



# **NIST/EPA/NIH Mass Spectral Library 2023**

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## User Manual

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# PUBLISHER'S NOTE

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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 scientists have come to rely on.

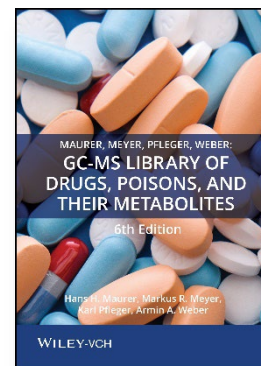
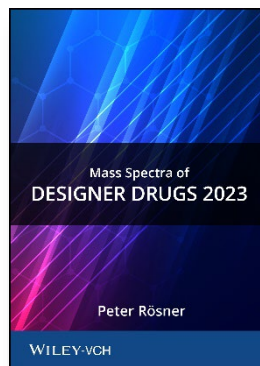
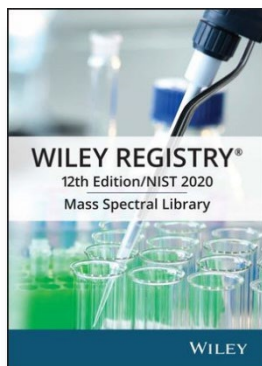
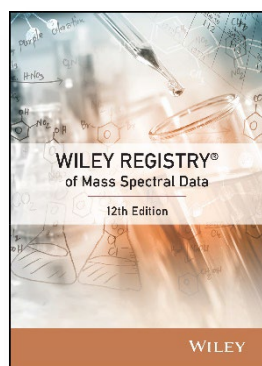
Thoroughly updated and more comprehensive than ever, the 2023 release of the *NIST/EPA/NIH Mass Spectral Library* is the one of the most trusted, versatile mass spectral collections ever published. It is made up of three types of libraries, an Electron Ionization (EI) mass spectral library, a MS/MS library, and a GC Retention Index library.

# COMPOUND SEARCH

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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.



# CONTACT INFORMATION

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## Editorial Correspondence

Wiley welcomes contributions of spectra for compounds, especially novel compounds not presently covered in the spectral library. Wiley can handle data in any machine-readable format. Data submissions, editorial notes, and 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  
Email: [dbinquiry@wiley.com](mailto:dbinquiry@wiley.com)  
Website: <https://sciencesolutions.wiley.com/>

## Customer Care

Customer care is available online or through correspondence at:

### Customer Care Center – Consumer Accounts

10475 Crosspoint Blvd.  
Indianapolis, IN 46256 USA  
<https://support.wiley.com/s/>

# COMPLIANCE

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Products manufactured by WTS are in compliance with Directive 2011/65/EU of the European Parliament and of the Council of 8 June 2011 on the restriction of the use of certain hazardous substances in electrical and electronic equipment (also known as “RoHS Recast”). In addition, this declaration of conformity is issued under the sole responsibility of WTS. Specifically, products manufactured do not contain the substances listed in the table below in concentrations greater than the listed maximum value.

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

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## Hardware and Software Recommendations

- Operating System: Microsoft Windows (Windows 10 or 11 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.

## License

Unless specified otherwise in writing, this product is sold as a single computer license (for the avoidance of doubt, not networked). Multiple license and network licenses are available. For additional licenses, please contact your sales representative or e-mail [dbinquiry@wiley.com](mailto:dbinquiry@wiley.com).

Help keep the cost of libraries down by reporting all copyright and license violations to the publisher at [dbinquiry@wiley.com](mailto:dbinquiry@wiley.com).

# COMPATIBILITY

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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

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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	SetupNIST23ChemStation.exe	C:\Database\{libraryname}\{filename}
MassHunter	SetupNIST23MassHunter.exe	C:\MassHunter\Library\{libraryname}\{filename}
MS Search	SetupNIST23MSSearch.exe	C:\NIST23\MSSEARCH\{libraryname}\{filename}
TurboMass	SetupNIST23TurboMass.exe	C:\TurboMass\ldendb\{libraryname}\{filename} C:\TurboMass\ldendb\STRUCTDB\{libraryname}\{filename}
GCMSsolution	SetupNIST23GCMSsolution.exe	C:\GCMSsolution\Library\{libraryname}\{filename}
MassLynx	SetupNIST23MassLynx.exe	C:\MassLynx\ldendb\{libraryname}\{filename} C:\MassLynx\ldendb\STRUCTDB\{libraryname}\{filename}

# QUICK-START

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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**

10475 Crosspoint Blvd.  
Indianapolis, IN 46256 USA



# 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.

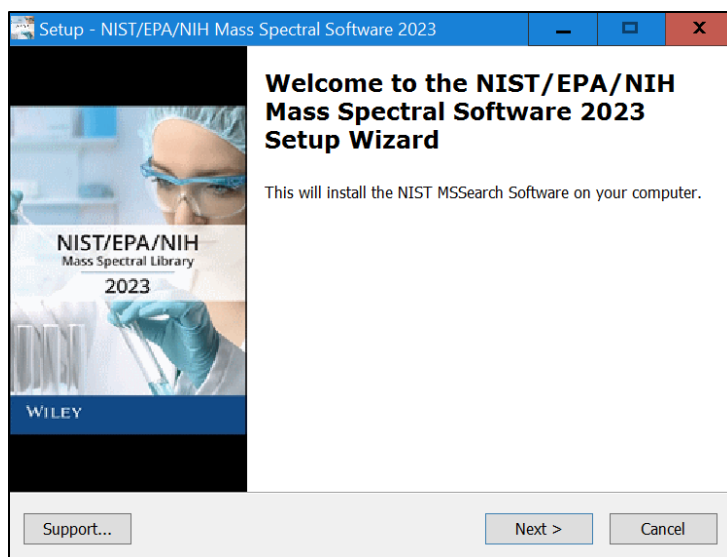
2. Insert the flash drive for installation. One file "Installation.htm" is included on the drive to simplify installation by using your web browser. Choose the format(s) you wish to install. Choosing to run the installer will bring you to a set-up wizard splash screen. Choose "Next."

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.**

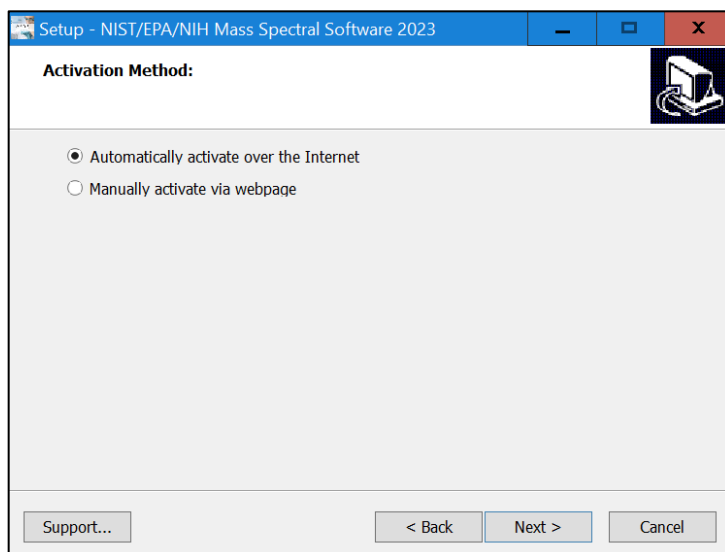
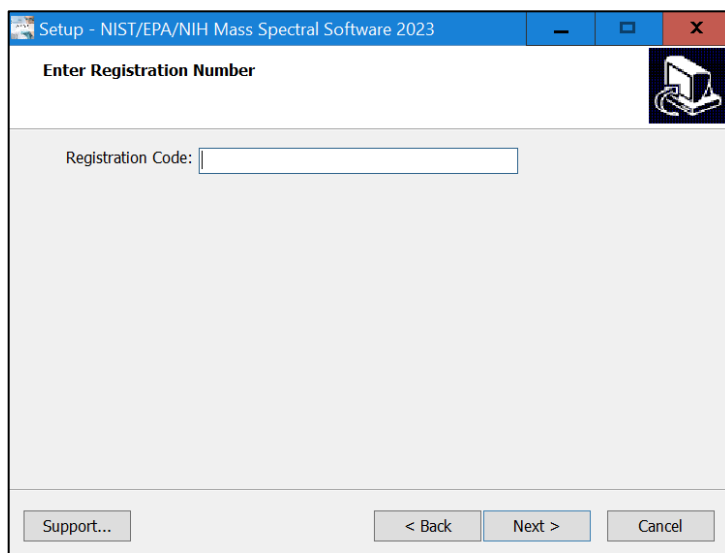


### 3. Registration Code and Machine ID

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.

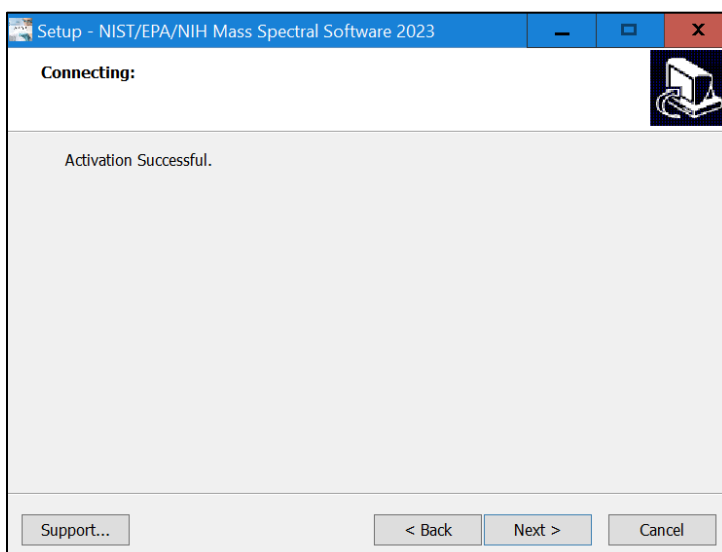
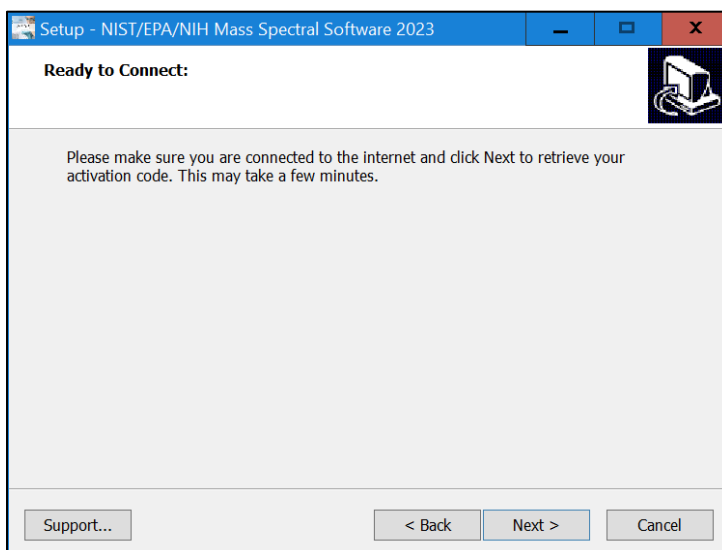
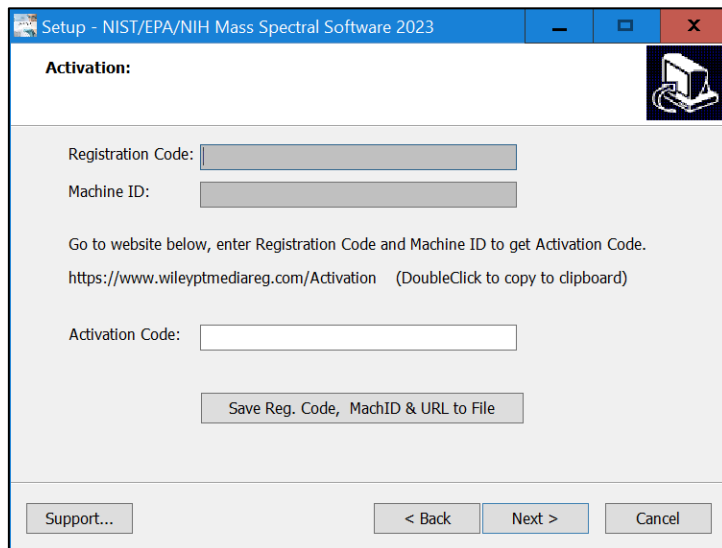
If the Registration Code is correct, you will be brought to the Activation screen. If your machine has internet connectivity, choose to "Automatically activate over the internet" and then click "Next" to begin internet activation.



- 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.



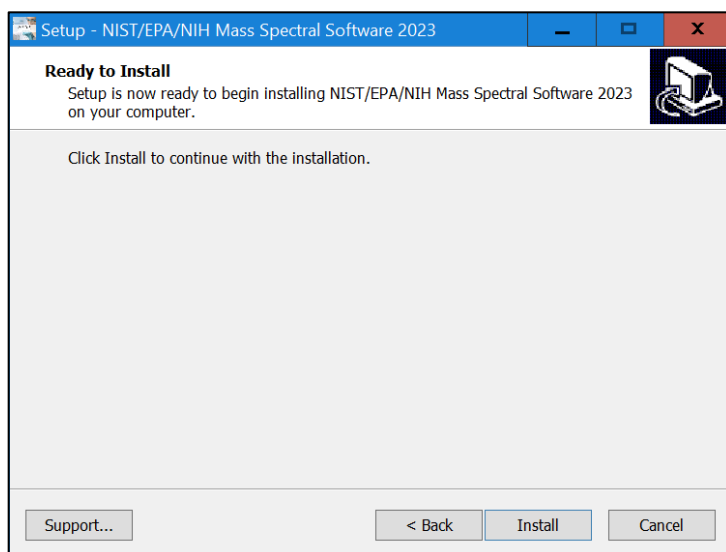
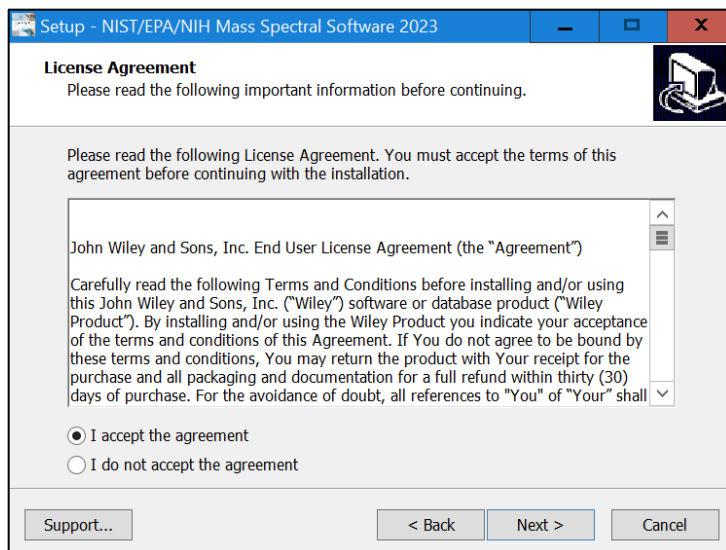
5. Once your activation is successful, proceed by pressing "Next." The next screen contains the End User License Agreement (97).

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.

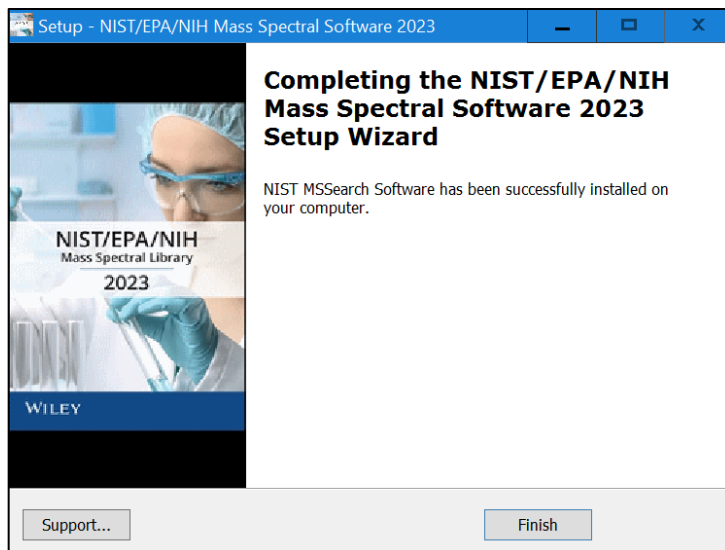
6. Press "Next" to proceed to the next step. At this point, the installer will unpack and install the library in the format you have selected. Confirm the target directory and destination location before proceeding.

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.



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/>

# GENERAL DATABASE CONTENT

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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 2023 – Thoroughly updated and more comprehensive than ever, the 2023 release of the NIST/EPA/NIH Mass Spectral Library is the one of the most trusted, versatile mass spectral data collections ever published.

Wiley Registry® – A complete, general-purpose high-quality library for analytical laboratories. Often used as the foundation library for research, quality control, deformation, and for forensic, toxicology, and homeland defense applications.

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 2023* and a specialized library such as the *Maurer, Meyer, Pfleger, Weber: GC-MS Library of Drugs, Poisons, and Their Metabolites, 6th Edition* 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	394,054	2,374,064	---
Compounds	347,100	51,501	180,618

## CAS-RN Field

Some mass spectrometry software programs rely on a field labeled "CAS-RN" to link spectral records with corresponding structure records. 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:** 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.

Most of CAS numbers in intervals [1000002-79-6, 1000562-64-8] and [1010004-87-4, 1010562-65-1] are not real CAS numbers if their check digits are incorrect (see Format section in [https://en.wikipedia.org/wiki/CAS\\_Registry\\_Number](https://en.wikipedia.org/wiki/CAS_Registry_Number)). Their last 6 digits are NIST registry number + 1,000,000,000 or 1,010,000,000. The second interval was used when the 1st produces correct check digit. These fake CAS numbers are used to link a spectrum to the corresponding chemical structure.

CAS r.n. above 21474836-4-3 were replaced for displaying purposes:

True CASRN	Replacement
2147718463	1047718466
2148923242	1048923245
2150476609	1050476602
2152153814	1052153817
2152883322	1052883325
2154283766	1054283769
2155618021	1055618024
2156314348	1056314341
2158976588	1058976581
2159083222	1059083225
2160555519	1060555512
2160555520	1060555523
2160555531	1060555534
2160555553	1060555556
2160555597	1060555590
2160569402	1060569405
2161566421	1061566424
2163571693	1063571696
2163724001	1063724004
2163847763	1063847766
2166085896	1066085899
2166566001	1066566004
2166598485	1066598488
2166915020	1066915023
2167319164	1067319167
2167325111	1067325114

2167949439	1067949432
2168229670	1068229673
2168407187	1068407180
2168553840	1068553843
2169309173	1069309176
2169458799	1069458792
2169498502	1069498505
2170110344	1070110347
2170219017	1070219010
2170550384	1070550387
2171492365	1071492368
2172698621	1072698624
2173386553	1073386556
2173565552	1073565555
2177287339	1077287332
2177288547	1077288540
2178996579	1078996572
2179307889	1079307882
2180247178	1080247171
2180543035	1080543038
2180924198	1080924191
2207805578	1007805573
2208818793	1008818798
2213087671	1013087676
2215083864	1015083869
2215437640	1015437645
2215567352	1015567357

2216965034	1016965039
2217145101	1017145106
2219319409	1019319404
2219320917	1019320912
2219324259	1019324254
2219324328	1019324323
2219331936	1019331931
2219332484	1019332489
2221100703	1021100708
2221100714	1021100719
2222298668	1022298663
2224446813	1024446818
2226434382	1026434387
2227542494	1027542499
2230013428	1030013423
2230662641	1030662646
2230706097	1030706092
2230715123	1030715128
2230798759	1030798754
2231672867	1031672862
2231674512	1031674517
2231674590	1031674595
2234276812	1034276817
2234307414	1034307419
2237296998	1037296993
2237297004	1037297009
2237961225	1037961220

2237963390	1037963395
2237963403	1037963408
2237963414	1037963419
2241239507	1041239502
2241239529	1041239524
2241239585	1041239580
2241239676	1041239671
2241373099	1041373094
2241684831	1041684836
2243815189	1043815184
2243973137	1043973132
2244443943	1044443948
2244737980	1044737985
2244864900	1044864905
2248014686	1048014681
2249872191	1049872196
2250019475	1050019470
2254710580	1054710585
2260975173	1060975178
2271590691	1071590696
2274162455	1074162450
2278261280	1078261285
2279683008	1079683003
2279917109	1079917104
2281697138	1081697133
2281748523	1081748528
2281777204	1081777209
2281918327	1081918322
2283389751	1083389756
2283789751	1083789756
2285245761	1085245766
2286078371	1086078376
2287683570	1087683575
2288022568	1088022563
2295336682	1095336687
2300734432	1100734437
2301169402	1101169407
2304610657	1104610652
2304915055	1104915050
2304915066	1104915061
2304915077	1104915072
2305155671	1105155676
2306686053	1106686058
2306823016	1106823011
2306823276	1106823271
2306823389	1106823384
2306823572	1106823577
2306823754	1106823759
2306825318	1106825313

2306825523	1106825528
2306827121	1106827126
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2306827552	1106827557
2306827881	1106827886
2306827938	1106827933
2306960132	1106960137
2307112485	1107112480
2307367800	1107367805
2307421323	1107421328
2307421436	1107421431
2307421469	1107421464
2307421776	1107421771
2307421801	1107421806
2307422597	1107422592
2307425416	1107425411
2307425687	1107425682
2307691832	1107691837
2308496957	1108496952
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2309383091	1109383096
2309383115	1109383110
2309383137	1109383132
2309383159	1109383154
2311933852	1111933857
2316839708	1116839703
2319878221	1119878226
2321352332	1121352337
2321936110	1121936115
2322064424	1122064429
2322211798	1122211793
2322759704	1122759709
2325222986	1125222981
2325347575	1125347570
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2326943615	1126943610
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2327168841	1127168846
2329070860	1129070865
2329072651	1129072656
2329293823	1129293828
2331254421	1131254426
2334114031	1134114036
2334480167	1134480162
2338332219	1138332214
2338332242	1138332247
2341528172	1141528177

2344231474	1144231479
2344231725	1144231720
2345373897	1145373892
2347179206	1147179201
2347745315	1147745310
2349358810	1149358815
2351142339	1151142334
2353459966	1153459961
2355385270	1155385275
2359227737	1159227732
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2361294122	1161294127
2361296628	1161296623
2361922327	1161922322
2362020026	1162020021
2362037485	1162037480
2364584723	1164584728
2365040704	1165040709
2365340389	1165340384
2365470977	1165470972
2365470999	1165470994
2365471027	1165471022
2365471038	1165471033
2365471050	1165471055
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2365542294	1165542299
2368252111	1168252116
2368931944	1168931949
2369641030	1169641035
2370977174	1170977179
2374285579	1174285574
2374320199	1174320194
2374892518	1174892513
2374983238	1174983233
2376189374	1176189379
2377403499	1177403494
2377403819	1177403814
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2379667168	1179667163
2380011572	1180011577
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2383722367	1183722362
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2666932450	1266932459
2666932552	1266932551
2666934547	1266934546
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2740821843	1340821842
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2748160985	1348160984
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2748301268	1348301267
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2748485143	1348485142
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2749326643	1349326642
2749326881	1349326880
2749391497	1349391496
2749394770	1349394779
2749394816	1349394815
2749428564	1349428563
2749618673	1349618672
2749897343	1349897342
2749985655	1349985654
2750249955	1350249954
2783144136	1383144135
2785346758	1385346757
2794878434	1394878433
2797119721	1397119720

**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.

Most of CAS numbers in intervals [900002-79-6, 900562-65-1] and [910011-95-2, 910562-64-3] are not real CAS numbers if their check digits are incorrect (see Format section in [https://en.wikipedia.org/wiki/CAS\\_Registry\\_Number](https://en.wikipedia.org/wiki/CAS_Registry_Number)). Their last 6 digits are NIST registry number + 900,000,000 or 910,000,000. The second interval was used when the 1st produces correct check digit.

These fake CAS numbers are used to link a spectrum to the corresponding chemical structure and synonyms.

Below are sorted lists of CAS r.n.

(1) A list of 6,357 CAS r.n. > 999,999,999, which were replaced with fake CAS r.n. for displaying purposes.

(2) A list of true 1,623 CAS r.n. in range 900,000,000 - 999,999,999 present in the library.

(1) The following are 6,357 CAS r.n. > 999,999,999, which were replaced with fake CAS r.n. for displaying purposes:

CAS r.n. 100018063 replaced with 900018066
CAS r.n. 1000018109 replaced with 900018102
CAS r.n. 1000018223 replaced with 900018226

CAS r.n. 1000174242 replaced with 900174245
CAS r.n. 1000189172 replaced with 900189175
CAS r.n. 1000313007 replaced with 900313000

CAS r.n. 1000313018 replaced with 900313011
CAS r.n. 1000339138 replaced with 900339131
CAS r.n. 1000339252 replaced with 900339255
CAS r.n. 1000339263 replaced with 900339266
CAS r.n. 1000339309 replaced with 900339302
CAS r.n. 1000339332 replaced with 900339335
CAS r.n. 1000339581 replaced with 900339584
CAS r.n. 1000339605 replaced with 900339608
CAS r.n. 1000339649 replaced with 900339642
CAS r.n. 1000339729 replaced with 900339722
CAS r.n. 1000339730 replaced with 900339733
CAS r.n. 1000339945 replaced with 900339948
CAS r.n. 1000339990 replaced with 900339993
CAS r.n. 1000340168 replaced with 900340161
CAS r.n. 1000340339 replaced with 900340332
CAS r.n. 1000340340 replaced with 900340343
CAS r.n. 1000340395 replaced with 900340398
CAS r.n. 1000340646 replaced with 900340649
CAS r.n. 1000341229 replaced with 900341222
CAS r.n. 1000341252 replaced with 900341255
CAS r.n. 1000341514 replaced with 900341517
CAS r.n. 1000341569 replaced with 900341562
CAS r.n. 1000342686 replaced with 900342689
CAS r.n. 1000342711 replaced with 900342714
CAS r.n. 1000342880 replaced with 900342883
CAS r.n. 1000342937 replaced with 900342930
CAS r.n. 1000342959 replaced with 900342952
CAS r.n. 1000343134 replaced with 900343137
CAS r.n. 1000343269 replaced with 900343262
CAS r.n. 1000343463 replaced with 900343466
CAS r.n. 1000343587 replaced with 900343580
CAS r.n. 1000343894 replaced with 900343897
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CAS r.n. 1000516584 replaced with 900516587
CAS r.n. 1000533038 replaced with 900533031
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CAS r.n. 1000775187 replaced with 900775180
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CAS r.n. 1000933196 replaced with 900933199
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CAS r.n. 1001026567 replaced with 901026560
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(2) The following are true 1,623 CAS r.n. in range 900,000,000 - 999,999,999 present in the library:

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