



NIST/EPA/NIH Mass Spectral Library 2020

User Manual

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Installation Manual Copyright © 2022 John Wiley and Sons, Inc., Hoboken, New Jersey. All Rights Reserved.

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PUBLISHER'S NOTE

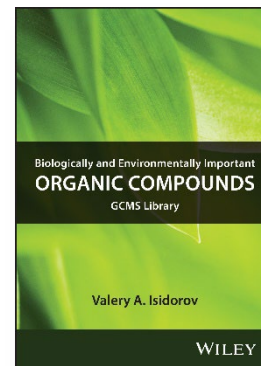
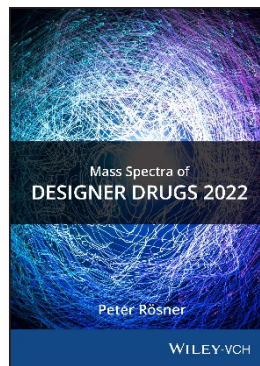
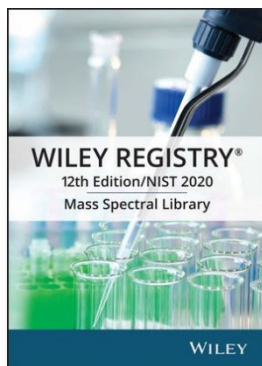
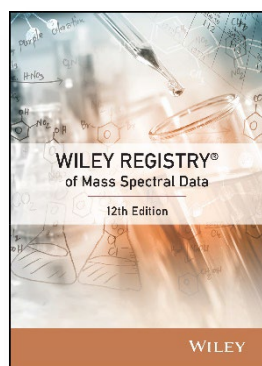
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Thoroughly updated and more comprehensive than ever, the 2020 release of the *NIST/EPA/NIH Mass Spectral Library* is the one of the most trusted, versatile mass spectral collections ever published. It is made up of three types of libraries, an Electron Ionization (EI) mass spectral library, a MS/MS library, and a GC Retention Index library.

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 spectral libraries.



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Editorial Correspondence

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10475 Crosspoint Blvd.

Indianapolis, IN 46256 USA

<https://support.wiley.com/s/>

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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 10 recommended)
- 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, 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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COMPATIBILITY

Wiley has provided you with a 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:

- Agilent ChemStation
- Agilent MassHunter
- NIST MS Search
- PerkinElmer TurboMass
- Shimadzu GCMSsolution
- Waters MassLynx

DIRECTORY ASSISTANCE

The table below lists the format, installation file, and their default target directory. 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	SetupNIST20ChemStation.exe	C:\Database\{libraryname}\{filename}
MassHunter	SetupNIST20MassHunter.exe	C:\MassHunter\Library\{libraryname}\{filename}
MS Search	SetupNIST20MSSearch.exe	C:\NIST20\MSSEARCH\{libraryname}\{filename}
TurboMass	SetupNIST20TurboMass.exe	C:\TurboMass\Idendb\{libraryname}\{filename} C:\TurboMass\Idendb\STRUCTDB\{libraryname}\{filename}
GCMSsolution	SetupNIST20GCMSsolution.exe	C:\GCMSsolution\Library\{libraryname}\{filename}
MassLynx	SetupNIST20MassLynx.exe	C:\MassLynx\Idendb\{libraryname}\{filename} C:\MassLynx\Idendb\STRUCTDB\{libraryname}\{filename}

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.
 - a. **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 Activation Code and use it to complete on-screen installation prompts on the computer.
 - b. **Computer ID – No internet:** Contact Wiley Customer Support at <https://support.wiley.com/s/> or by telephone at (877) 762-2974.
3. **Installation:** Please note installation requires the Registration Code that accompanied your 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

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STEP-BY-STEP INSTALLATION

* This installation process mirrors installation on the NIST MS Search software.

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.

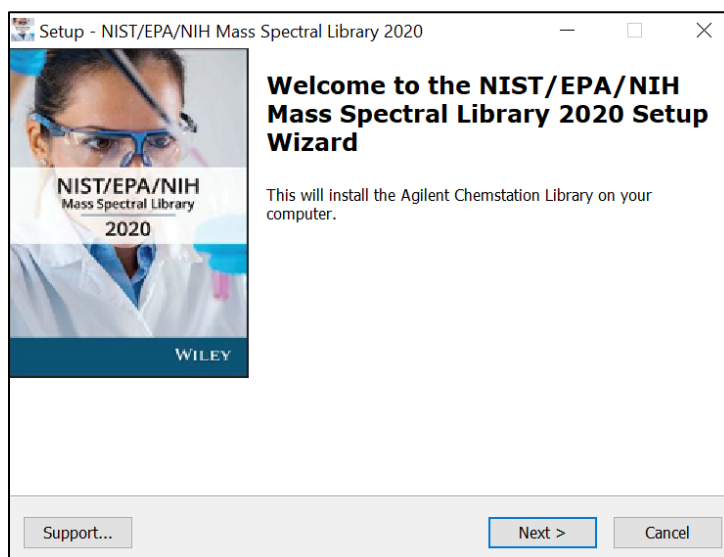
2. Insert the flash drive for installation. One file "Installation.htm" is included on the drive to simplify installation by using your web browser. Choose the format(s) you wish to install. Choosing to run the installer will bring you to a set-up wizard splash screen. Choose "Next."

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.

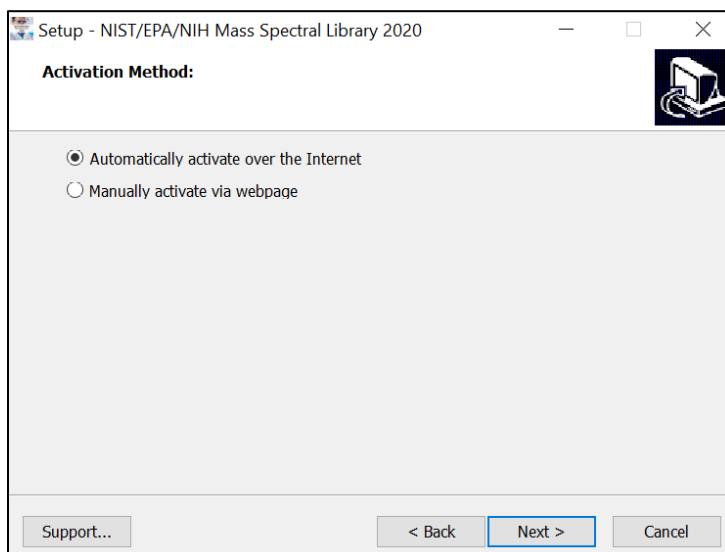
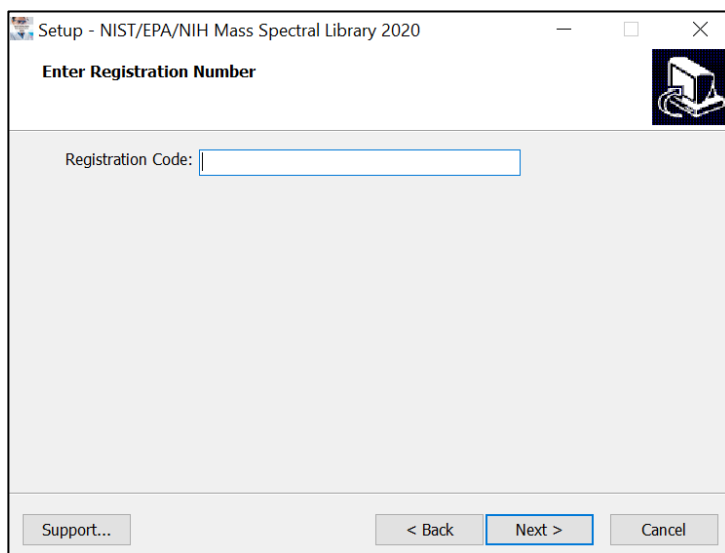


3. Registration Code and Machine ID

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.

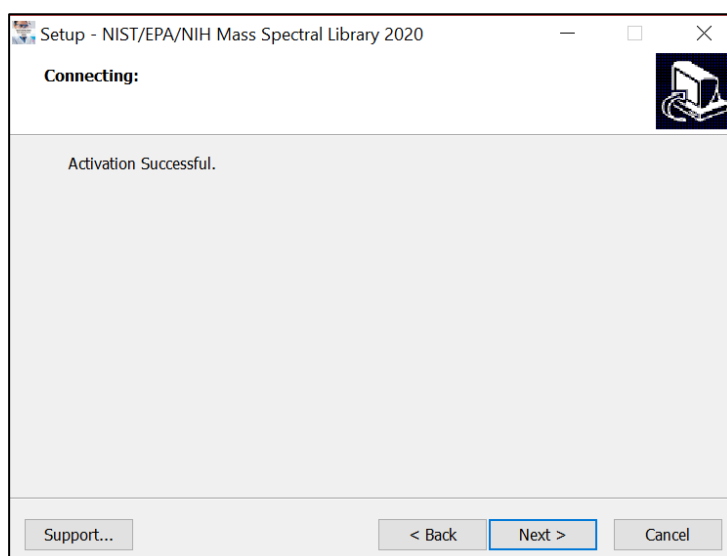
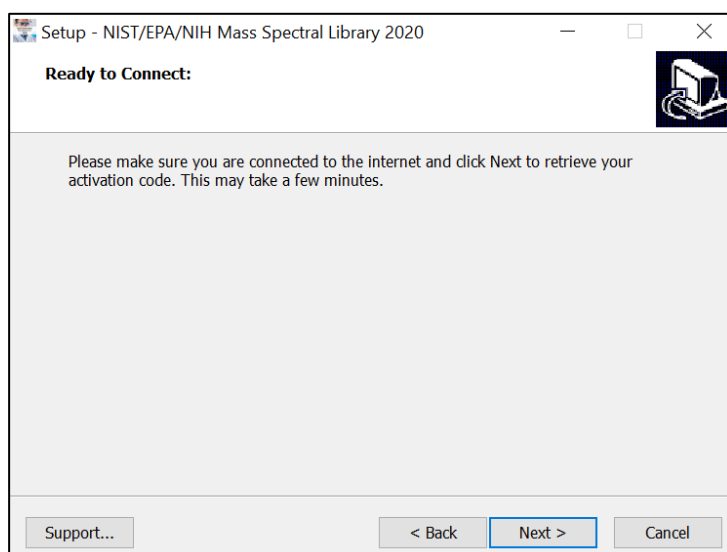
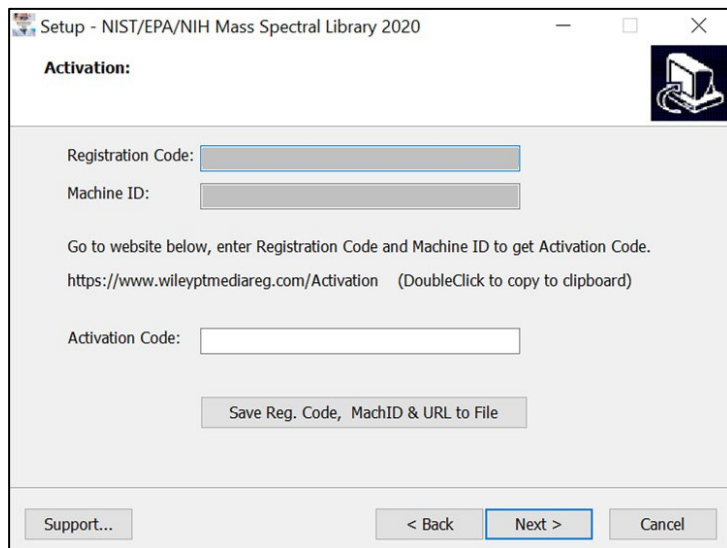
If the Registration Code is correct, you will be brought to the Activation screen. If your machine has internet connectivity, choose to "Automatically activate over the internet" and then click "Next" to begin internet activation.



- 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.



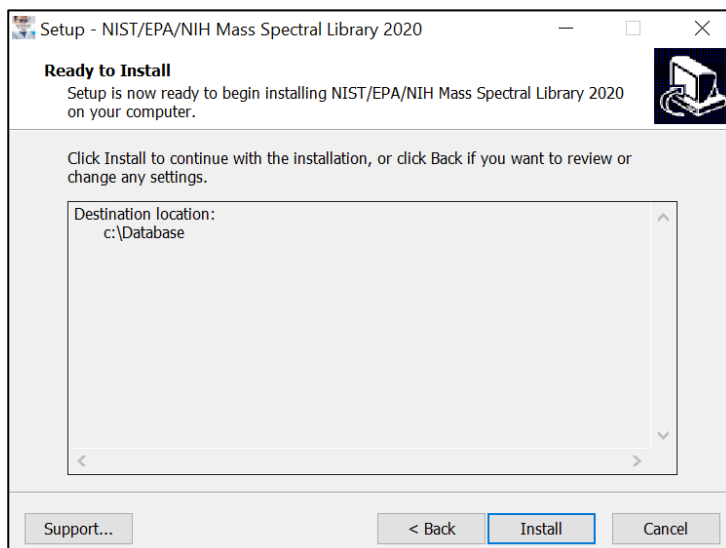
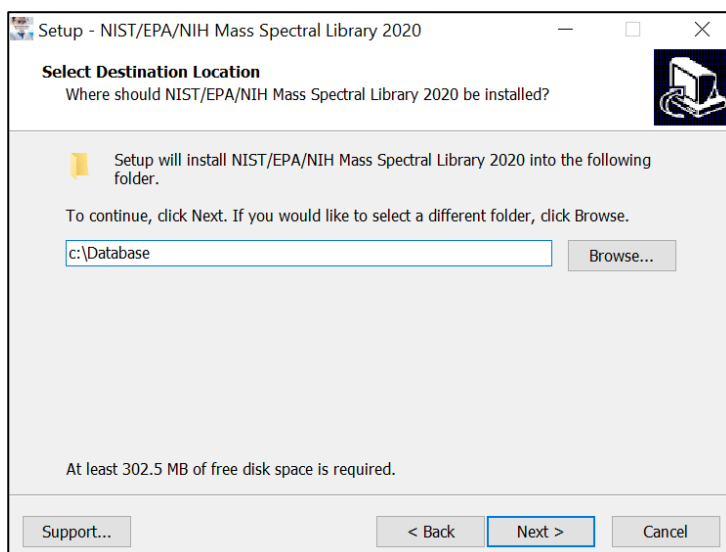
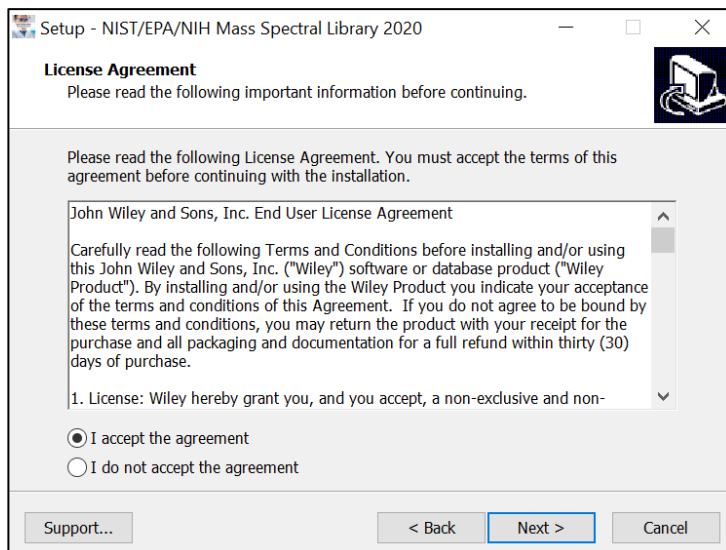
5. Once your activation is successful, proceed by pressing “Next.” The next screen contains the End User License Agreement (14).

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.

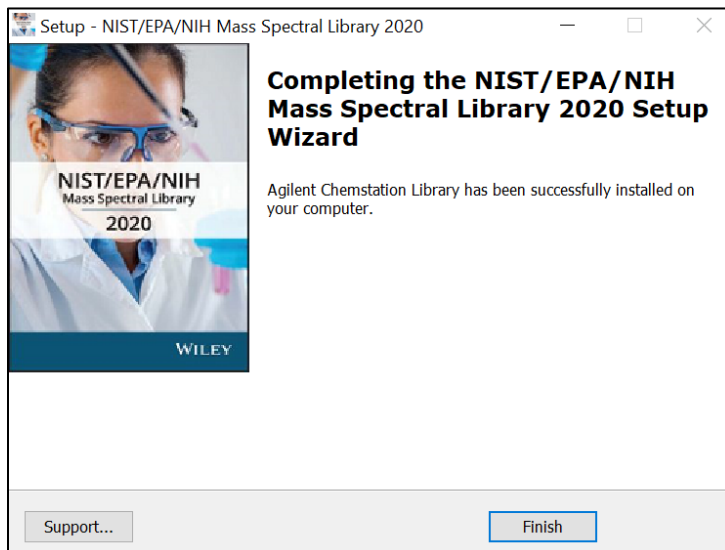
6. Press “Next” to proceed to the next step. At this point, the installer will unpack and install the library in the format you have selected. Confirm the target directory and destination location before proceeding.

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.



- 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/>

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.

NIST/EPA/NIH Mass Spectral Library 2020 – Thoroughly updated and more comprehensive than ever, the 2020 release of the NIST/EPA/NIH Mass Spectral Library is the one of the most trusted, versatile mass spectral data collections ever published.

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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 *NIST/EPA/NIH Mass Spectral Library 2020* and a specialized library such as *MS and GC Data of Drugs, Poisons, Pesticides, Pollutants, and Their Metabolites* or the *Mass Spectra of Flavors and Fragrances of Natural and Synthetic Compounds, 3rd Edition*.

Search Tips

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.

Specifications

	EI Library	MS/MS Library	GC Retention Library
Spectra	350,643	1,320,389	---
Compounds	306,869	30,999	139,693

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.

Agilent ChemStation/PerkinElmer TurboMass: For linking MS records to the respective structure records in the structure add-on files, the values in the CAS Registry Number field of the library are used. Since not for all records a CAS Registry Number is available, 'pseudo' CAS Registry Numbers were created to be able to link to the chemical structure. Please note that in these cases the entries don't represent real CAS Registry numbers and are used here only for referring to the structure record in the separate structure database file. These pseudo IDs used are created as 9-digit numbers with a leading '998' to make them distinguishable to real CAS Registry numbers. The NIST20 library does not contain any real 9-digit CAS Registry Numbers starting with '998'. Each individual pseudo CAS Registry Number is created as 998.000.000 + the NISTNO of the corresponding NIST record.

PerkinElmer TurboMass: Since the database format doesn't support entries with more than 9 digits, (real) CAS Registry Numbers with 10 digits were replaced with pseudo CAS Registry Numbers too (same format as for records without a CAS Registry Number).

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- Tandem MS (MSn)
- MS-TOF exact mass
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- 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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