\MSSEARCH\{libraryname}\{filename}
Thermo Xcalibur	SetupMPW5e_Xcalibur.exe	C:\Program Files\NISTMS\MSSearch\{libraryname}\{filename}
Waters MassLynx	SetupMPW5e_MassLynx.exe	C:\MassLynx\Idendb\{libraryname}\{filename}
Perkin Elmer TurboMass	SetupMPW5e_TurboMass.exe	C:\TurboMass\Idendb\{libraryname}\{filename}
ACD Labs	SetupMPW5e_SpecManager.exe	C:\Program Files\ACD2016\{libraryname}\{filename}
Shimadzu GCMS Solutions	SetupMPW5e_GCMS-Solution.exe	C:\Program Files\GCMSsolution\{libraryname}\{filename}

QUICK-START

1. Registration Code: After reading the EULA, enter the **Registration Code** accompanying the disc packaging.

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 <http://support.wiley.com> 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

Customer Care Center – Consumer Accounts

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Indianapolis, IN 46256
USA

STEP-BY-STEP INSTALLATION

- * **This installation process mirrors installation on a NIST MSSearch program**

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

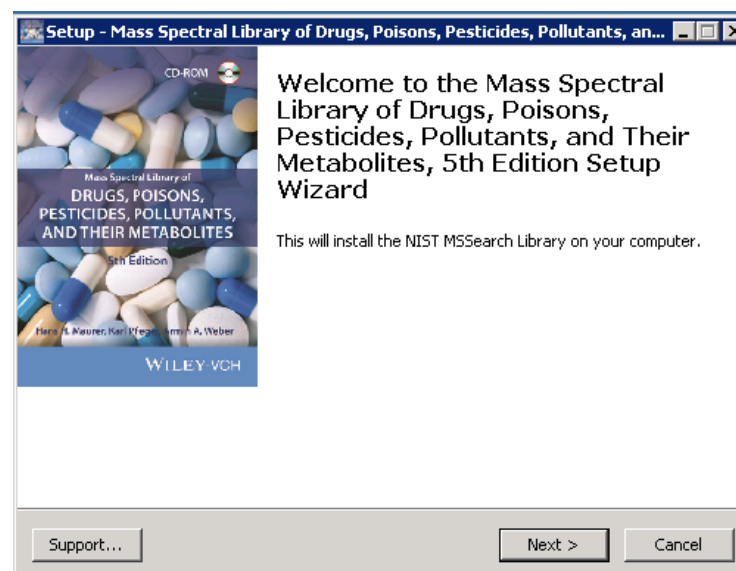
You will be unable to install this library without a Registration Code. Carefully read the End User License Agreement contained on the disc or the accompanying packaging before using and/or installing this product.

Step 2. Read this carefully – if you already have NIST/EPA/NIH MSSearch installed on your system, you will have the opportunity to choose a different directory, but it will change your system's win.ini file to specify this new version of NIST MS Search.

Step 3. 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.

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.

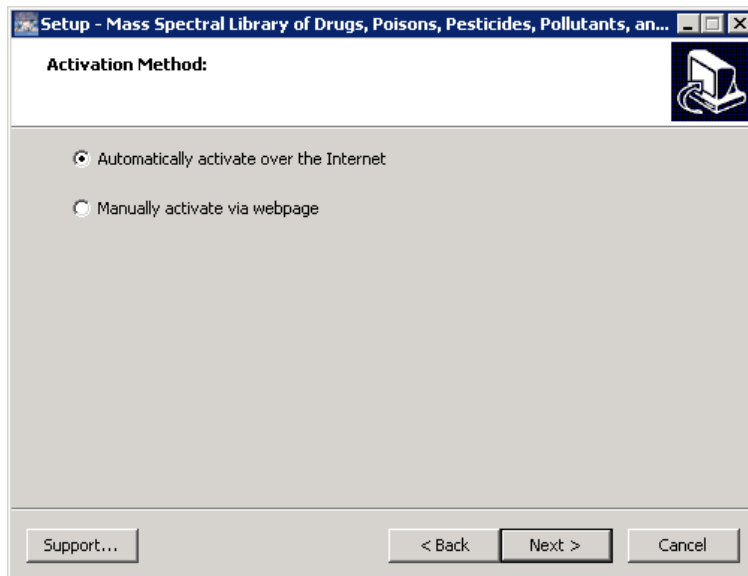
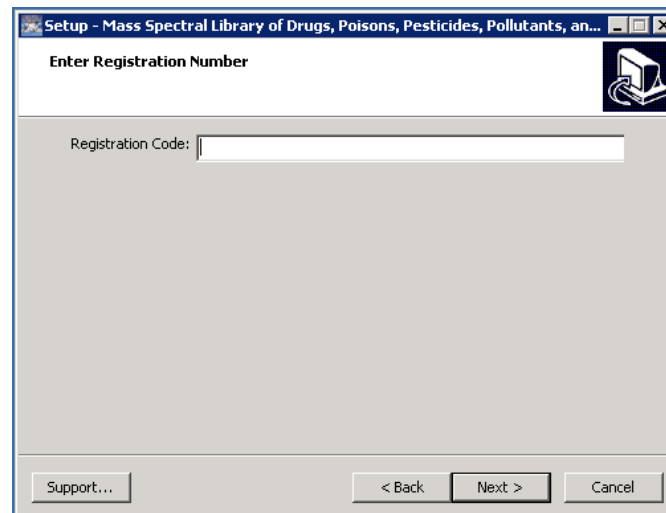


Step 4. Registration Code and Machine ID

Choosing to run the installer will bring you to a splash screen. Choose “next”. Your Registration number appears on instructions accompanying your packaging.

Enter the Registration Code 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 your installation



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.

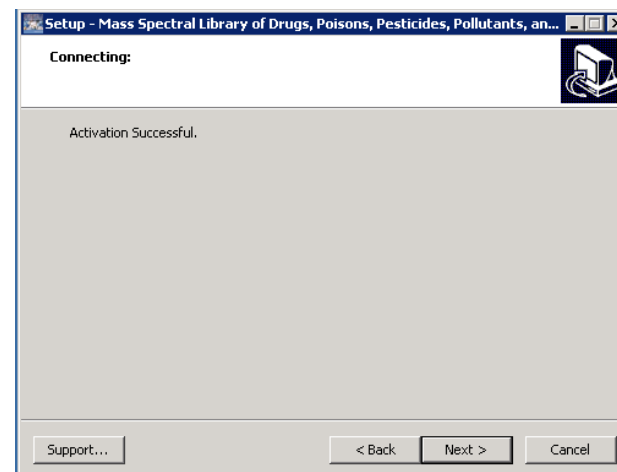
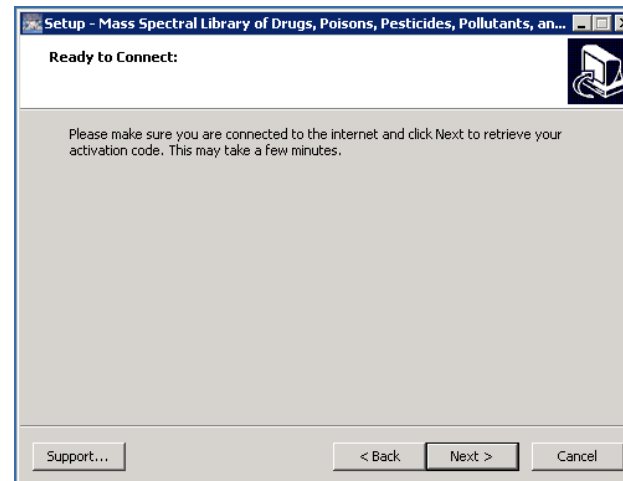
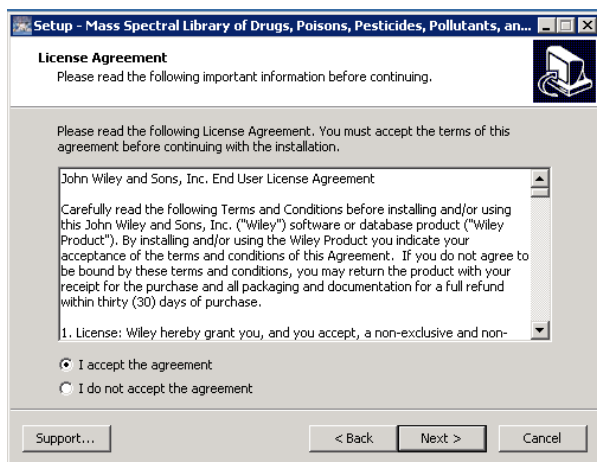
Alternatively you may save the Registration Code, Machine ID and URL to a text file that will be saved to the root directory.

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

Step 6. Once your activation is successful, proceed by pressing "Next".

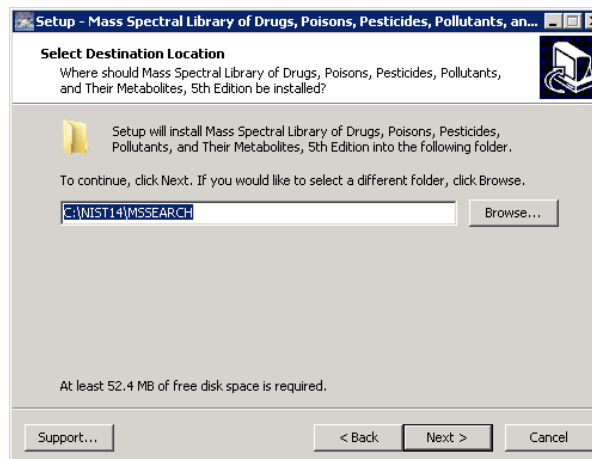
The next screen contains the End User License Agreement (13).

Read the agreement carefully and select the radio button labeled "I accept the terms in the license agreement" to proceed to install the library. Spectral libraries should only be used by qualified individuals who meet the requirements outlined in the Agreement.

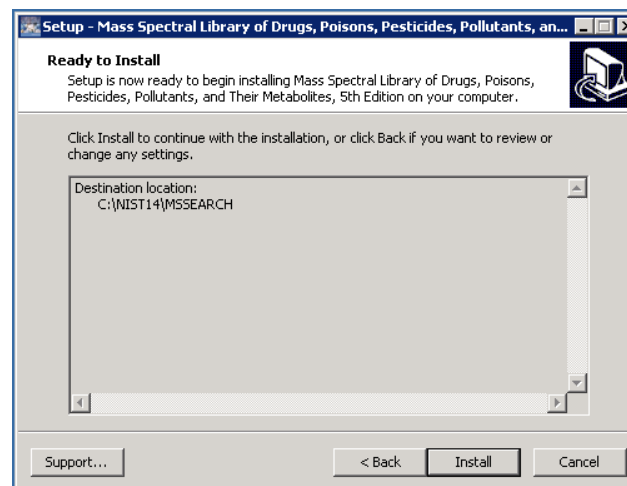


Step 7. Press “NEXT” to proceed to the next step. At this point, the installer will unpack and install the library in the format you have selected.

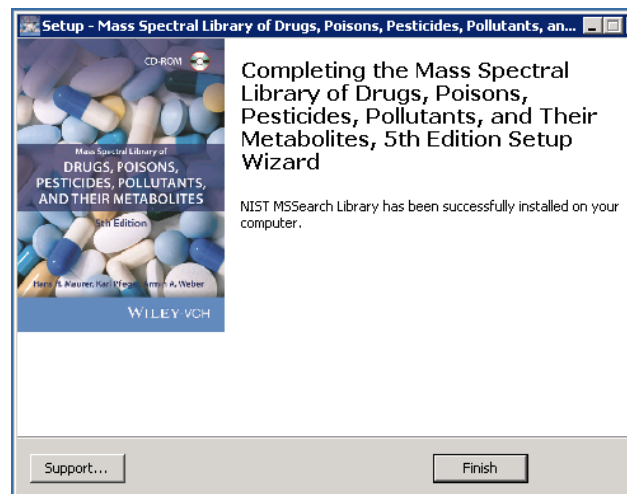
Confirm the target directory and destination location before proceeding.



Step 8. Ready to install? After selection of the destination folder, click the install button to begin installation. Allow installation



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. to finish before closing out any applications.



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 1) to go to:

<http://support.wiley.com>

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.

Mass Spectral Library of Drugs, Poisons, Pesticides, Pollutants, and their Metabolites, 5th Edition- A reference library with 1,780 new data sets, a total of 10,430 mass spectra and GC retention indices. Featuring compounds of 175 categories including older and new psychoactive substances, almost all relevant therapeutic drugs as well as 7,800 of their metabolites.

Wiley Registry 11th/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 www.wiley.com/go/databases for other mass spectrometry, NMR, IR, and enterprise spectroscopy software from Wiley-VCH and John Wiley and Sons, Inc.

BASIC FUNCTIONS

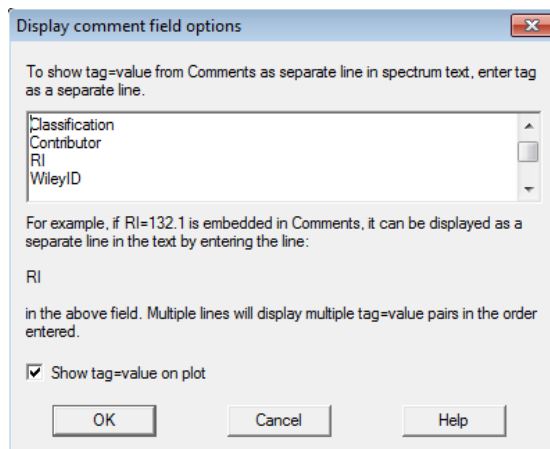
The enclosed library, *Mass Spectral Library of Drugs, Poisons, Pesticides, Pollutants, and their Metabolites, 5th Edition*, can be used as the primary search library or can be searched along with other libraries. We recommend, for mission-critical tasks, that users consult both a general library such as *Wiley Registry of Mass Spectral Data 11th Edition* and a specialized library such as *Designer Drugs 2016* or *Mass Spectra of Flavors and Fragrances of Natural and Synthetic Compounds 3rd Edition*.

SEARCH TIPS

Tags in Comments: For some fields there is no field in the NIST MSSearch library format. For specifying additional fields to hold this data, the 'Tags in Comment' field option has been used. For displaying the data as separate data fields, select the Comment field options dialog available from the main menu bar's view item.

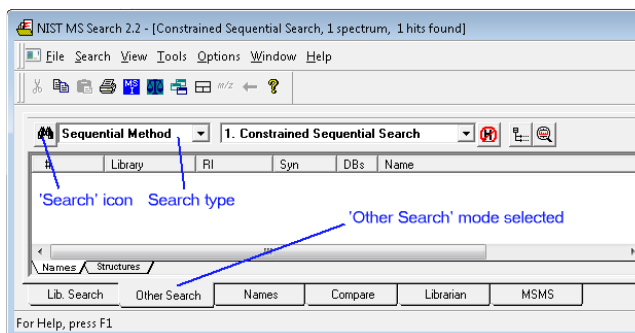
Available 'special' fields for the MPW5E library are:

- Classification
- Contributor
- RI
- WileyID



These special, 'Tags in Comment' fields could be used for searching the same way as 'hard-wired' data fields. Select the 'Other Search' tab, then 'Sequential Search' and click the Search icon (showing a binocular):

Clicking the 'Search' icon brings up a dialog window. Check the 'Tags in Comment' box and type your query in the text field. Additional search options like greater or less than as well as range searches are available for numerical values. For text searching it is also possible to define exact, substring or exclusions are possible. The 'Options' tab is available to select the libraries to be searched.



CAS RN NUMBERS

Within the **Agilent .L** and **Waters MassLynx/PE TurboMass** library formats the CAS Registry Number data field is used for linking the mass spectra records to their corresponding chemical structure records in the structure add-on files. For records for which no CAS Registry Number is given, a 'pseudo' CAS number is created. These 'pseudo' CAS numbers consist of a fixed prefix (in this case here: '99600') combined with the record's ID (0001 to 0430, in the form -00-0 to -43-0 to mimic the CAS number syntax). Again, please note that not all of the values in the CAS Registry Number field actually represent real CAS Registry numbers and are used here only for referring to the structure record in a separate database file.

The 'pseudo' CAS numbers used were created as 9-digit numbers with a leading '99600' to make them distinguishable to real CAS Registry numbers. No real/actual CAS Registry Number starts with 99600.

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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:

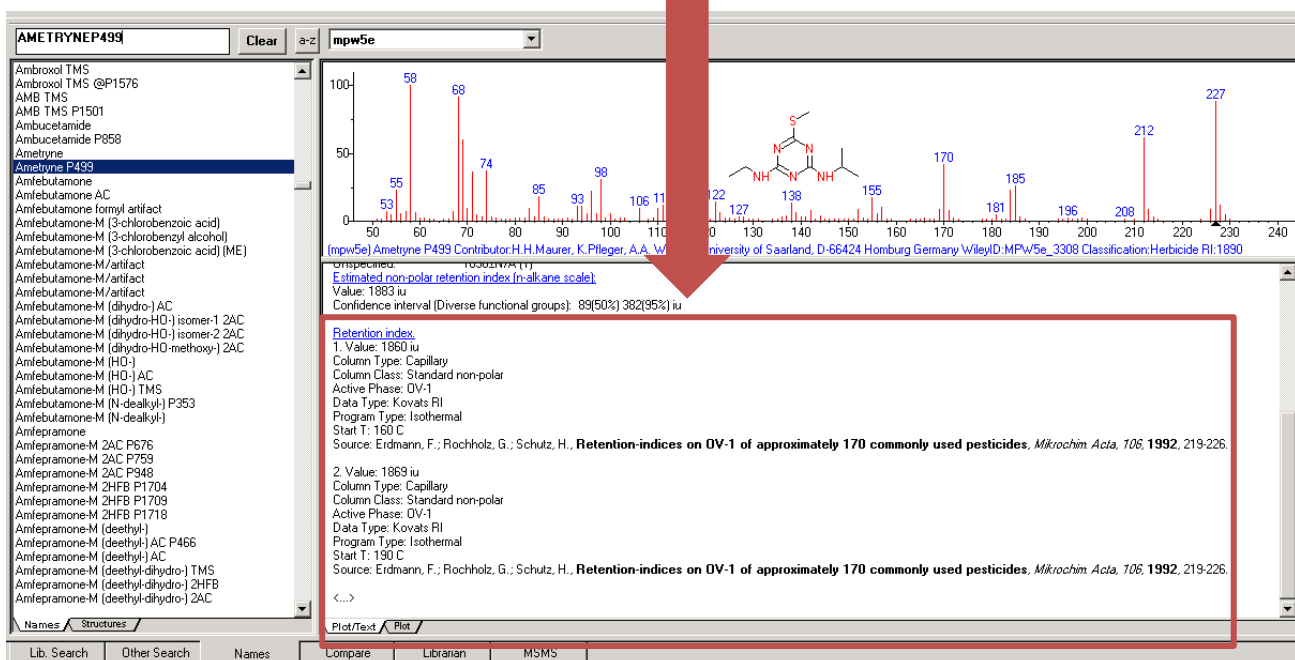
- Classical EI-MS
- Tandem MS (MSⁿ)
- MS-TOF exact mass
- C-NMR, H-NMR, P-NMR, Si-NMR, X-NMR
- FT-IR, Raman, UV-Vis, Near-Infrared, Diamond-ATR

Data proposals, sample data, or inquiries are best sent to dbinquiry@wiley.com

You might send the original TIC file (Xcalibur (*.raw), ChemStation (DATA.MS)) 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.

DATABASE DATA DESCRIPTION

*The RI values automatically displayed in the highlighted sections above are not part of the library and were not measured by the authors. These estimated non-polar retention index values are values given by NIST not from the testing for MPW 5e.



Operating on Shimadzu instrumentation software?

- The "presearch" option filters library compounds before calculation of similarity index.
- The "presearch" option is meant for a PC with slow CPU.
- The recommend default setting to use is the "No PreSearch" option.

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