

**USER MANUAL**

**VERSION 1.0**



# LIPIDS

Mass Spectral Database

**LUIGI MONDELLO**

**WILEY**

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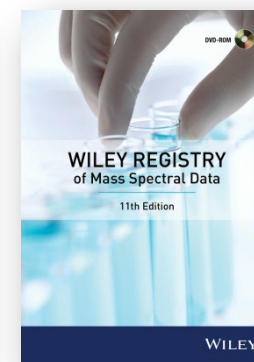
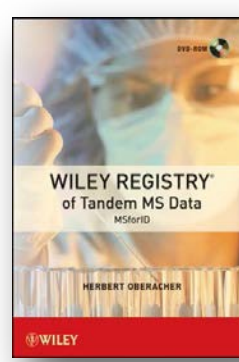
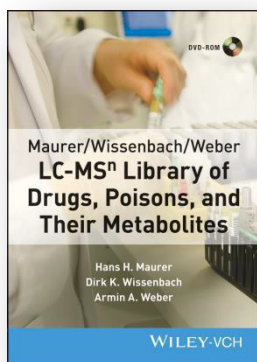
For over 45 years, John Wiley and Sons and Wiley-VCH have worked with the world's leading researchers and practitioners to deliver the spectral libraries mass spectrometrists have come to rely on as the gold standard in mass spectrometry.

Lipids are one of the major constituents of food and they have an essential role in human diet, metabolism, physiological and pathological processes. Mass spectrometry is the most important technology for lipid analysis. The **Lipids Mass Spectral Database** gives a significant support for peak assignment in complex mixtures and can be a valid support in many research fields, such as food analysis, clinical and medical applications. This Library contains 430 lipid-like molecules classified in 11 different classes and almost one LRI for each molecule.

## 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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**WileyScience 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

Email: [dbinquiry@wiley.com](mailto:dbinquiry@wiley.com)

Website: <http://www.wiley.com/go/databases>

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10475 Crosspoint Blvd.

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<b>Substance</b>	<b>Maximum Limit (ppm)</b>
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
- \* Memory: At least 2GB
- \* Disk Space: At least 2GB free disc space
- \* Software: 32-bit or 64-bit software

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 is present on the Certificate of Authenticity that 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 contains the following manufacturer formats:

- Agilent Chemstation
- Agilent MassHunter
- NIST MS Search
- Thermo Xcalibur
- ACD Labs
- PerkinElmer TurboMass
- Waters MassLynx

## 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
<b>Chemstation</b>	SetupLM_LIPIDS_Chemstation.exe	C:\Database\{libraryname}\{filename}
<b>MassHunter</b>	SetupLM_LIPIDS_MassHunter.exe	C:\MassHunter\Libraries\{libraryname}\{filename}
<b>MassLynx</b>	SetupLM_LIPIDS_MassLynx.exe	C:\MassLynx\ldendb\{libraryname}\{filename} C:\MassLynx\ldendb\STRUCTDB\{libraryname}\{filename}
<b>ACD Labs</b>	SetupLM_LIPIDS_SpecManager.exe	C:\Program Files\ACD2016\{libraryname}\{filename}
<b>MS Search</b>	SetupLM_LIPIDS_MSSearch.exe	C:\NIST14\MSSEARCH\{libraryname}\{filename}
<b>TurboMass</b>	SetupLM_LIPIDS_TurboMass.exe	C:\TurboMass\ldendb\{libraryname}\{filename} C:\TurboMass\ldendb\STRUCTDB\{libraryname}\{filename}
<b>Thermo Xcalibur</b>	SetupLM_LIPIDS_Xcalibur.exe	C:\ProgramFiles\NISTMS\MSSearc h\{libraryname}\{filename}

**QUICK-START**

- 1. Registration Code:** After reading the EULA provided in the CD packaging, note the **Registration Code** featured on the Certificate of Authenticity and begin the installation process.
- 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. INSTALLATION:** Please note installation requires the Registration Code that accompanied you disc packaging. Install the formats you wish to use on a single computer, following the on-screen prompts to “run” the installer. NB: You must “run” the installers from the CD-ROM or in a directory containing the Registrationprocess.dll

**Customer Care Center – Consumer Accounts**

10475 Crosspoint Blvd.  
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 provided code does not work or your disc is not accompanied by a Registration Code, alert Wiley customer service at <http://support.wiley.com>

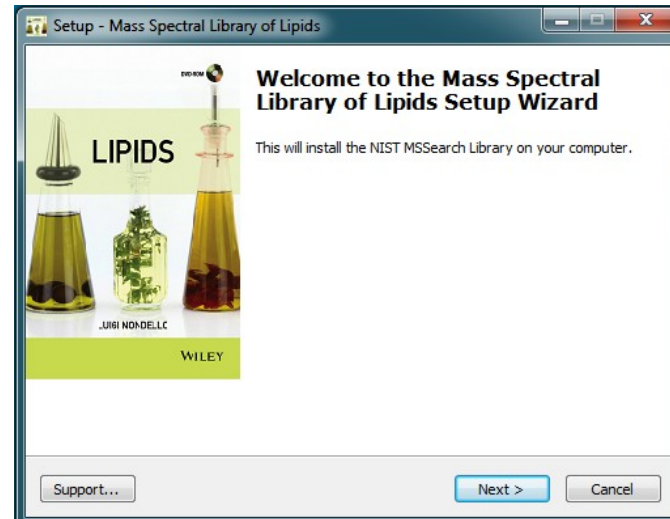
You will be unable to install this library without a Registration Code.

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

**Step 2.** 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 set-up wizard splash screen. Choose "next".

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.

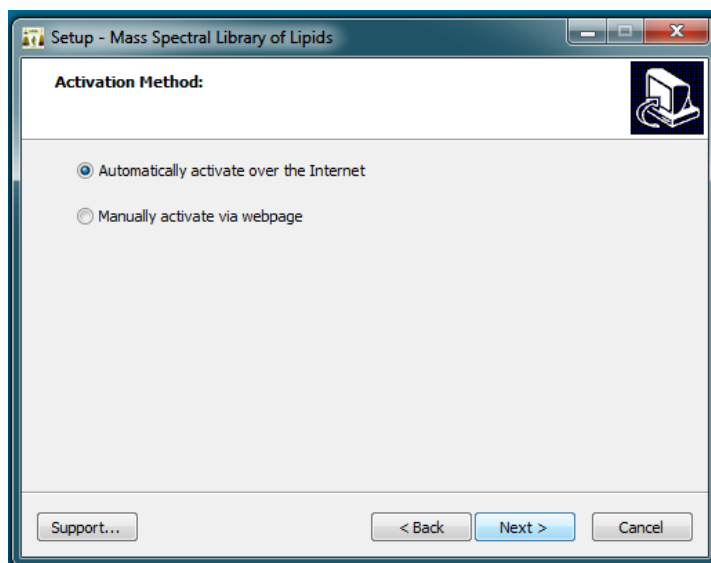
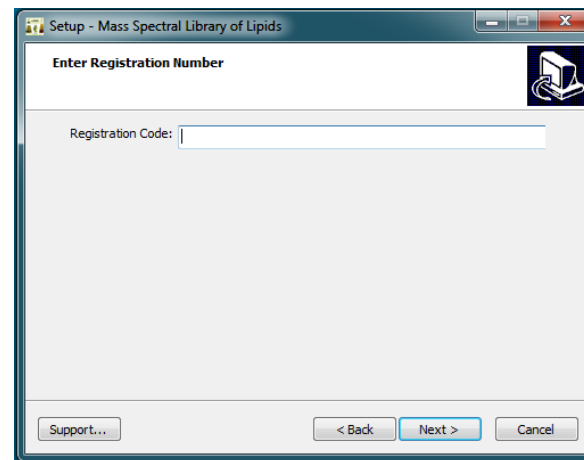


**Step 3. Registration Code and Machine ID**

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 your installation. Choose "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.

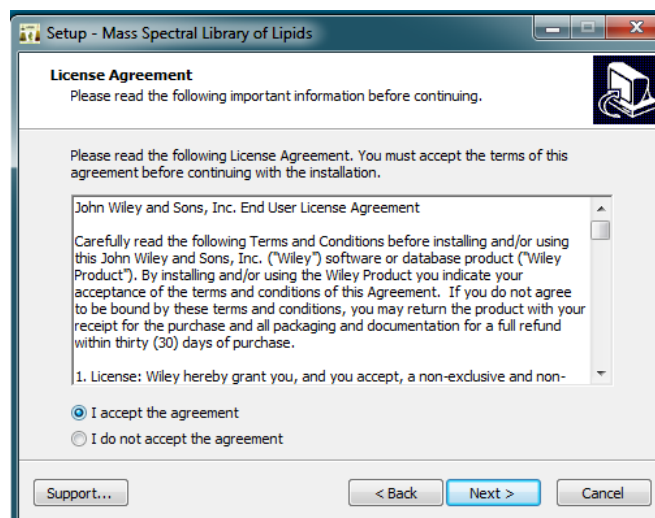
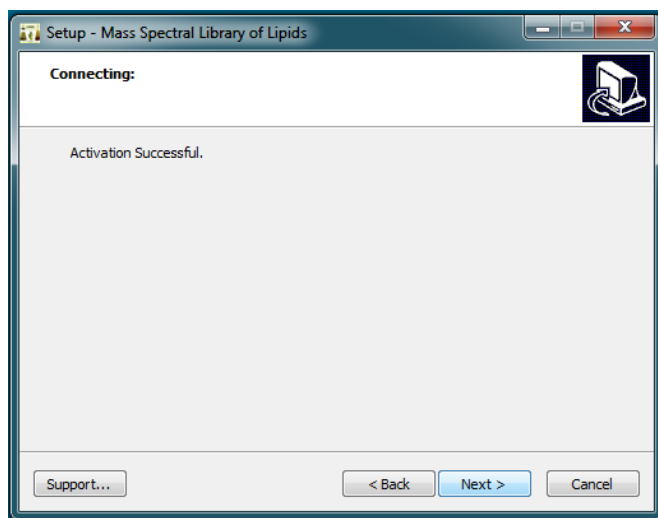
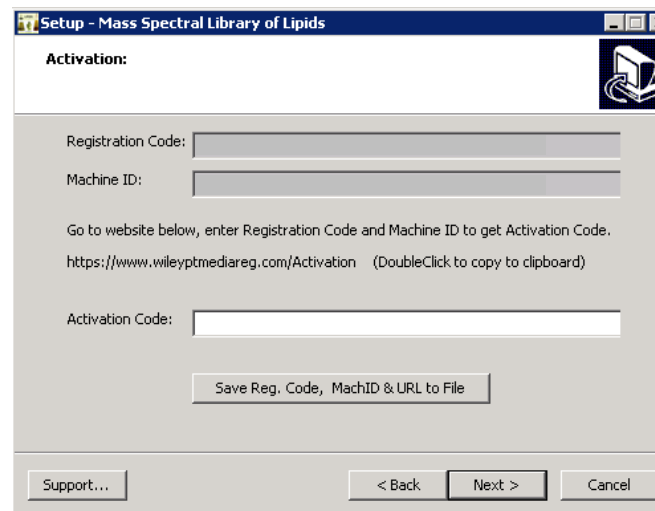
Alternatively you may save the Registration Code, Machine ID and URL to a text file that will be saved to the root directory.

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 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 (17).

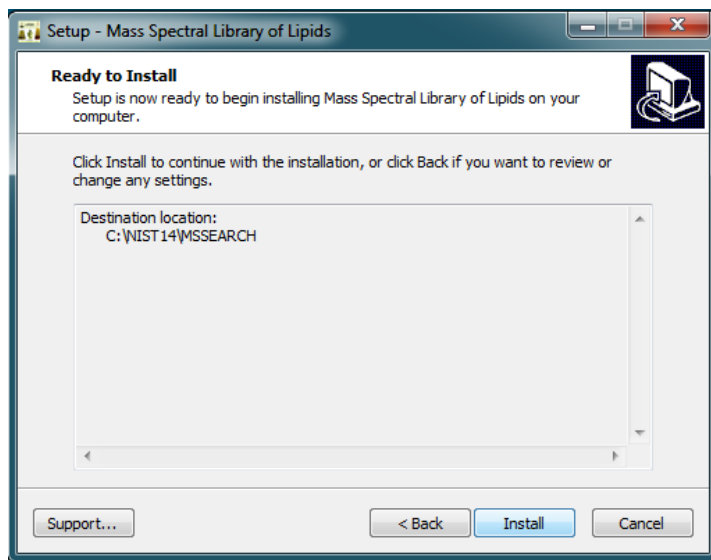
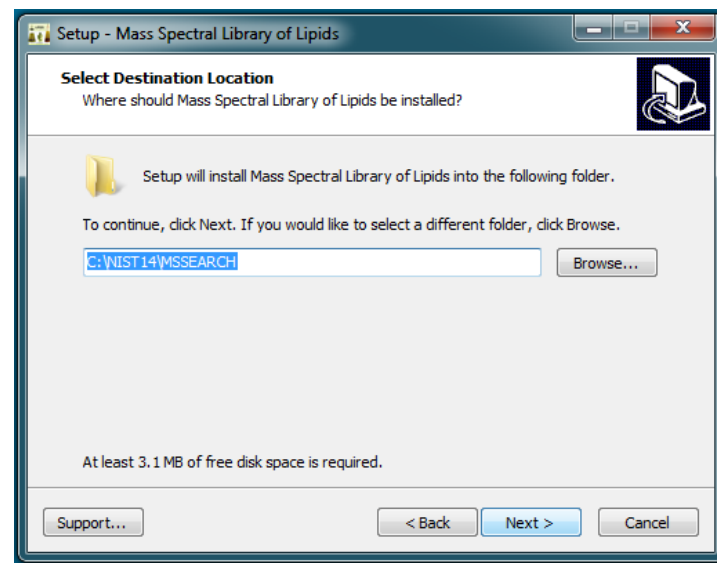
Read the agreement carefully and select the radio button labeled "I accept the agreement" to proceed to install the library. Spectral libraries should only be used by qualified individuals who meet the requirements outlined in the Agreement.



**Step 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.

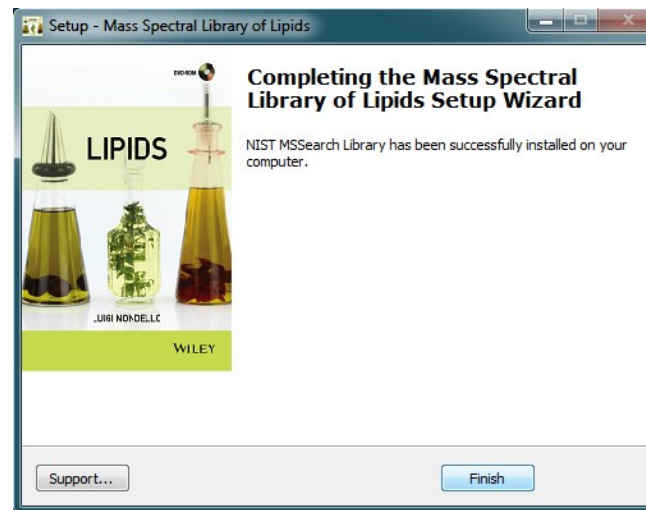
**Step 7.** Ready to install? After selection of the destination folder, choose the “Install” button to begin installation. Allow installation to finish before closing out any applications.



**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 1) to go to:

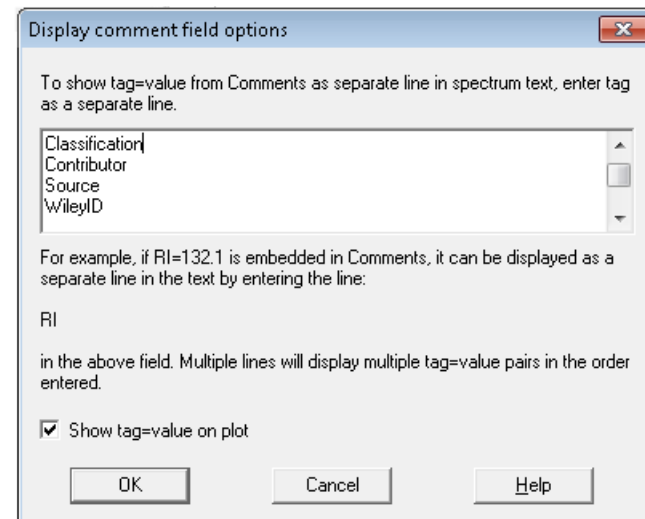
<http://support.wiley.com>

## SEARCH TIPS

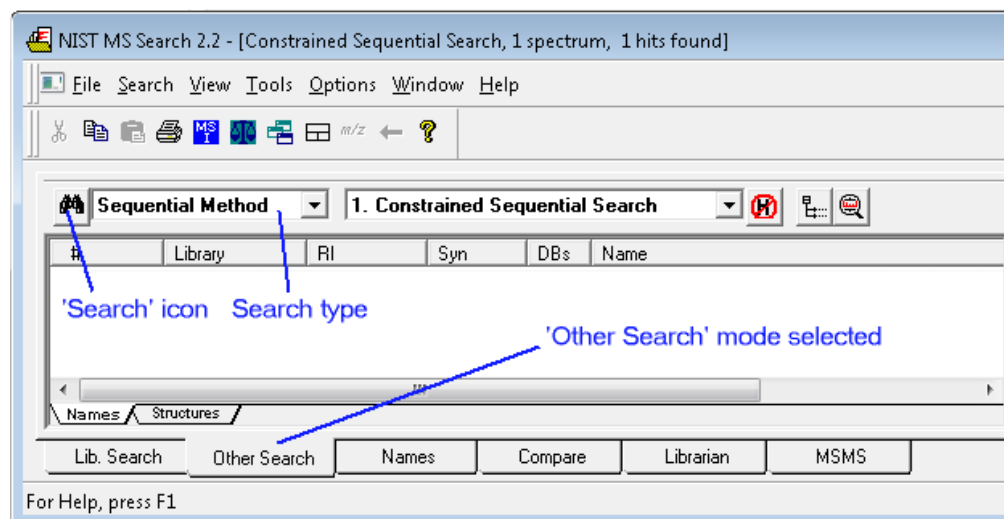
For some fields there is no field in the NIST MSSearch library format. For specifying additional fields to hold this data, the 'Tags in Comment' field option has been used. For displaying the data as separate data fields, select the Comment field options dialog, as seen here, available from the main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

Available 'special' fields for the LM\_LIPIDS library are:

- Classification
- Contributor
- Source
- WileyID
- RI 1, 2, 3, 4, 5
- SampleInfo

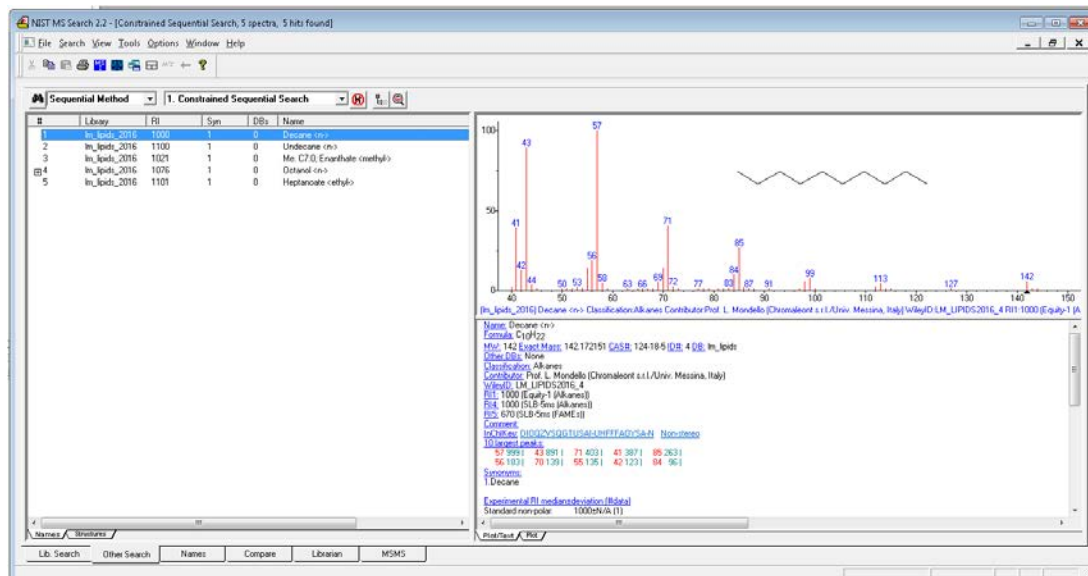


\*\* These special 'Tags in Comment' fields could be used for searching the same way as 'hard-wired' data fields. Select the 'Other Search' tab, then 'Sequential Search' and click the Search icon. Clicking the 'Search' icon brings up a dialog window where you could specify your query.



## GENERAL DATABASE CONTENT

Seen in the example below is a constrained sequential search for Retention Index values being exactly 1000 from the RI1 data field as well as a range search (RI1 being between 1000 and 1100). 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.



See [www.wiley.com/go/databases](http://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 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 the featured library, *Lipids Mass Spectral Database* or *Mass Spectra of Flavors and Fragrances of Natural and Synthetic Compounds 3rd Edition*.

### 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 number is prefixed with the number 991.**

**Please note that IDs prefixed with the number 991 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. Wiley accepts data in the following areas:

- ClassicalEI-MS
- Tandem MS (MS<sup>n</sup>)
- 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](mailto: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](mailto: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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