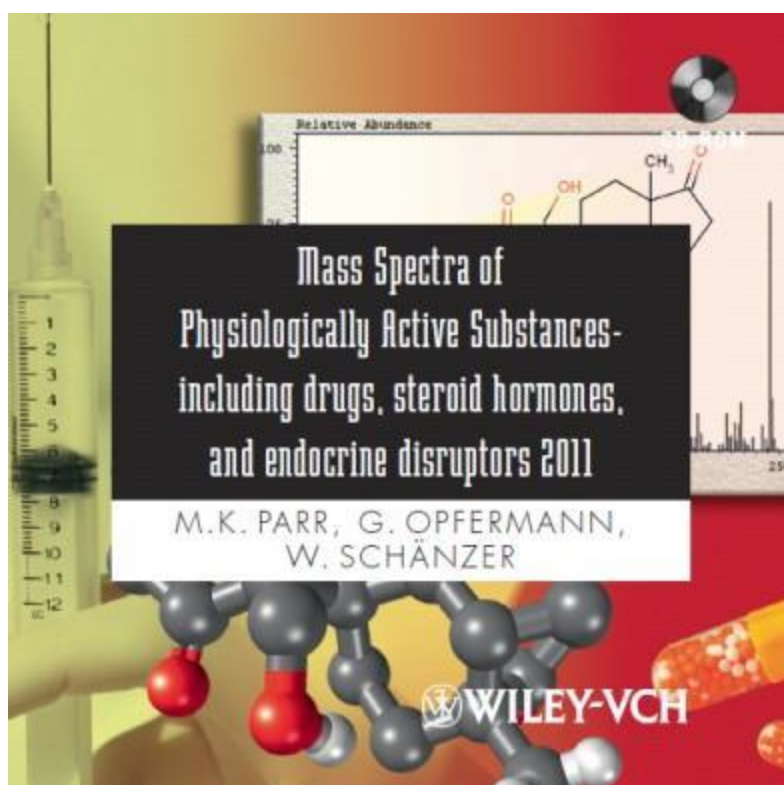


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## *INSTALLATION MANUAL*

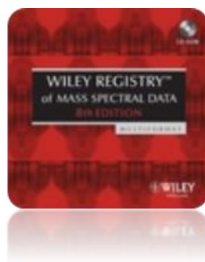
## *VERSION 1.0*



 **WILEY-BLACKWELL**

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# Wiley-Blackwell Data Collections



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John Wiley and Sons, Inc. 111 River Street, Hoboken, NJ 07030

 Please do not print this manual.



# Wiley-Blackwell Data Collections



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## FOREWORD

This latest edition contains:

- **Over 4180 spectra and chemical structures**

This library package contains the library **POS 2011** in the following manufacturer formats:

ACD/Labs *	INCOS
Agilent Chemstation	NIST MSSEARCH *
Finnigan GCQ	PerkinElmer TurboMass *
Finnigan SSQ	Shimadzu GCMS (QP-5000/QP-2010) *
Finnigan TSQ	Thermo Galactic SpectralID *
Finnigan ICIS	Varian Saturn
Finnigan INCOS	VG Labbase *
Finnigan Iontrap	VG Masslab *
Finnigan ITS40	Waters Masslynx *
Finnigan Magnum	Xcalibur *

\* Formats marked with an asterisk come with chemical structures.

Only one manufacturer format plus the NIST MS Search format may be installed on one machine. In case you purchased the collection from an instrument manufacturer, the license keys are provided through their sales staff. If you purchased a license from Wiley, you will be asked for the desired database format and get the appropriate keys.

**Helpful Hint:** License Keys are provided to you by the party from which you purchased the **POS 2011** collection.



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Since the format with which the database is delivered on this CD ROM is compatible with several programs, please check the manual of your specific software on how to install an additional library to your system. In particular, please check the destination folder to which the database files should be installed to for your spectrometer software to be able to open the files. In general, the destination directory given by default in the installer is **C:\POS2011\**, except for Agilent Chemstation, NIST/Xcalibur, PerkinElmer Turbomass, Shimadzu GCMS, Thermo Galactic SpectralID and Waters Masslynx formats. For the latter formats listed the default destination directories are:

ACD/Labs	C:\Program Files\ACD12\DATABASE
Agilent Chemstation	C:\Database\POS2011.L\
NIST / Xcalibur	C:\NIST08\MSSEARCH\POS2011\
PerkinElmer Turbomass	C:\TurboMass\ldendb\
Shimadzu GCMS	C:\GCMSsolution\Library\
Thermo Galactic SpectralID	C:\Program Files\Galactic\Data
Waters Masslynx	C:\Masslynx\ldendb\

The contents of this disc are compressed, which may require additional time decompressing the data.

Additional Information: If you have any question, please do not hesitate to contact us. E-mail: [techhelp@wiley.com](mailto:techhelp@wiley.com); phone: US (317) 572-3994; or Internet [www.wiley.com](http://www.wiley.com).



# Wiley-Blackwell Data Collections



## ACKNOWLEDGEMENTS

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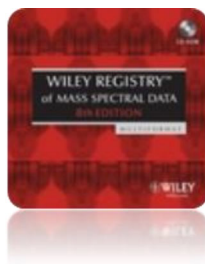
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### Market

Hospitals; Endocrinology; Sports universities; Governmental institutions; Crime laboratories; Doping control laboratories; Investigation laboratories.

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## Content

Steroids are of considerable therapeutic importance and play a substantial role in endocrinology, a medicine branch dealing with disorder of the endocrine system, an integrated system of small organs that involve the release of extracellular signaling molecules known as hormones.

On the other hand, steroids are increasingly being abused for performance enhancement by professional athletes, Olympians and even amateurs.

The identification of small amounts of steroids in body fluids is an analytical challenge. GC/MS is one of the key analytical techniques applied in these areas. For the fast and reliable identification of steroids, mass spectral reference data are essential.

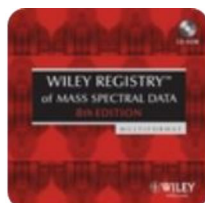
This newly expanded collection contains 4182 mass spectra and chemical structures of androgens and estrogens and their trimethylsilyl-, O-methoxyoxime- and acetal derivatives. Most spectra have been obtained on the same mass spectrometer under identical conditions. The data records include chemical name, chemical structure, molecular formula, and synonyms.

Average number of peaks: 145

**Some words about the new data being taken up (beta-2-agonists), about the change of the libraries name from Androstans, Estrogens and Other Steroids... (AES...) into Physiologically Active Substances... (POS...)????**

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## CONTACT INFORMATION

### Wiley Scientific, Technical and Medical Data Collections

John Wiley & Sons, Inc.  
111 River Street  
Hoboken, NJ 07030-5774  
USA

Telephone: +1-201-748-6000  
Fax: +1-201-748-8888

More information about data collections offered by STM Databases is available at

<http://www.wiley-vch.de/stmdata> and <http://www.wiley.com/go/databases> .

### Customer Care Center – Consumer Accounts

10475 Crosspoint Blvd.  
Indianapolis, IN 46256  
Phone: (877) 762-2974  
Fax: (800) 597-3299  
Web: <http://support.wiley.com>

## LICENSE

- Unless specified otherwise in writing, the *POS 2011* collection is sold as a single CPU license.
- Users are entitled to install the library in NIST MS Search and up to one (1) manufacturer format (e.g., Agilent, PerkinElmer, or Waters).
- Multiple license and network licenses are available.
- For additional licenses/copies e-mail [dbinquiry@wiley.com](mailto:dbinquiry@wiley.com) or [stmdata@wiley-vch.de](mailto:stmdata@wiley-vch.de).
- 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).

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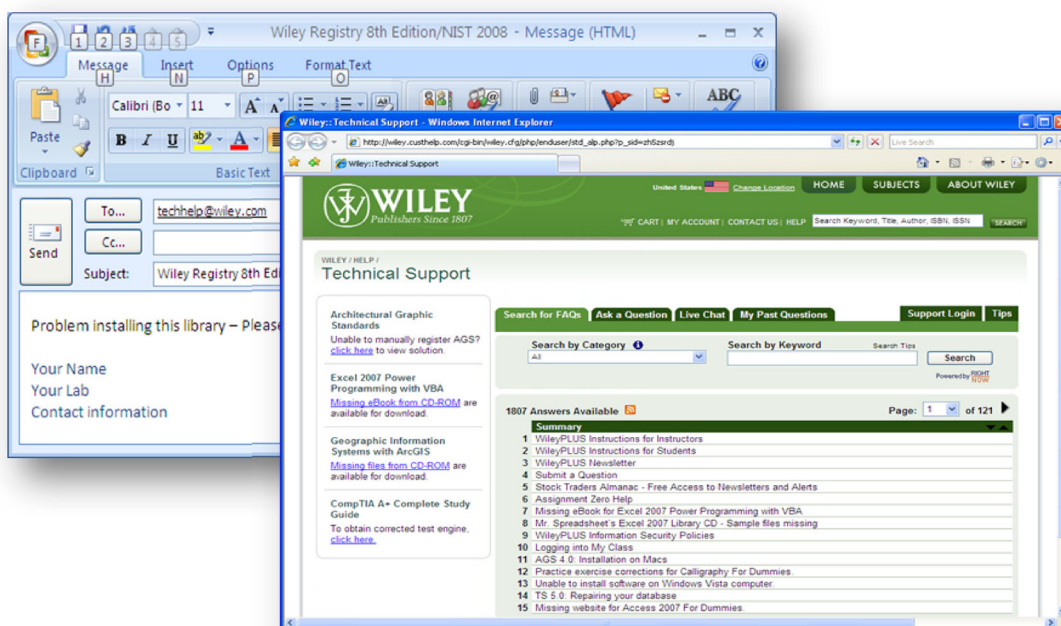
## GETTING STARTED

### Hardware and Software Requirements

The enclosed library comes in multiple manufacturer formats, but without manufacturer software. You must have mass spectrometry software installed on your computer prior to installing the mass spectrometry library, in all formats. Mass spectral data searching software is also available free from Standard Reference Data Program of the National Institute of Standards and Technology. NIST MSSearch Fully Functional Demo Program: [http://chemdata.nist.gov/mass-spc/Srch\\_v1.7/NISTDEMO\\_05.exe](http://chemdata.nist.gov/mass-spc/Srch_v1.7/NISTDEMO_05.exe). AMDIS Deconvolution Software is also available at: <http://chemdata.nist.gov/mass-spc/amdis>

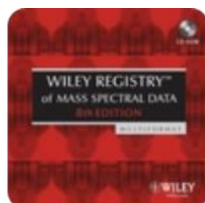
### Getting Help

Getting Help – you can choose 1) to go to <http://support.wiley.com> or 2) email [techhelp@wiley.com](mailto:techhelp@wiley.com)



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## 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 8e/NIST 2009 Mass Spectral Library* and a specialized library such as *POS 2011*.

## Searching 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 MSSearch, 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 illegal variants of designer drugs are only available in our specialized collections.

## Additional data files

On the installation CD you will find two files in Microsoft Excel (.xls) format containing additional information for each data record as well as data which could not be imported into some of the database formats. The two files, POS2011\_data\_list.xls and POS2011\_data\_list\_ordered\_by\_basepeak.xls, contain the same information. The only difference is the sort order of the data records appearing in these files. Users of the Finnigan GCQ, SSQ, TSQ, ITS-40, Magnum, ICIS, INCOS, Iontrap or the Varian Saturn format might find the second file helpful, since it shows the records in the same sort order (sorted by ascending base peak position) as in the respective databases.

## Adding Data

Please submit data to Wiley STM Data Collections directly at our offices in Hoboken or at [dbinquiry@wiley.com](mailto:dbinquiry@wiley.com)



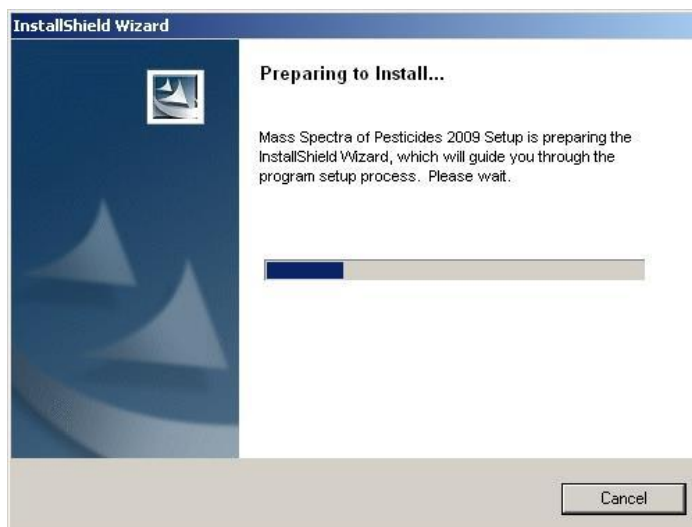
# Wiley-Blackwell Data Collections



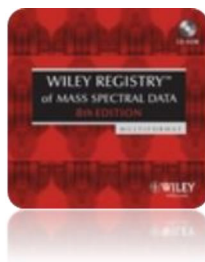
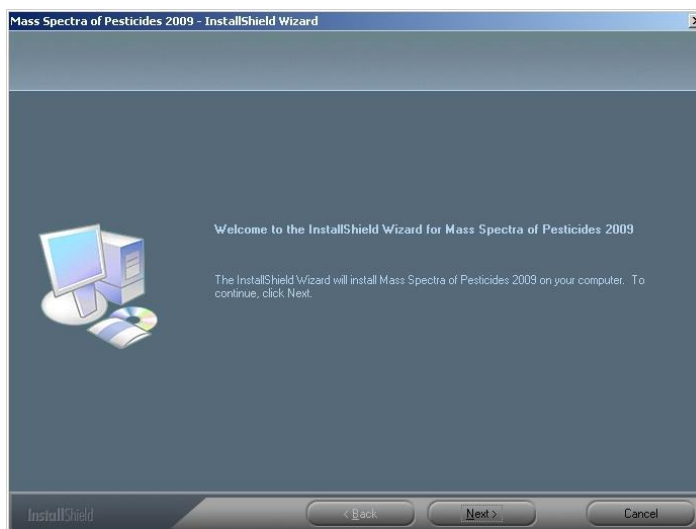
## Instructions for installing the library:

Insert the CD-ROM into your CD drive and start the installation by double-clicking the setup launcher program 'setup.exe' from the top-level directory of the CD-ROM.

The screenshots shown were taken during the installation of a different collection, but all steps described here apply analogously to the installation of the POS 2011 collection.



As soon as the setup launcher has finished his preparatory work a 'Welcome' screen is displayed:



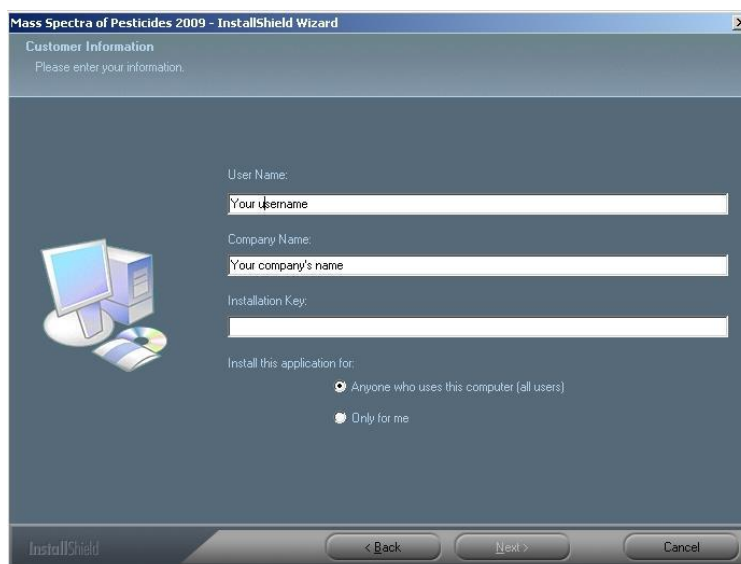
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Carefully read the End User License Agreement. If you agree to the terms, click “I accept..” and press the “next” button.



Include your name and your organization’s name in the Customer Information dialog. This information is only stored on your computer. Insert the license key for the format you would like to install and press “Next”.



In the exemplary installation shown here the license key for the NIST MSSEARCH format was used.

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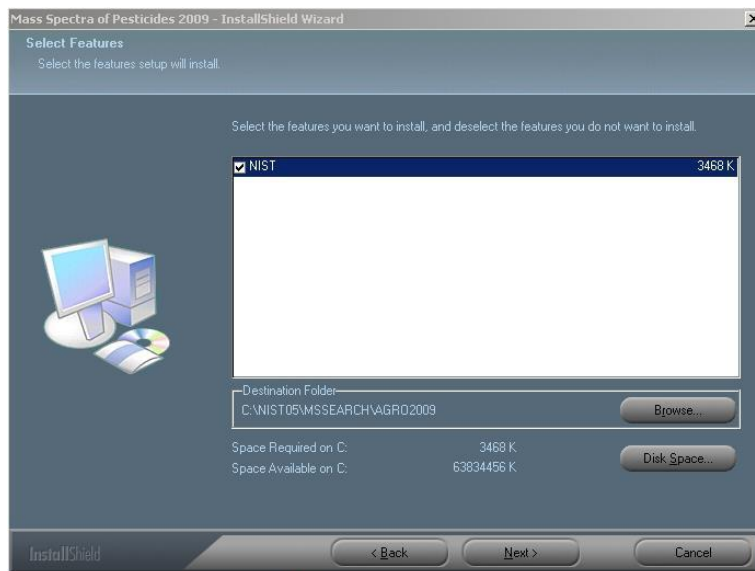
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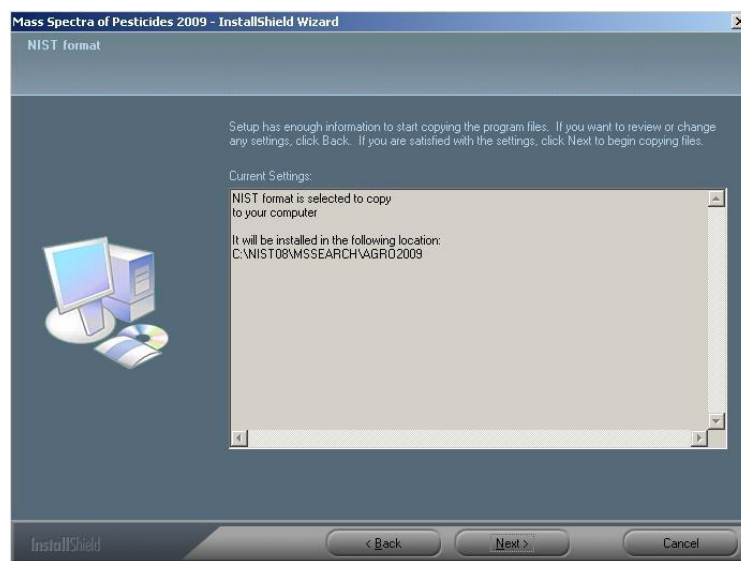
# Wiley-Blackwell Data Collections



The installation program will allow you to modify the target directory of the installation. This is not recommended without first consulting your software-specific user manual.

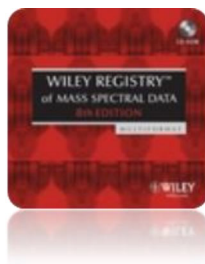


The last option screen provides an installation summary. Review the summary carefully before installing the library onto the computer hard drive. If you are not satisfied with the settings you made, you could use the 'Back' button to re-enter into the previous screen.



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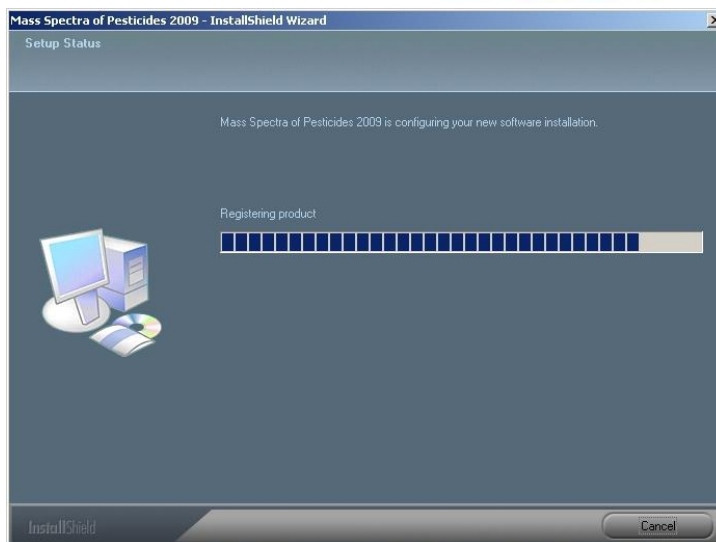
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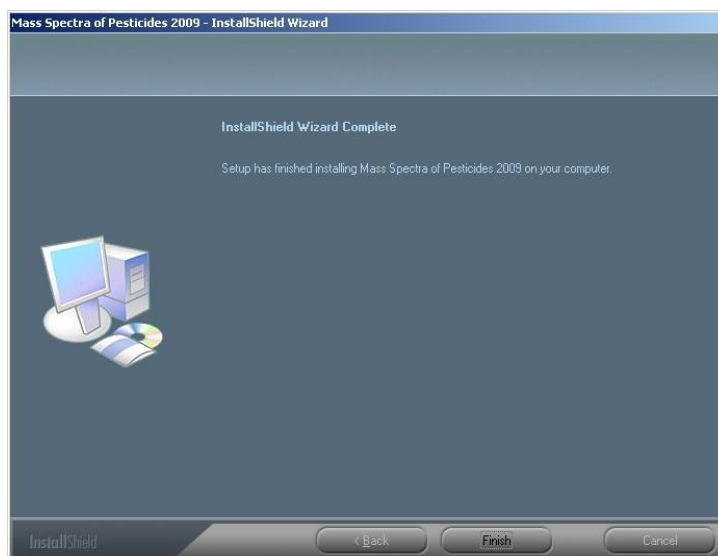
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The InstallShield Wizard then copies the files for the selected format to your hard disk and registers the format with the Windows system.



Click "Finish" to complete the installation.



The next section describes how to install an additional database format.



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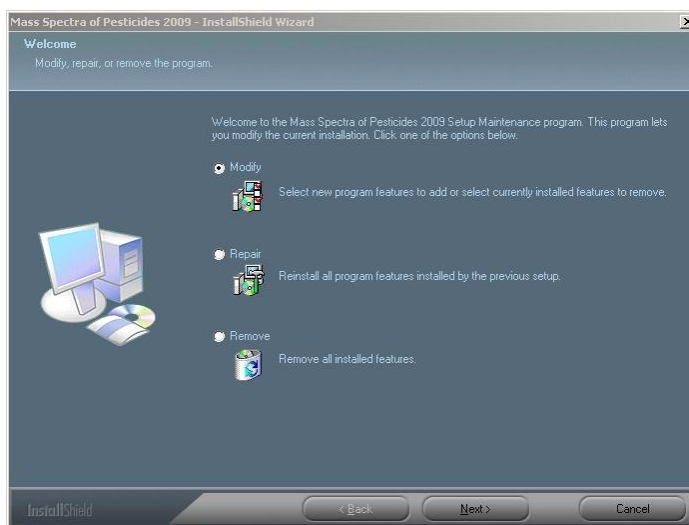


## *Modify the installation / Install an additional database format*

The modify option allows to install additional formats to your computer. Please note that changes to already installed databases **are not possible** using the 'Modify' option. **E.g. changing the installation directory of an already installed database could be selected, but will not work.** If

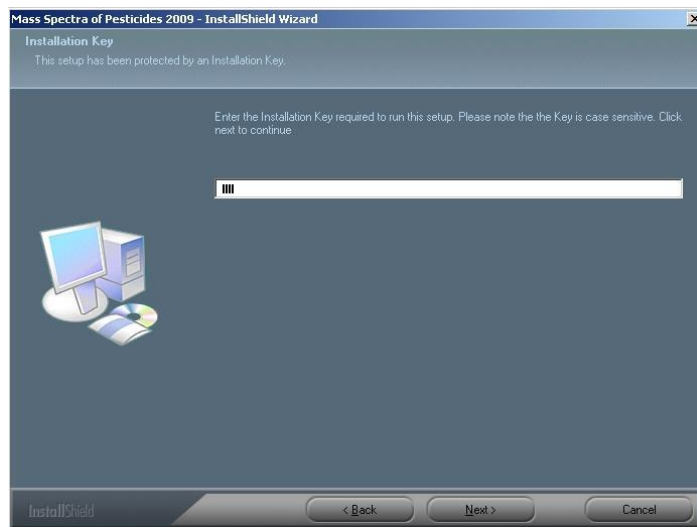
you need to change the location of an already installed database format, please uninstall the format first and re-install with the changed destination directory eventually. Please see the chapter 'Uninstalling database formats' for further instructions.

Start the setup launcher program again (double-click' the file 'setup.exe' located in the top-level directory of the CD-ROM). Select the 'Modify' option and click on the 'Next >' button.



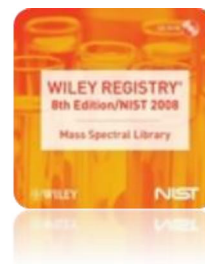
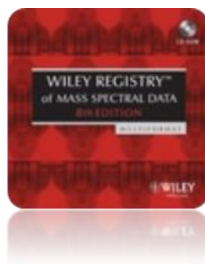
A Window shows up with an input area for the **installation key**. As described in the previous section, the license key should have been provided to you by your instrument manufacturer or Wiley.

**Helpful Hint:** License Keys are provided to you by the party from which you purchased the **POS 2011** collection.



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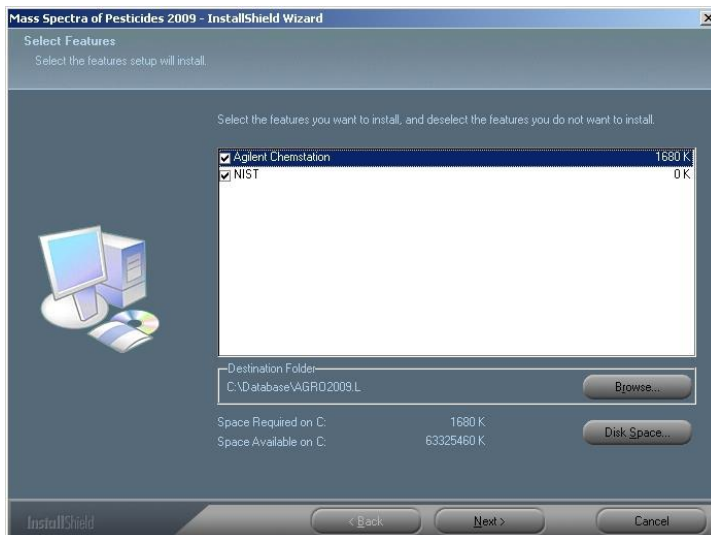
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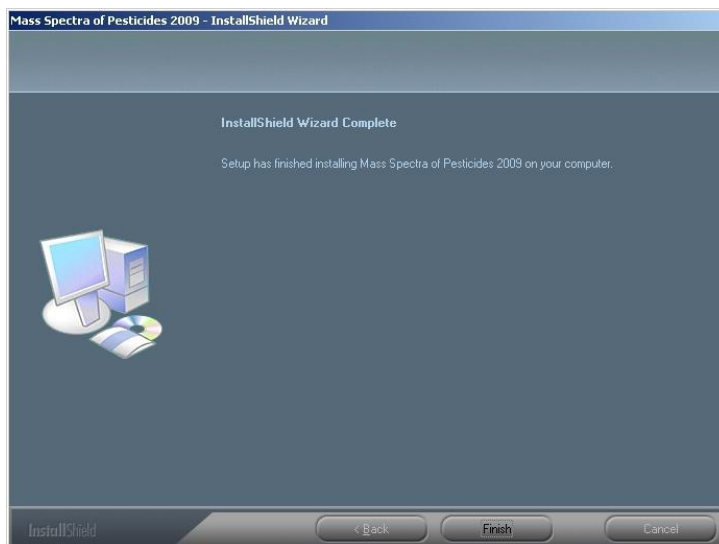
# Wiley-Blackwell Data Collections



In the example shown here the Agilent Chemstation format will be installed in addition to the NIST format installed before.

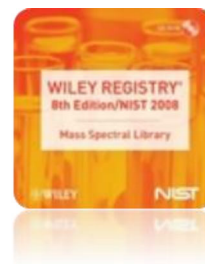
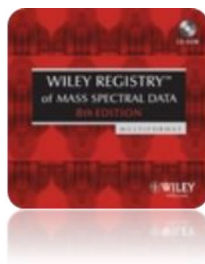


After the installation process finishes the installer returns with the 'Maintenance Complete' screen. Select the 'Finish' button to exit the installer application.



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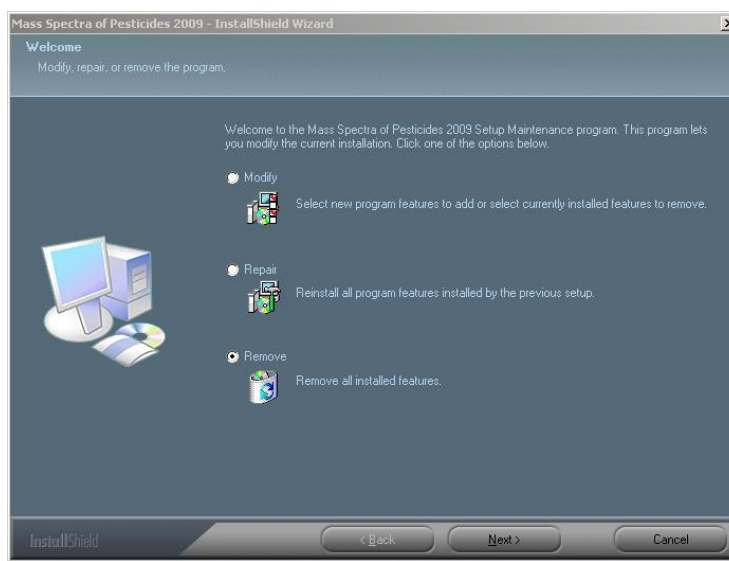
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## Uninstalling the POS 2011 Library

Use the Windows Control Panel to uninstall the library. After the InstallShield Wizard comes up, check the 'Remove' radio button and click 'Next'.

Please note that the Remove option doesn't allow to do a selection for specific database formats to be removed. **The Remove option always removes all installed database formats** which were installed with the specific installer before (it does not, however, remove any other database which was installed with a different installer, e.g. the POS 2011 installer. Remove option does not affect the installation of e.g. the Wiley Registry of Mass Spectral Data or any other files or programs).



Before the installer commences to remove all installed database formats the user is given a last chance to cancel the process by clicking the 'No' button. If you want to proceed with the complete deinstallation of all installed formats click the 'yes' button:



Once the uninstaller finishes its work the screen with the 'Finish' button comes up. Click the button to close the InstallShield Wizard.

**Hints:** *Windows Vista users: If you want to uninstall a format by using the Start/Programs option you need to select 'Run as Administrator' by a right mouse click. Folders will not be removed if 'Run as Administrator' has not been selected.*

*Windows XP users: Folder might not be removed if an application (e.g. Files Manager) locks the directory.*

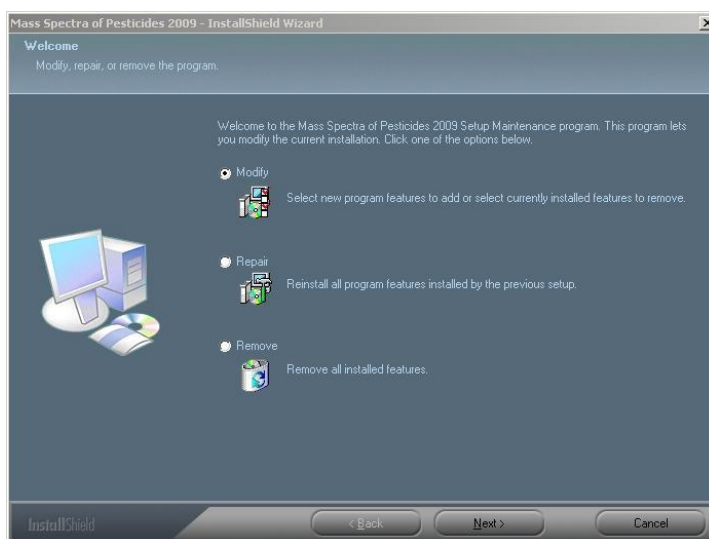


# Wiley-Blackwell Data Collections

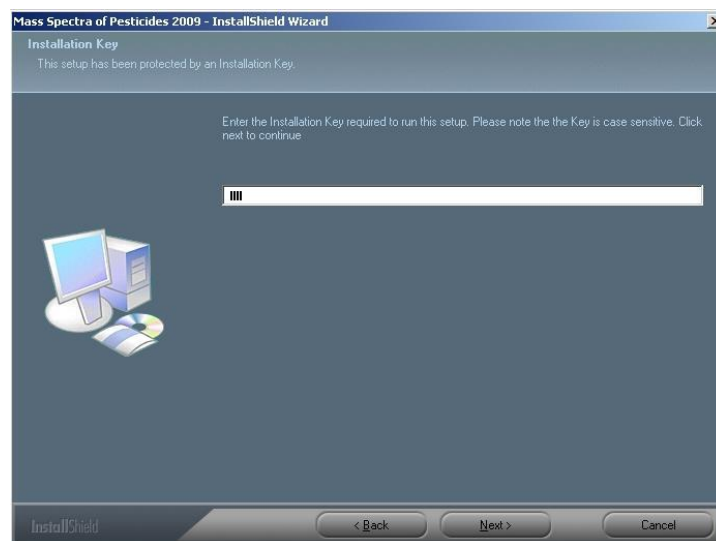


## *Removing selected database formats*

Individual database formats can be uninstalled by using the Modify option.

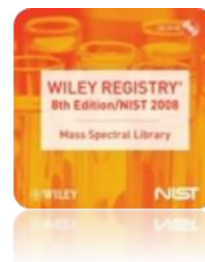
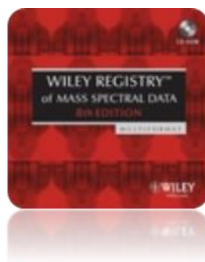


To display the formats stored on your computer you need to type in an installation key of one of the installed formats.



18

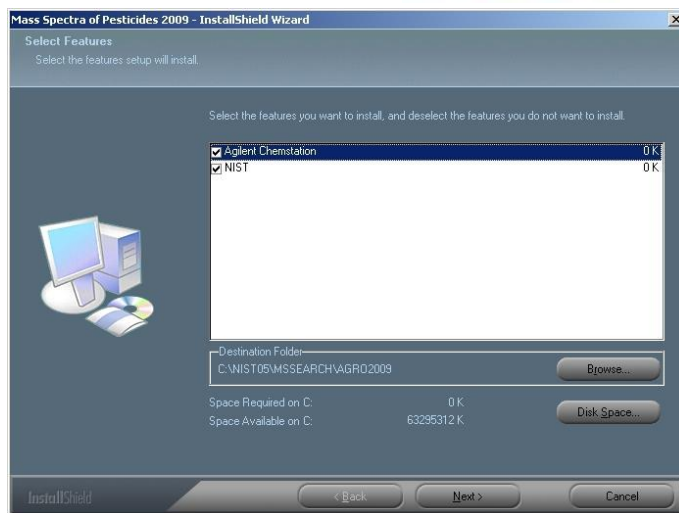
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# Wiley-Blackwell Data Collections

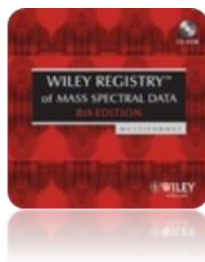
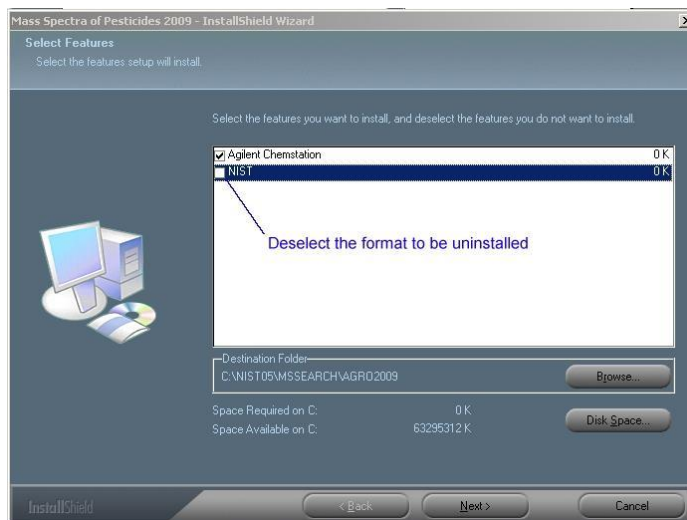


In the given example two database formats are installed – Agilent Chemstation and NIST. Note that the space requirements on the right side are set to '0 K' (zero kilobyte), indicating that these formats are already installed (and thus won't take up any additional space (i.e. 0 K) on your hard disk).



For removing only the NIST deselect the check box on the left of 'NIST'. Click on 'Next >' to initiate the uninstallation.

While the uninstallation is in progress the Installer screen will display a progress bar, after which you can click the "Finish" button to close the InstallShield Wizard (screenshots not shown here).



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## Special Note: ACD/Labs format

The ACD/Labs database has been created with the latest available software from ACD/Labs (ACD/Spectrum Database V12.0 and ACD/SpecManager V12.0) in the '.ND9' format. The database might thus not be compatible with older versions of the software.

The screenshot displays the ACD/SpecDB software window. On the left, the chemical structure of a steroid metabolite is shown, featuring four trimethylsilyloxy (TMS) groups and a fluorine atom. On the right, a mass spectrum plot shows relative intensity versus m/z, with a base peak at m/z 50. Below the structure and spectrum, the 'Structure User Data' section provides the following information:

CAS Registry Number	Original number	WILEY-ID
C32H63FO4Si4	DSHS_50_0004	50_4

Additional data includes the molecular formula C<sub>32</sub>H<sub>63</sub>FO<sub>4</sub>Si<sub>4</sub>, molecular weight 643.181, and nominal mass 642. The source is identified as 'Fluoxymesterone metabolite, 0,0',0'',0'''-tetrakis-TMS'. The retention time is 10.56 minutes. A small inset image shows the cover of the book 'Mass Spectra of Androgens, Estrogens, and other Steroids 2010'.

Screenshot of the POS 2011 database opened in ACD/SpecDB .



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## *Special Note: Agilent Chemstation*

The Agilent Chemstation software references chemical structures in the corresponding chemical structure database files POS2011.ind and POS2011.sdb (located in directory STRUCTDB below the ...\\POS2011.L installation directory) via the entries in the CAS Registry Number data field. Since not for all chemical structures CAS Registry numbers were available, additional pointers were added to the CAS Registry number data field. Due to format specifications these numbers look like real CAS Registry numbers. To allow these additional pointers to be easily distinguishable from real CAS Registry numbers the pointers are of form '99900x-xx-x', where 'x-xx-x' is the Library Entry number of the respective data record (e.g. for record **4** for which no CAS Registry Number is given, the pointer '99900**0-00-4**' is used). For additional information see the screenshot on next page and the separately provided PDF file named 'POS2011\_Appendix\_CASRN\_like\_Structure\_Pointers.pdf'.

### **Using the chemical structure database files with Agilent Chemstation software:**

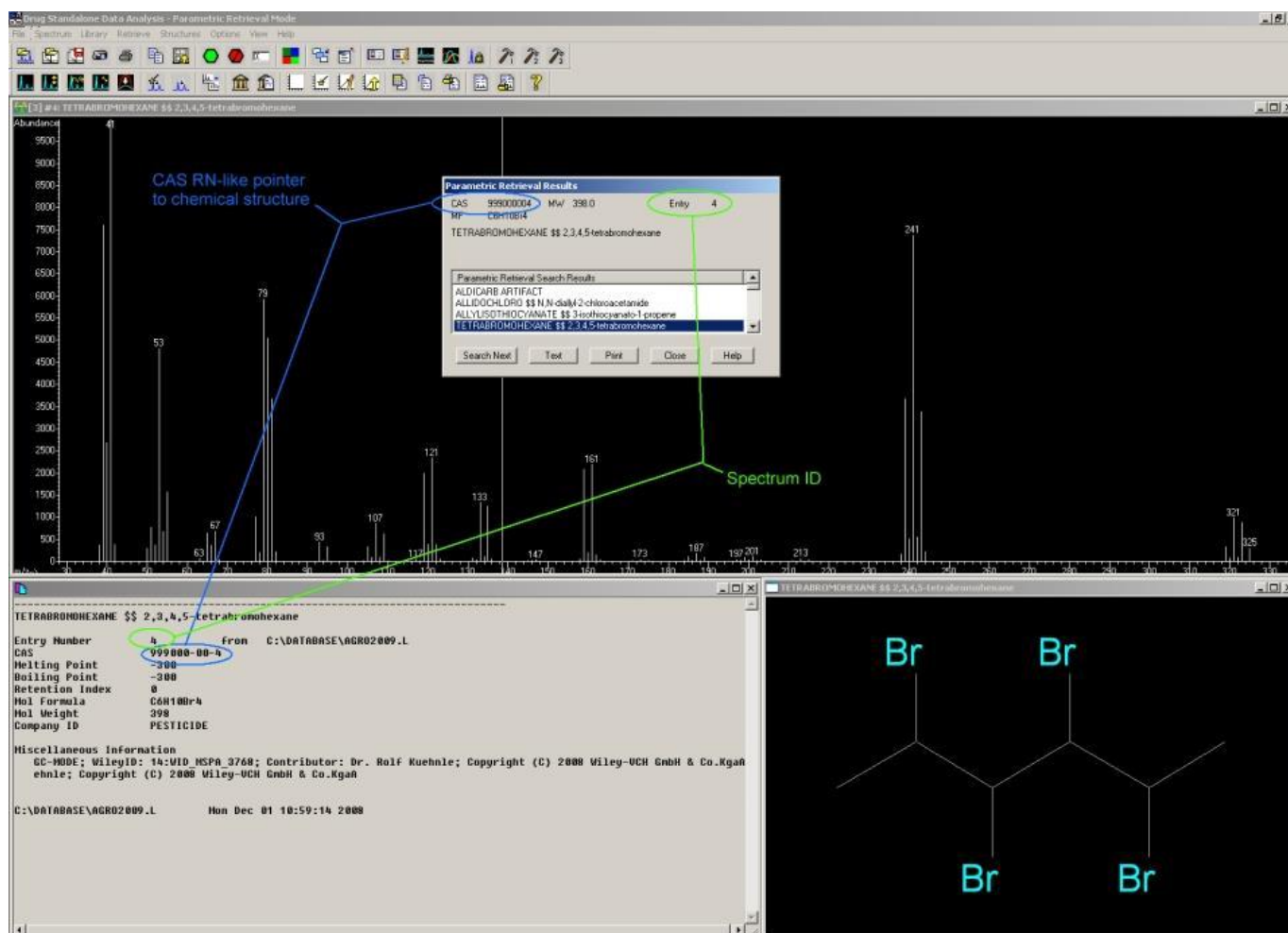
The Agilent Chemstation database files containing the spectral data (files CAS.IND, CONDENSE, CONDENSE.IND, HEADER, HEADER.IND, and ROOT) are installed into the C:\\DATABASE\\POS2011.L directory. The files containing the chemical structure data are placed in a subdirectory below the POS2011.L main installation folder.

To access the structure database files from you Chemstation software two options are available: From the Standard Menu select 'Define Chemical Structure Subsets...' from the Library menu item. This displays a new window from which the structure database files could be selected after clicking the 'Add New File ...' button in the lower right corner. Navigate to the directory where you installed the Chemstation database and go into the STRUCTDB subdirectory. Select the file POS2011.sdb and click the 'Open' button. The new structure database now appears in the list in the 'Chemical Structure Databases' window. Click 'OK' to finish up the registration of the structure database.

When you are in 'Parametric Retrieval Mode' (shown on the uppermost frame bar of the application window) use 'Select Structure Database...' from the 'Structures' menu item. Then proceed as described in the paragraph above to register the structure database files with your Chemstation software.



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Screenshot of the Agilent Chemstation user interface showing an exemplary data record (from a different database) where a CAS Registry Number like structure pointer was used to reference the chemical structure in the chemical structure data files



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## *Special Note: Waters Masslynx, PerkinElmer TurboMass and VG Labbase/Masslab formats*

The Waters Masslynx, Perkin-Elmer Turbomass and the VG Labbase/Masslab software suites reference chemical structures in the corresponding chemical structure database files (STRUCT.DB and STRUCT.IN) via the entries in the CAS Registry Number data field. Since not for all chemical structures CAS Registry numbers were available, additional pointers were added to the CAS Registry number data field. To allow these additional pointers to be easily distinguishable from 'real' CAS Registry numbers the pointers are of form '99900x-xx-x', where 'xx-xx-x' is the Library Entry number of the respective data record (e.g. for record **1046** for which no CAS Registry Number is given, the pointer '99900**1-04-6**' is used). For more information see the screenshot on next page and the separately provided PDF file named 'POS2011\_Appendix\_CASRN\_like\_Structure\_Pointers.pdf'.

### **Using the mass spectra database files with Waters Masslynx, Perkin-Elmer Turbomass and VG Labbase/Masslab software:**

The database files containing the spectral data (files .idb, .idi, .pdb and .pdi) are installed into the Idendb directory of your MassLynx or Turbomass installation. For a default installation that is in C:\Masslynx\Idendb and C:\TurboMass\Idendb, respectively. For the VG software the files are installed by default to C:\POS2011. The database files containing the chemical structure records are installed into a directory named C:\Masslynx\STRUCTDB\POS2011 or C:\TurboMass\STRUCTDB\POS2011, respectively. The structure files for the VG formats are installed below the path specified to install the mass spectrum database files. To access the POS2011 spectra database files select File/Search List... from the respective Search Library module. In the dialog window coming up select the Add... functionality to add the database to the list of databases to be searched.

### **Using the chemical structure database files with Waters Masslynx software:**

To access the POS2011 chemical structure database select File/Structures... from the Search Library module in your spectral software package. In the file browser window coming up select the STRUCT.DB file from the directory where the POS2011 chemical structure database files were copied into.

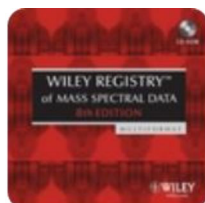


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File	Compound Name	rev	Library
1	Ergocalciferol II	270	DD:2008
2	Warfarin	261	DD:2008
3	Opipramol-M (OH) ZAC I	213	DD:2008
4	Fluocortafen	224	DD:2008
5	Chlorprothixen-M (Bisnor) AC	249	DD:2008
6	Opipramol-M (OH) ZAC 2	205	DD:2008
7	Chlorprothixen-M (Bisnor) AC	238	DD:2008
8	Chlorprothixen-M (Nor) AC	243	DD:2008
9	Chlorprothixen-M (Nor) AC	227	DD:2008
10	Warfarin AC	247	DD:2008
11	N,N-Ethyl-propyl-lysargamide AC	250	DD:2008
12	Lysargine	174	DD:2008
13	Ergocalciferol TMS IV	227	DD:2008
14	Cholecalciferol II	209	DD:2008
15	Chlorprothixen-M (Nor,-OH) AC	231	DD:2008
16	Chlorprothixen-M (-C2H6N,Ox) AC	201	DD:2008
17	Ergocalciferol DMBS IV	223	DD:2008
18	Cholecalciferol IV	199	DD:2008
19	Cholecalciferol III	190	DD:2008
20	Fumestrand-A (-C5H7F5SO)	194	DD:2008

Above: Screenshot of the Masslynx user interface showing an exemplary data record (from a different database) where a CAS Registry Number-like structure pointer was used to reference the chemical structure in the chemical structure data files.





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