

Mass Spectra of Geochemicals, Petrochemicals,
and Biomarkers, 2nd Edition

USER MANUAL VERSION 1.1

USER MANUAL
VERSION 1.1

The cover image features a silhouette of an offshore oil rig against a bright orange and yellow sunset sky. A large, semi-transparent yellow circle is positioned behind the rig's cranes. The rig's structure, including its derrick and various platforms, is clearly visible against the darkening sea.

**Mass Spectra of
GEOCHEMICALS, PETROCHEMICALS,
AND BIOMARKERS**

J.W. De Leeuw

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TABLE OF CONTENTS

PUBLISHER'S NOTE	4
COMPOUND SEARCH	4
CONTACT INFORMATION	5
Editorial Correspondence.....	5
Customer Care.....	5
COMPLIANCE.....	5
GETTING STARTED.....	6
Hardware and Software Recommendations	6
Registration Code	6
License.....	6
COMPATIBILITY	7
DIRECTORY ASSISTANCE	7
QUICK-START	8
STEP-BY-STEP INSTALLATION.....	9
Getting Help	13
GENERAL DATABASE CONTENT	14
Basic Functions	14
Database Data Description	15
DATA SUBMISSION	16
JOHN WILEY AND SONS, INC. PRIVACY POLICY AND TERMS OF USE	17
JOHN WILEY AND SONS, INC. END USER LICENSE AGREEMENT.....	17

PUBLISHER'S NOTE

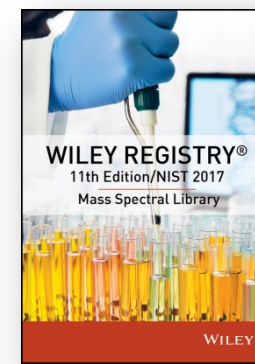
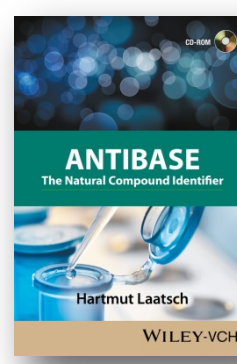
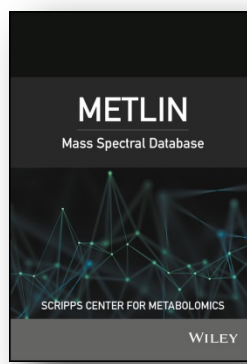
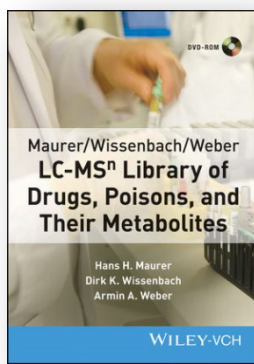
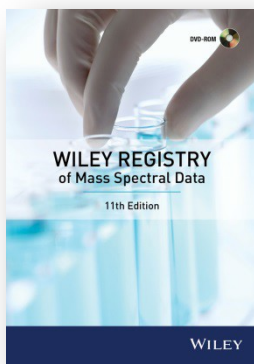
For over 45 years, John Wiley and Sons and Wiley-VCH have worked with the world's leading researchers and practitioners to deliver the spectral libraries mass spectrometrists have come to rely on as the gold standard in mass spectrometry.

This reference collection contains 1,100 mass spectra of well-defined compounds. The spectra have been measured by J. W. de Leeuw's group in the Department of Marine Biogeochemistry at the Netherlands Institute of Sea Research (NIOZ). The substances have been carefully isolated and purified. Chemical structures have been elucidated, if necessary, by a variety of techniques, including NMR spectroscopy and single-crystal X-ray structure analysis. The spectra were collected during extensive project on the occurrence of resistant biomacromolecules and lipids in sedimentary organic matter, and mechanisms of fossil fuel generation as well as the chemistry of organic sulphur in the geosphere. This comprehensive collection covers a wide range of components relevant to the geo- and petrochemical fields.

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**

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Substance	Maximum Limit (ppm)
Lead (Pb)	1000
Cadmium (Cd)	100
Mercury (Hg)	1000
Hexavalent Chromium (Cr ⁶⁺)	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:

- Agilent ChemStation
- Agilent MassHunter
- NIST MS Search
- Shimadzu GCMSsolution
- Thermo 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
Agilent ChemStation	SetupMSGeoPetroChemstation.exe	c:\Database\{libraryname}\{filename}
Agilent MassHunter	SetupMSGeoPetroMassHunter.exe	C:\MassHunter\Library\{libraryname}\{filename}
NIST MS Search	SetupMSGeoPetroMSSearch.exe	C:\NIST17\MSSEARCH\{libraryname}\{filename}
Shimadzu GCMSsolution	SetupMSGeoPetroGCMS_Solutio.exe	C:\GCMSsolution\Library\{libraryname}\{filename}
Thermo Xcalibur	SetupMSGeoPetroXcalibur.exe	C:\Program Files (x86)\NistMS\MSSearch\{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 <https://hub.wiley.com/community/support> or 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. 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.

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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 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**.

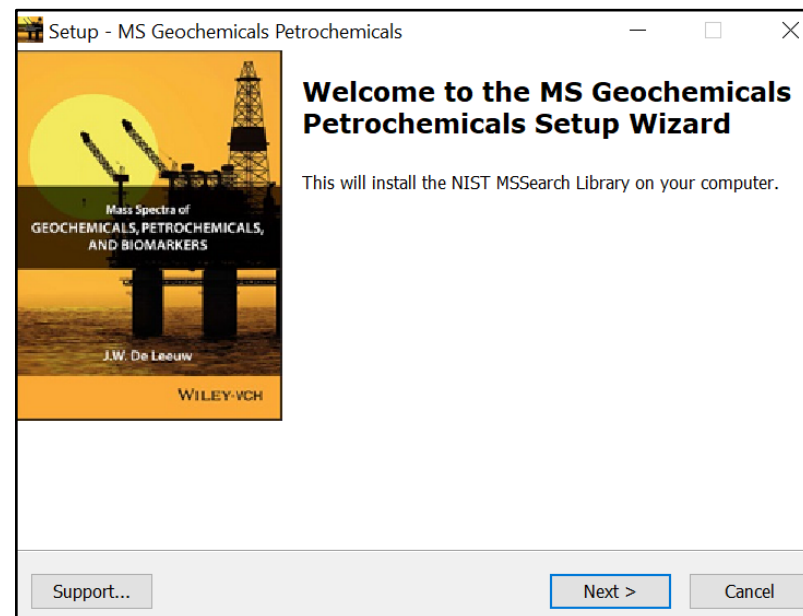
Step 2. Carefully read the End User License Agreement contained on the disc or the accompanying packaging before using and/or installing this product.

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.

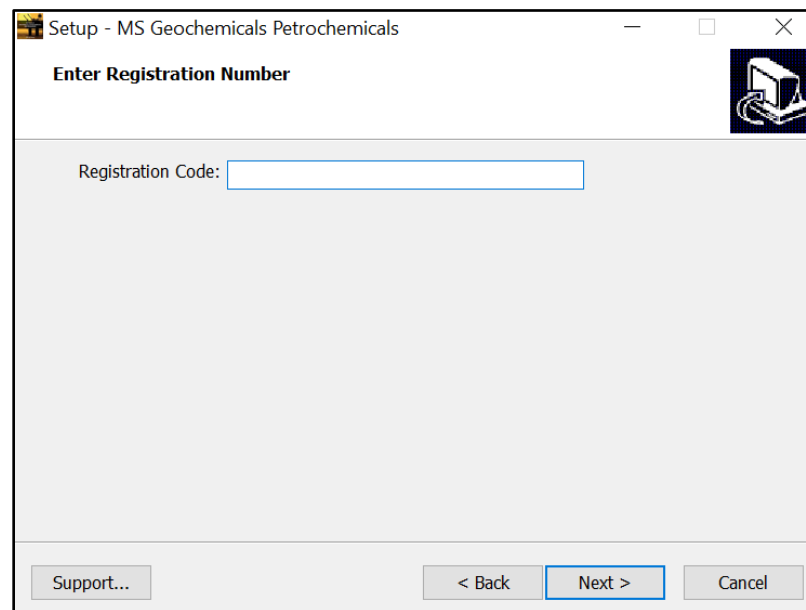
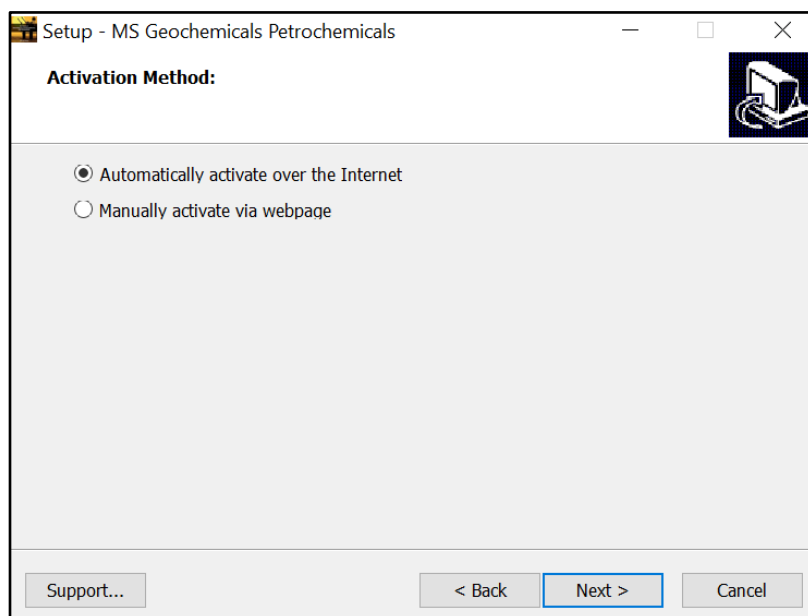


Step 3. Registration Code and Machine ID

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.

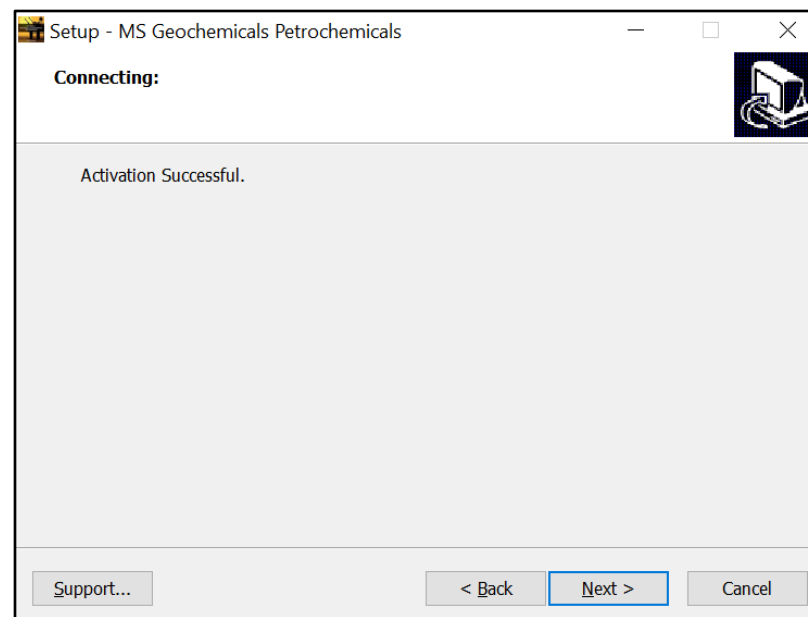
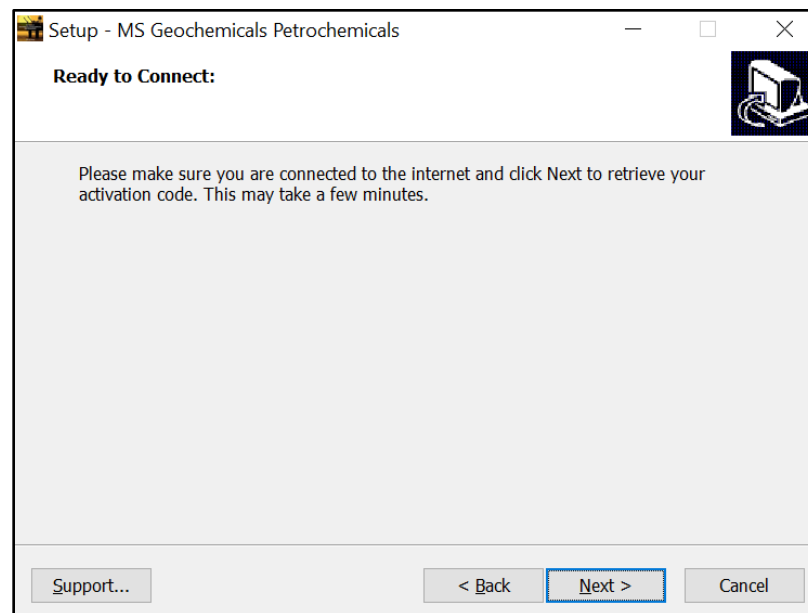
If the **Registration Code** is correct, you will be brought to the Activation screen. If your machine has internet connectivity, choose to “Automatically activate over the internet” and then click “Next” to begin internet activation.



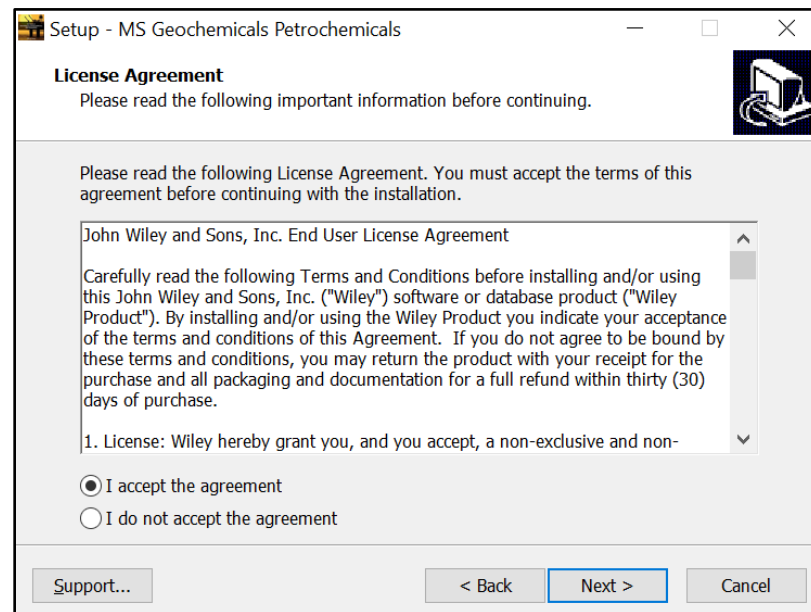
Step 4. If you choose to manually activate, the **Registration Code** and the Machine ID will be automatically filled in. You may either double click the web address to copy it to your computer's clipboard and paste it in a web browser, or enter the URL as listed in your web browser.

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

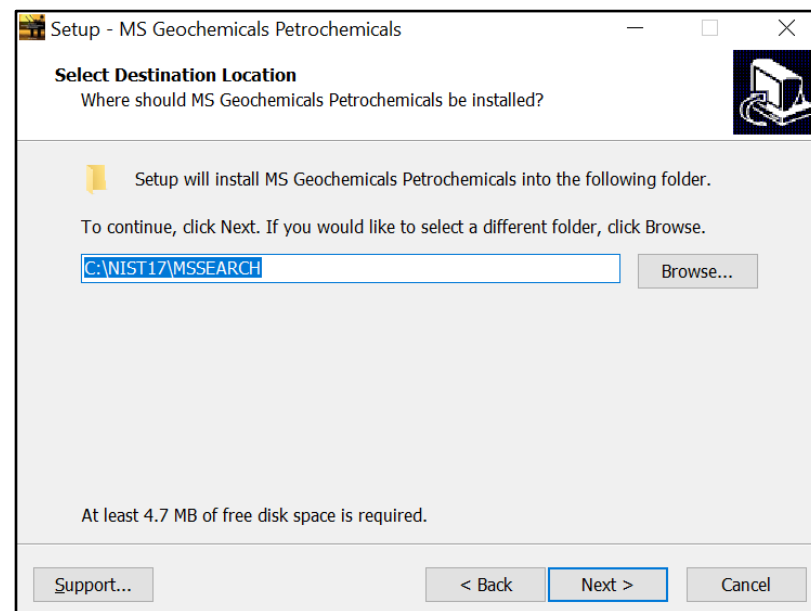
In the web browser, enter the **Registration Code** and the Machine ID. The next screen will provide the Activation Code. Copy this code down and save it, entering it into the Activation screen on the computer that you are installing the spectral library on.



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.

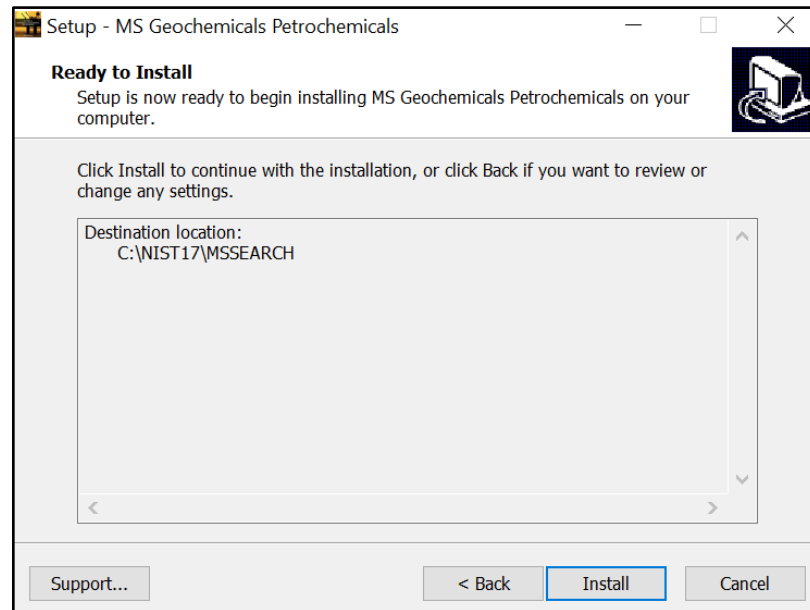


Step 7. Ready to install? After selection of the destination folder, choose the “Install” button to begin installation. Allow installation to finish before closing out any applications.

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.

Repairing or Uninstalling

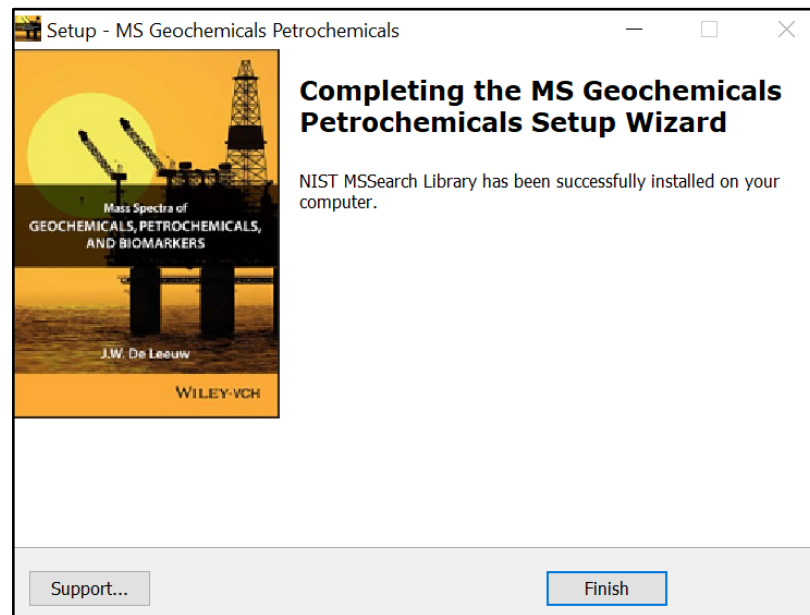
Repairing or uninstalling the library should be managed using the “Add/Remove Programs” utility in Windows. If the library is manually moved, removed, or installed using overwrite mode, the Windows utility may not work.



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.

This reference collection contains 1,100 mass spectra of well-defined compounds. The spectra have been measured by J. W. de Leeuw's group in the Department of Marine Biogeochemistry at the Netherlands Institute of Sea Research (NIOZ). The substances have been carefully isolated and purified. Chemical structures have been elucidated, if necessary, by a variety of techniques, including NMR spectroscopy and single-crystal X-ray structure analysis. The spectra were collected during extensive project on the occurrence of resistant biomacromolecules and lipids in sedimentary organic matter, and mechanisms of fossil fuel generation as well as the chemistry of organic sulphur in the geosphere. This comprehensive collection covers a wide range of components relevant to the geo- and petrochemical fields.

Substance classes include saturated, unsaturated and aromatic hydrocarbons, aromatic and nonaromatic sulphur and oxygen compounds, terpenes, steroids and their degradation products.

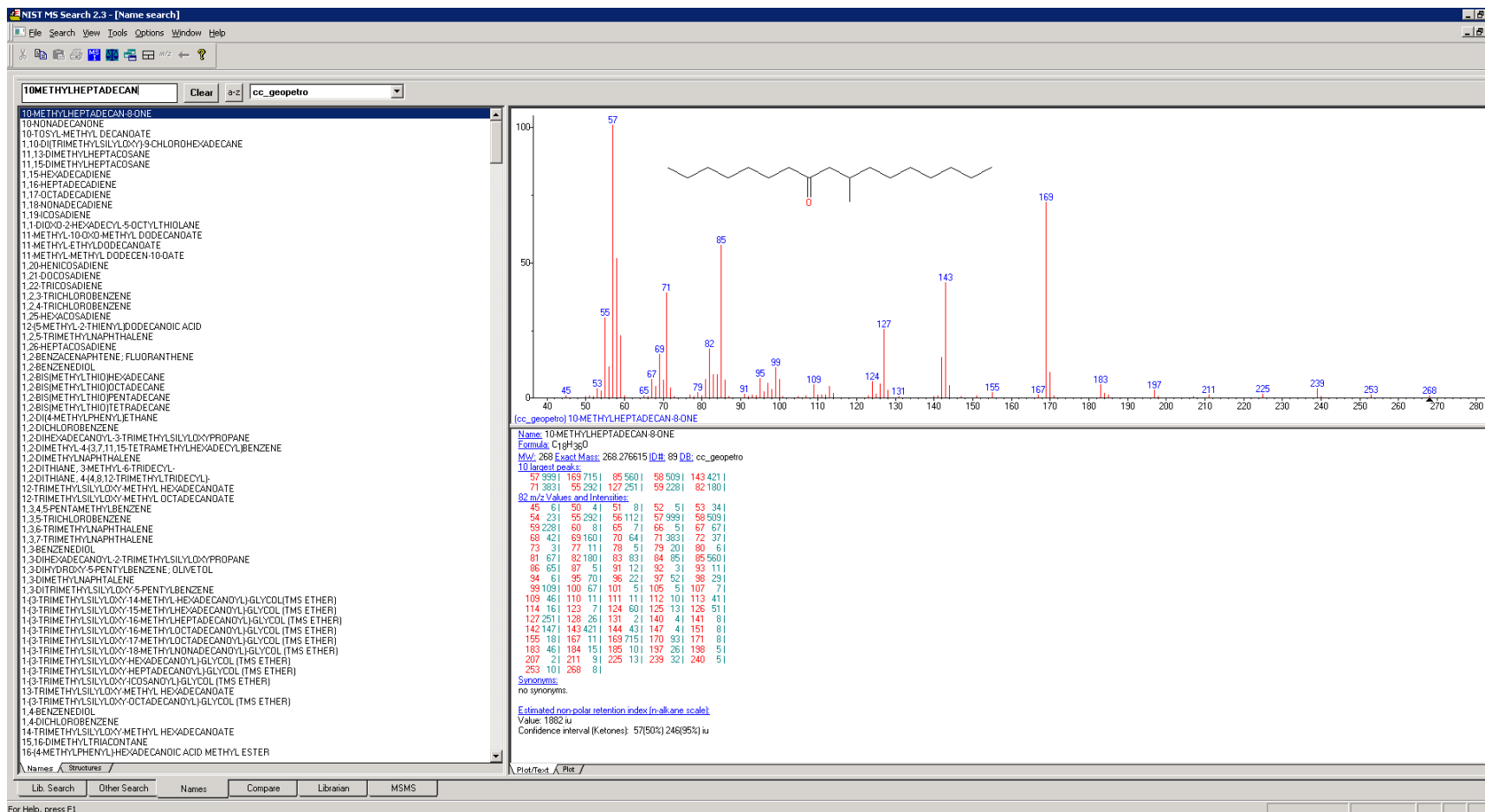
Practitioners and researchers are encouraged to evaluate their own needs and decide what libraries are appropriate for them.

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, *Mass Spectra of Geochemicals, Petrochemicals, and Biomarkers*, 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 Edition/NIST 2017 Mass Spectral Library* and a specialized library such as the featured *Mass Spectra of Geochemicals, Petrochemicals, and Biomarkers* library or the *Mass Spectra of Pesticides* library.

DATABASE DATA DESCRIPTION



Featured Data Fields:

- Chemical Structure
- Chemical Name
- Molecular Formula
- Molecular Weight
- Synonyms

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:

- ClassicalEI-MS
- Tandem MS (MSⁿ)
- MS-TOF exact mass
- C-NMR, H-NMR, P-NMR, Si-NMR, X-NMR
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Data proposals, sample data, or inquiries are best sent to dbinquiry@wiley.com.

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