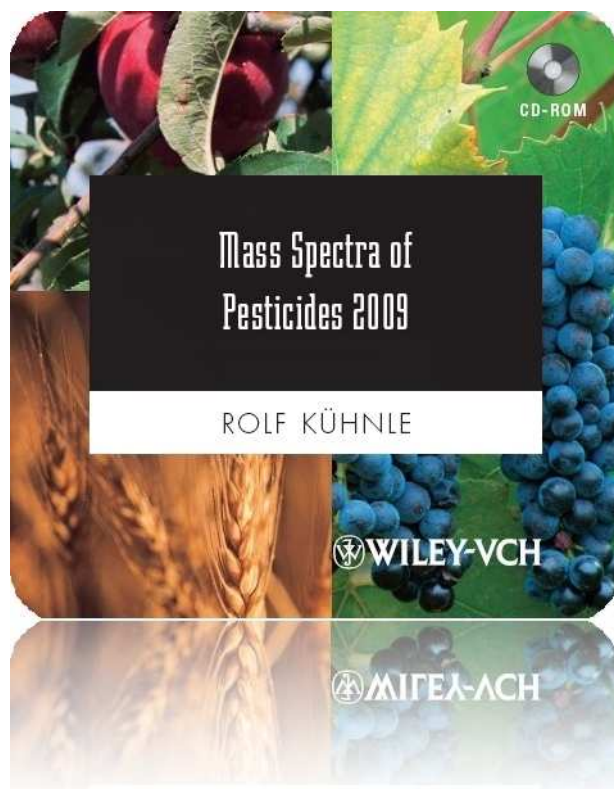


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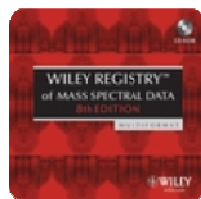
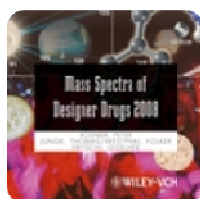


INSTALLATION MANUAL VERSION 1.0



 **WILEY-BLACKWELL**

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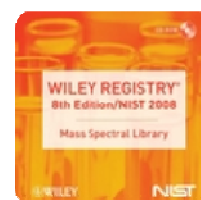
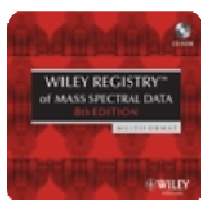
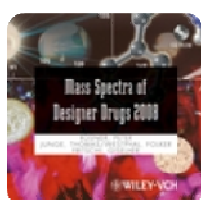
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 Please do not print this manual.

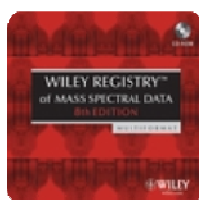
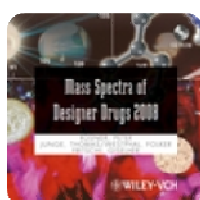


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FOREWORD

This latest edition contains:

- Over 1.230 spectra,
- Over 1.000 chemical structures

This library package contains the [Mass Spectra of Pesticides 2009](#) in the following manufacturer formats:

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

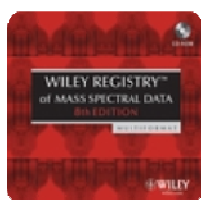
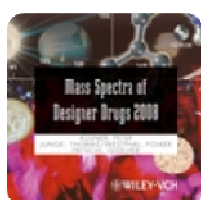
* Formats marked with an asterisk come with chemical structures.

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 [Mass Spectra of Pesticides 2009](#) collection.

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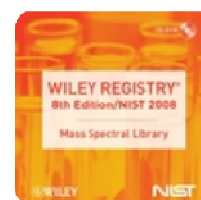
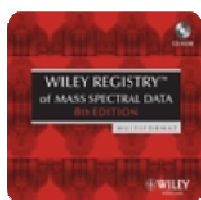
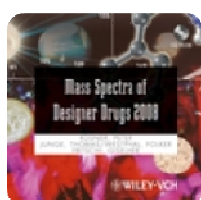


Since the format with which the database is delivered on this CD ROM is compatible with several programs, please check the manual of your specific software on how to install an additional library to your system. In particular, please check the destination folder to which the database files should be 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:\AGRO2009**, except for Agilent Chemstation, NIST/Xcalibur, PerkinElmer Turbomass, Shimadzu QP5000/QP2010, Thermo Galactic SpectralID and Waters Masslynx formats. For the latter formats listed the default destination directories are:

| | |
|----------------------------|--------------------------------|
| Agilent Chemstation | C:\Database\AGRO2009.L\ |
| NIST / Xcalibur | C:\NIST05\MSSEARCH\AGRO2009\ |
| PerkinElmer Turbomass | C:\TurboMass\ldendb\ |
| Shimadzu QP5000/QP2010 | 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; phone: US (317) 572-3994; or Internet www.wiley.com.



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ACKNOWLEDGEMENTS

Mass Spectra of Pesticides 2009

Dr. Rolf Kühnle

Regional Department of Criminal Investigation Niedersachsen, Germany

About the Author

Rolf Kühnle studied chemistry at the University of Hannover and got his PhD in chemistry in 1974. From 1971 to 1976 he worked at the Institute of Organic Chemistry. In 1976 he joined the Regional Department of Criminal Investigation Niedersachsen, Germany and took over responsibility for the mass spectrometry. 1995 he became group leader of the special division narcotics, toxic agents and body fluids.

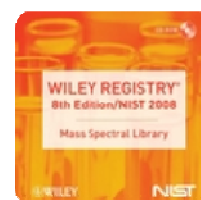
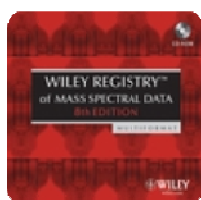
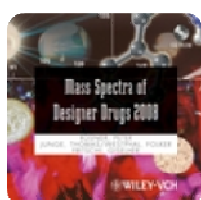


About the Author

A pesticide is any substance or mixture of substances intended for preventing, destroying, repelling, or mitigating any pest. Because most pesticides are designed to be toxic to their target pest and because any substance can be harmful if used improperly, pesticide use is strictly controlled. Environmental monitoring and reliable identification of pesticides in small amounts requires sophisticated analytical techniques such as mass spectrometry. To identify a pesticide, searchable mass spectral reference data are indispensable.

Content

This collection includes over 1.230 high quality mass spectra of pesticides such as insecticides, acaroids, nematicides, fungicides, rotenticides, molluscicides and repellents. The mass spectra are unreduced with an average number of peaks > 100. Chemical structure, CAS RN, synonym and



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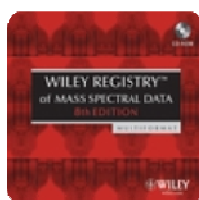
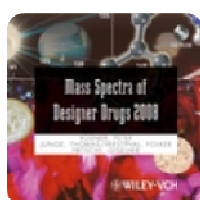
systematic name, molecular weight, molecular formula and experimental conditions complete the data record.

Market

Agricultural research and production; Toxicologists; Environmental chemists; Pharmacologists; Food Chemists; Scientists working in industry, government and academia looking at risk assessment; Treatment of poisoning and regulation; Mass spectrometry laboratories.

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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

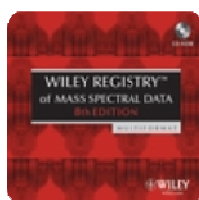
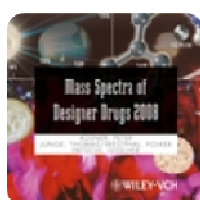
10475 Crosspoint Blvd.
Indianapolis, IN 46256
Phone: (877) 762-2974
Fax: (800) 597-3299
Web: <http://support.wiley.com>

LICENSE

- Unless specified otherwise in writing, the *Mass Spectra of Pesticides 2009* 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 or 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.

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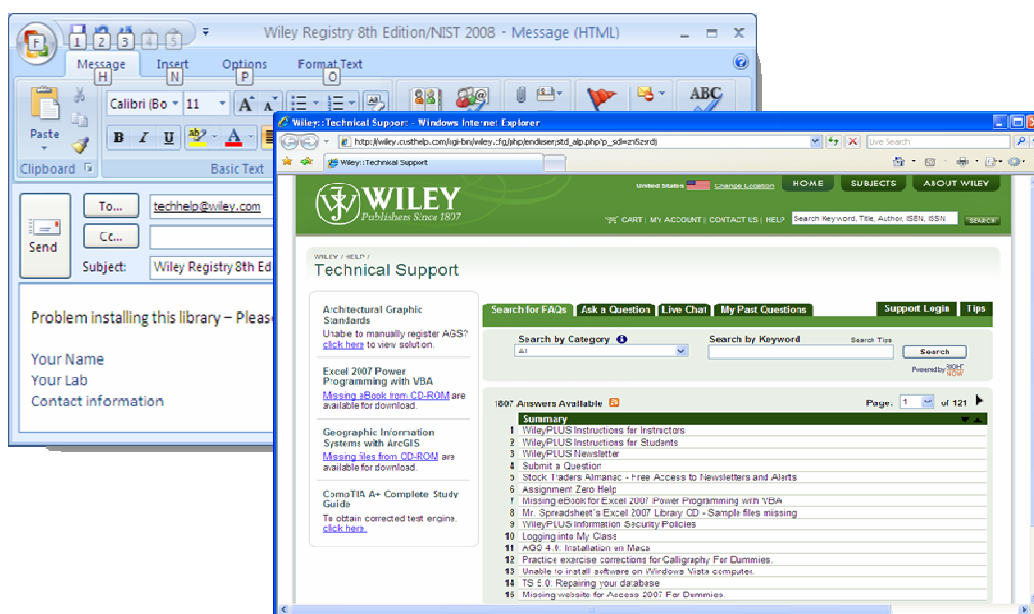
GETTING STARTED

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. AMDIS Deconvolution Software is also available at: <http://chemdata.nist.gov/mass-spc/amdis>

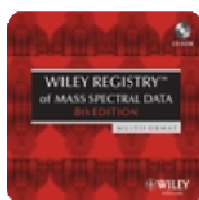
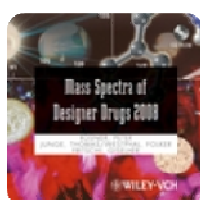
Getting Help

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



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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 2008 Mass Spectral Library* and a specialized library such as *FFNSC 1.3*.

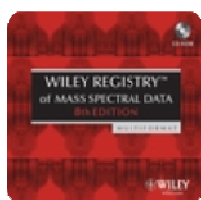
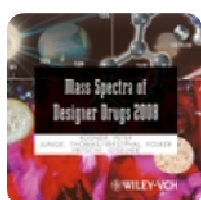
Searching Tips

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.

Adding Data

Please submit data to Wiley STM Data Collections directly at our offices in Hoboken or at dbinquiry@wiley.com

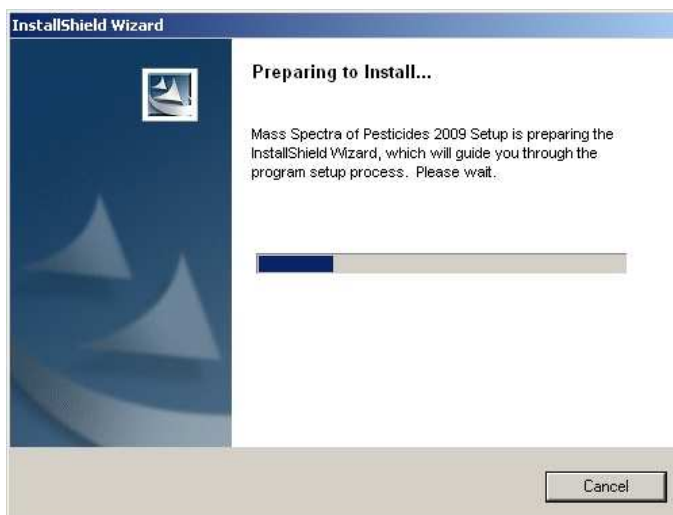


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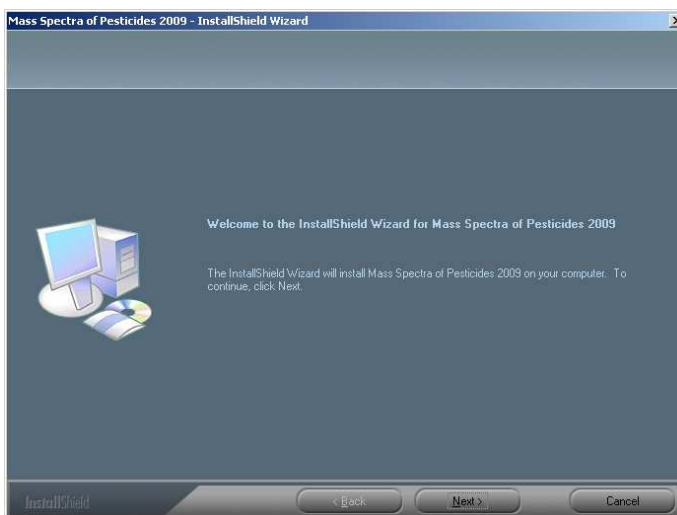


Instructions for installing the library:

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.

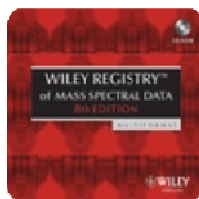
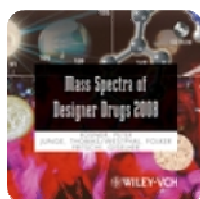


As soon as the setup launcher has finished his preparatory work a 'Welcome' screen is displayed:



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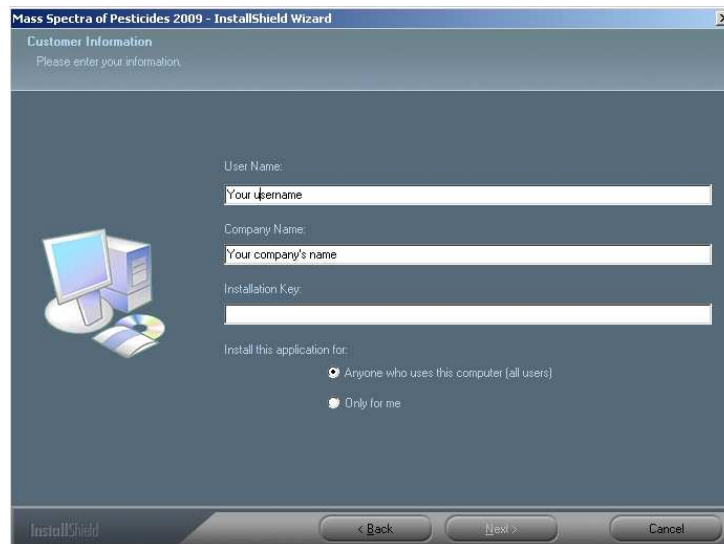
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Carefully read the End User License Agreement. If you agree to the terms, click "I accept.." and press the "next" button.



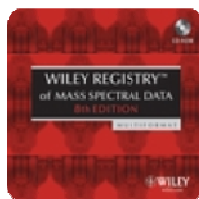
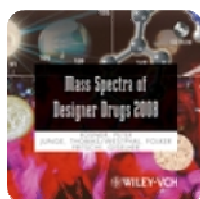
Include your name and your organization's name in the Customer Information dialog. This information is only stored on your computer. Insert the license key for the format you would like to install and press "Next".



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

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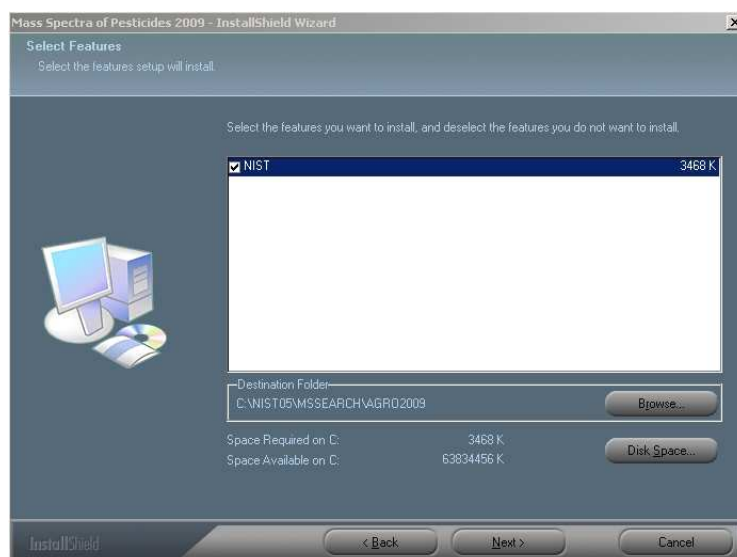
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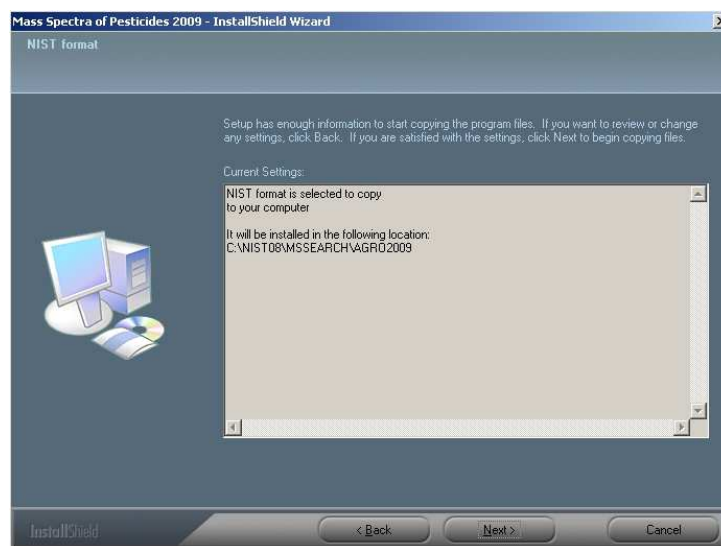
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The installation program will allow you to modify the target directory of the installation. This is not recommended without first consulting your software-specific user manual.

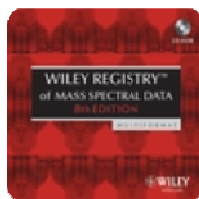
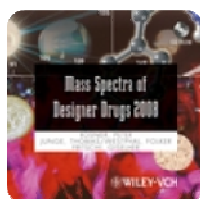


The last option screen provides an installation summary. Review the summary carefully before installing the library onto the computer hard drive. If you are not satisfied with the settings you made, you could use the 'Back' button to re-enter into the previous screen.



13

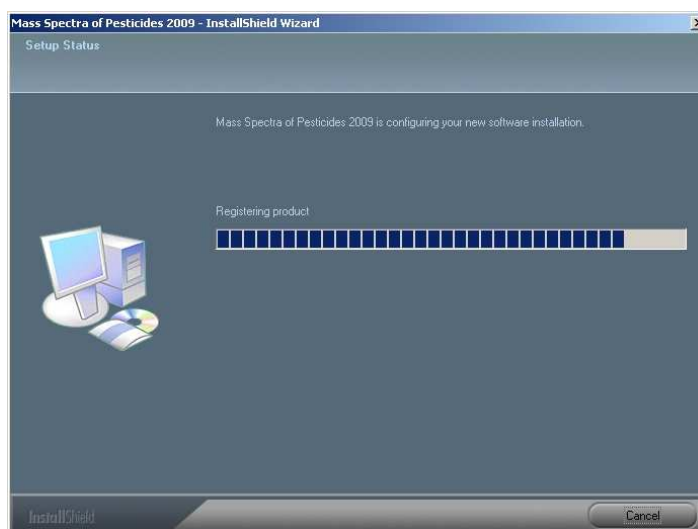
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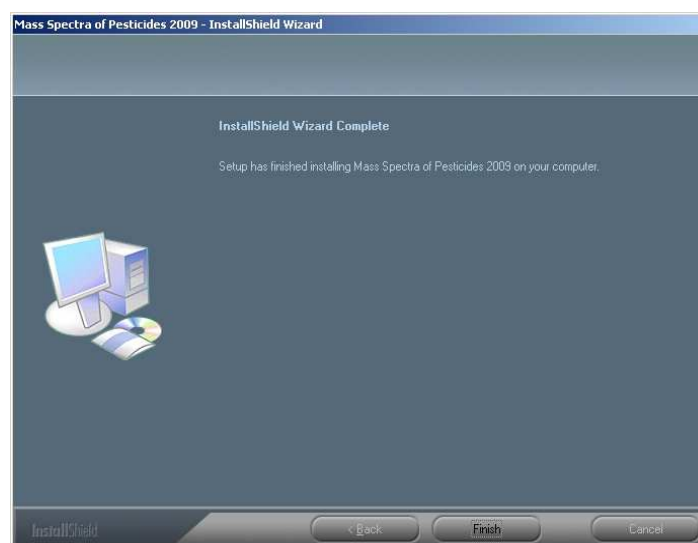
Wiley-Blackwell Data Collections



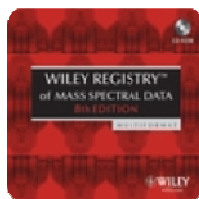
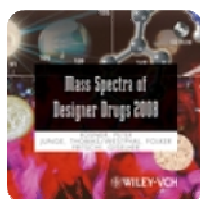
The InstallShield Wizard then copies the files for the selected format to your hard disk and register the format with the Windows system.



Click "Finish" to complete the installation.



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



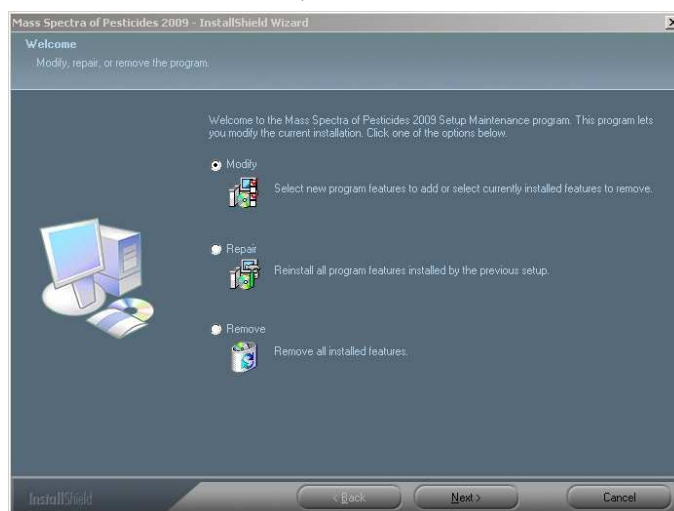
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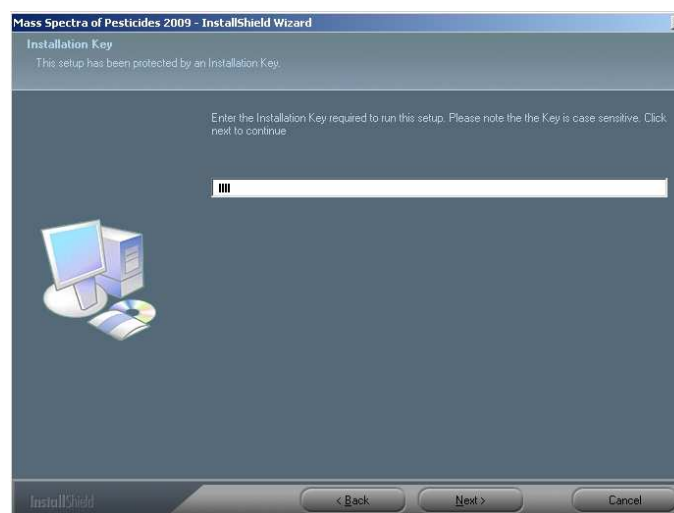
Modify the installation / Install an additional database format

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.

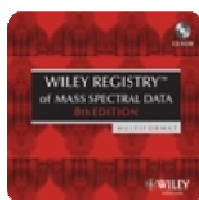
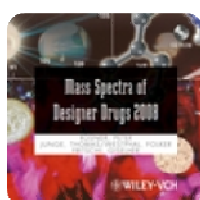


A Window shows up with an input area for the **installation key**. As described in the previous section, the license key should have been provided to you by your instrument manufacturer or Wiley.



15

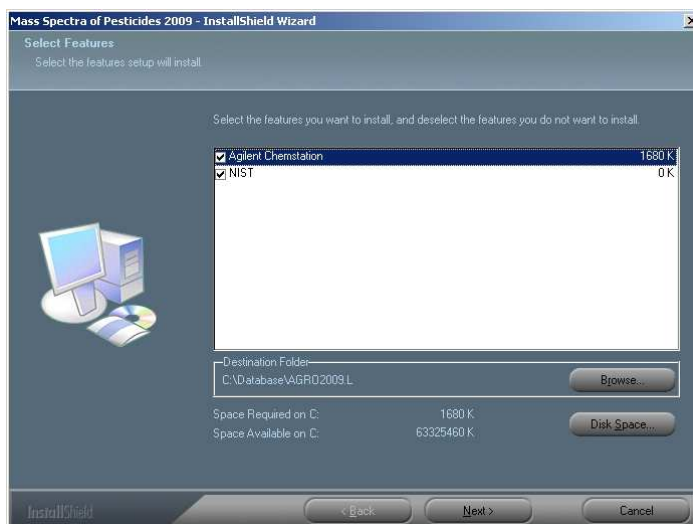
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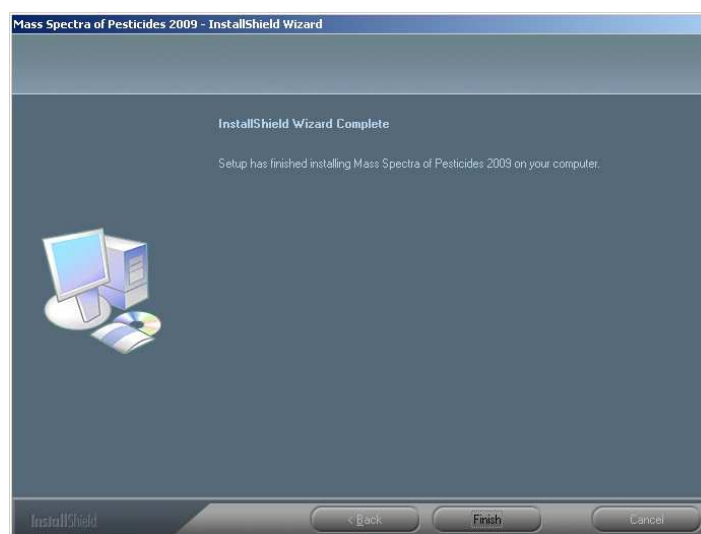
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In the example shown here the Agilent Chemstation format will be installed in addition to the NIST format installed before.

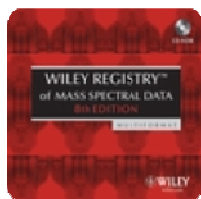
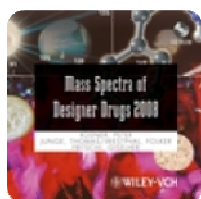


After the installation process finishes the installer returns with the 'Maintenance Complete' screen. Select the 'Finish' button to exit the installer application.



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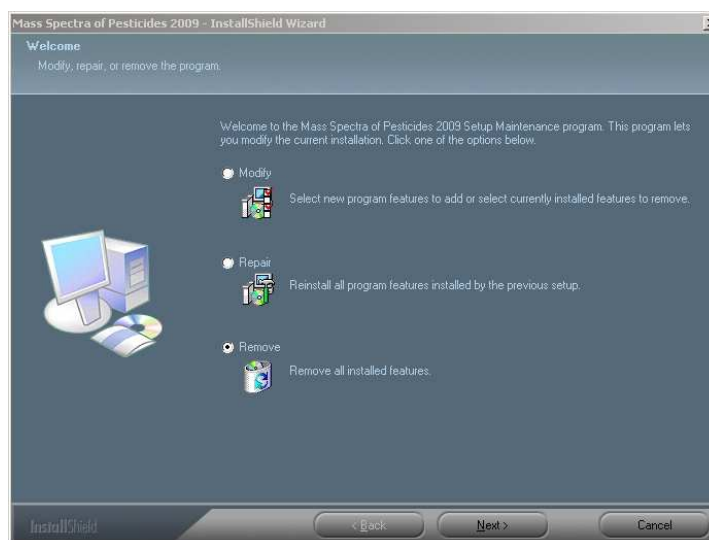
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Uninstalling the Pesticides 2009 Library

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 Pesticides 2009 installer Remove option does not affect the installation of e.g. the Wiley Registry of Mass Spectral Data or any other files or programs).



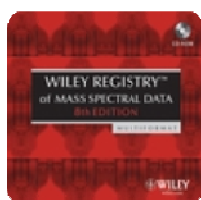
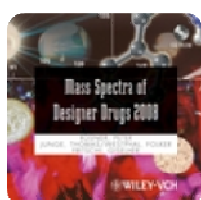
Before the installer commences to remove all installed database formats the user is given a last chance to cancel the process by clicking the 'No' button. If you want to proceed with the complete deinstallation of all installed formats click the 'yes' button:



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.

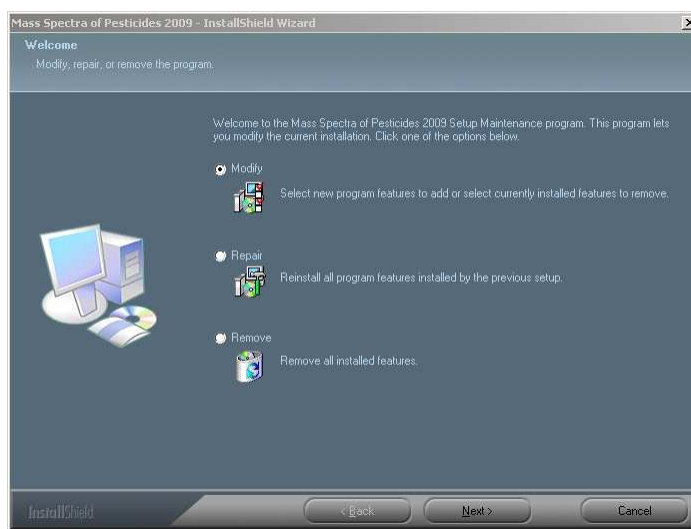


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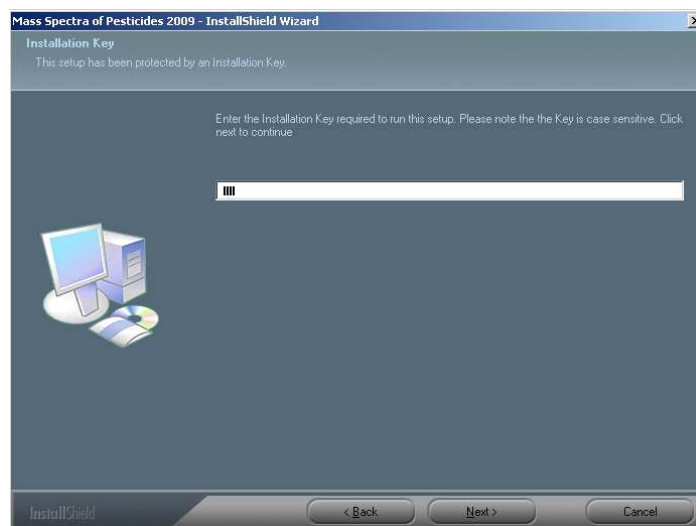


Removing selected database formats

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

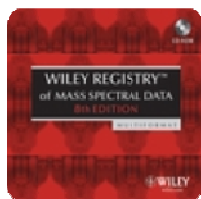
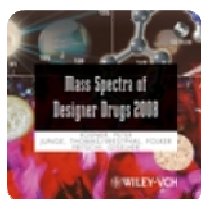


To display the formats stored on your computer you need to type in an installation key of one of the installed formats.



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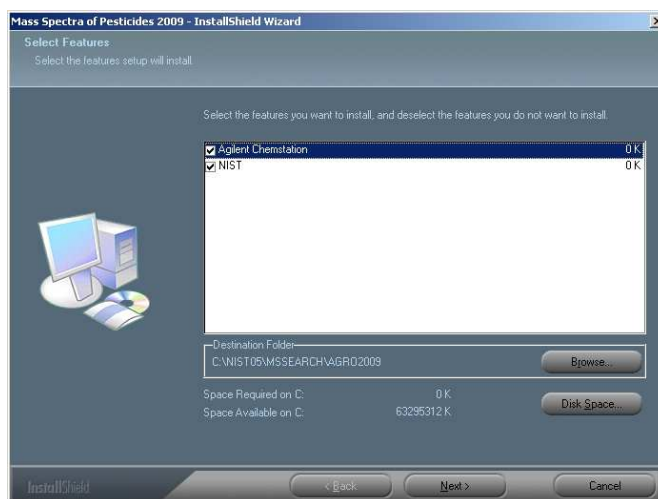
Wiley-Blackwell Data Collections
Hoboken • Weinheim • Chichester



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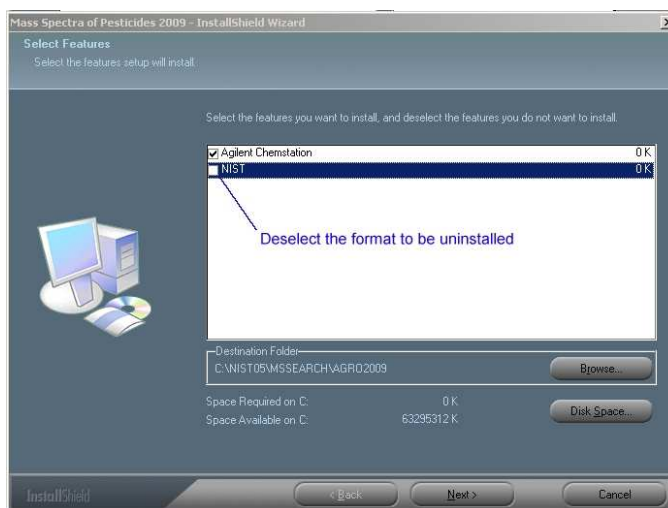


In the given example two database formats are installed – Agilent Chemstation and NIST. Note that the space requirements on the right side are set to '0 K' (zero kilobyte), indicating that these formats are already installed (and thus won't take up any additional space (i.e. 0 K) on your hard disk).



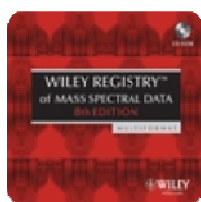
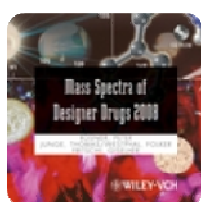
For removing only the NIST deselect the check box on the left of 'NIST'. Click on 'Next >' to initiate the uninstallation.

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 V11.0 and ACD/SpecManager V11.0) in the '.ND9' format. The database might thus not be compatible with older versions of the software.

The ACD/Labs format is provided together with a customized screen form which you could use with the database. After opening the database in ACD/SpecDB use the 'Screen Forms Manager available from View/Screen Forms/Manage Screen Forms... to load the form file 'AGRO2009.frm'. During the installation the 'AGRO2009.frm' is copied into the same folder as the database file (if you haven't changed the default path given in the installer, the two files are located in C:\AGRO2009).

ACD/SpecDB: Database Window - [D:\projects\databases\MS\KUEHNLE\P...CIDES_WORK\AGRO2009_MASTER\ACD\AGRO2009.nd9]

Structure User Data

| | | | | | | |
|---------------------------------------------------------|-----------------------------------------------------------------------------------------|------------------------------------------------|------------------|------------------|--------------|-----|
| FW: 444.5205 | CAS Registry Number | 56073-07-5 | WILEYID | T4:WID_MSPA_4360 | | |
| Formula: C ₃₁ H ₂₄ O ₃ | Molecular Formula | C ₃₁ H ₂₄ O ₃ | Molecular Weight | 444.52 | Nominal mass | 444 |
| Chemical Name | DIFENACOLUM | | | | | |
| Synonym Names | 3-[3-[1,1'-biphenyl]-4-yl-1,2,3,4-tetrahydro-1-naphthalenyl]-2-hydroxy-4H-chromen-4-one | | | | | |

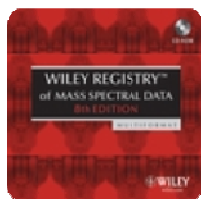
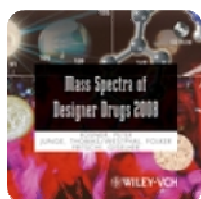
Technique: DI-MODE
Source of spectrum: Dr. Rolf Kühnle, Regional Department of Criminal Investigation Niedersachsen

Mass Spectra of Pesticides 2009
Source: Dr. Rolf Kühnle, Regional Department of Criminal Investigation Niedersachsen;
Copyright (C) 2009 John Wiley & Sons, Inc. - All Rights Reserved

ID: 1234 A: 1234/1238 B: 1238 MASS Single DB 12.11.2008 17:42:30

1-ChemSketch 2-Processor 3-Database

Screenshot of the Pesticides 2009 database opened in ACD/SpecDB making use of the customized screen form 'AGRO2009'.



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Special Note: Agilent Chemstation

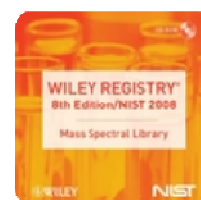
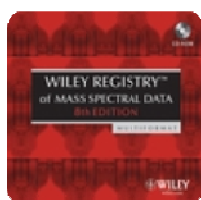
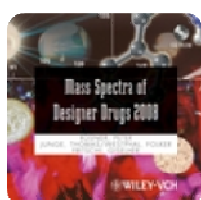
The Agilent Chemstation software references chemical structures in the corresponding chemical structure database files AGRO2009.ind and AGRO2009.sdb (located in directory STRUCTDB below the ...\\AGRO2009.L installation directory) via the entries in the CAS Registry Number data field. Since not for all 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**0-00-40**' is used). For additional information see the screenshot on next page and Appendix A.

Using the chemical structure database files with Agilent Chemstation software:

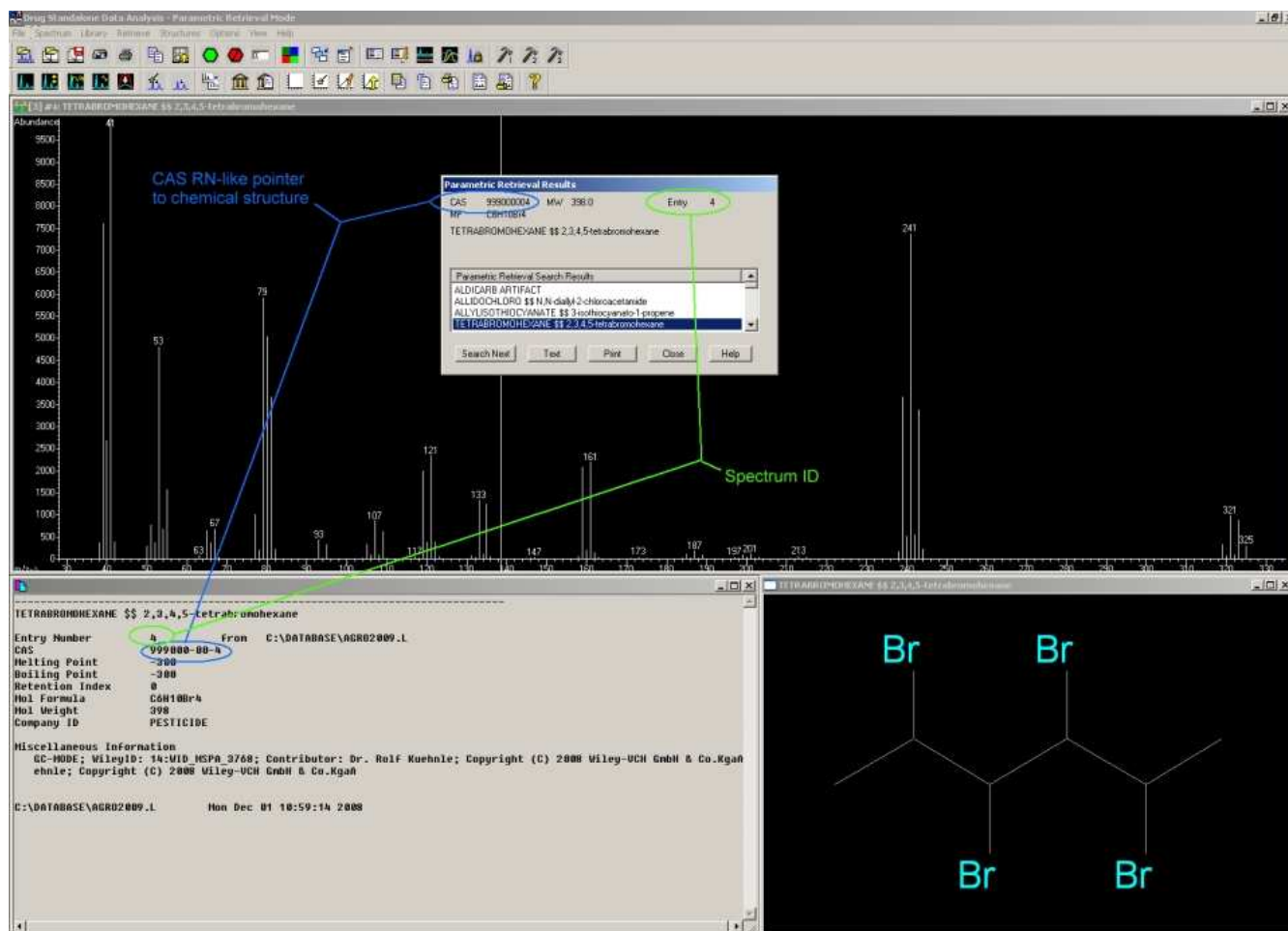
The Agilent Chemstation database files containing the spectral data (files CAS.IND, CONDENSE, CONDENSE.IND, HEADER, HEADER.IND, and ROOT) are installed into the C:\DATABASEVAES2008.L directory. The files containing the chemical structure data are placed in a subdirectory below the AES2008.L main installation folder.

To access the structure database files from your 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 AES2008.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.

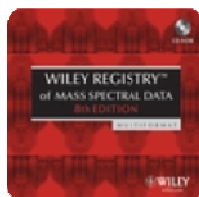
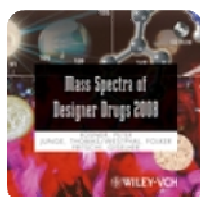
When you are in 'Parametric Retrieval Mode' (shown on the uppermost frame bar of the application window) use 'Select Structure Database...' from the 'Structures' menu item. Then proceed as described in the paragraph above to register the structure database files with your Chemstation software.



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



Wiley-Blackwell Data Collections



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

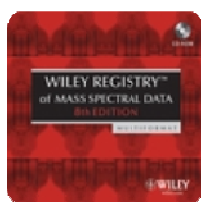
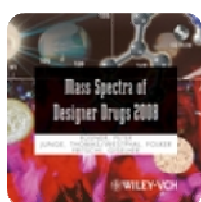
The Waters Masslynx, Perkin-Elmer Turbomass and the VG Labbase/Masslab software suites reference chemical structures in the corresponding chemical structure database files (STRUCT.DB and STRUCT.IN) via the entries in the CAS Registry Number data field. Since not for all chemical structures CAS Registry 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 '99600x-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 '996000-00-40' is used). For additional information see the screenshot on next page and Appendix A.

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

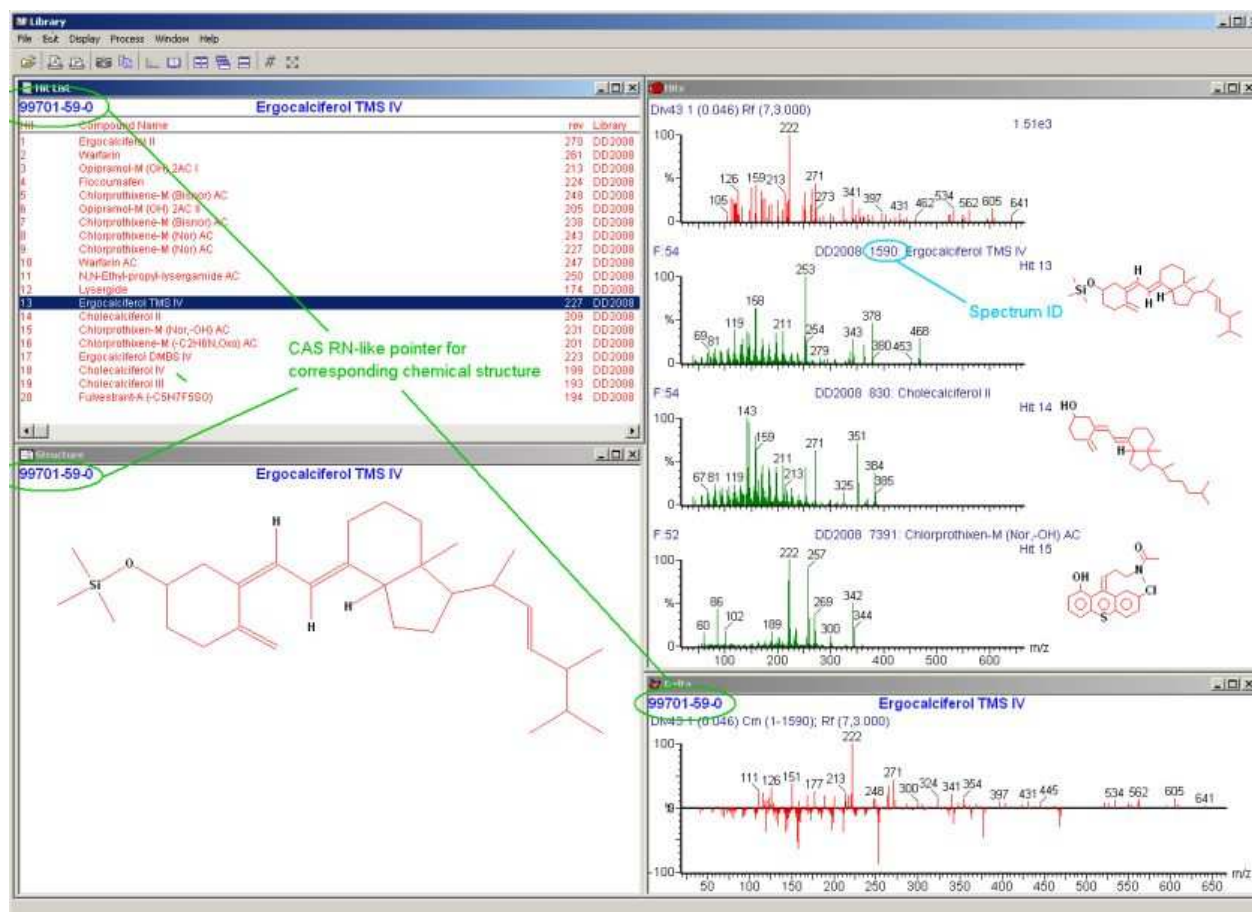
The database files containing the spectral data (files .idb, .idi, .pdb and .pdi) are installed into the Idendb directory of your MassLynx or Turbomass installation. For a default installation that is in C:\Masslynx\Iendb and C:\TurboMass\Iendb, respectively. For the VG software the files are installed by default to C:\AGRO2009. The database files containing the chemical structure records are installed into a directory named C:\Masslynx\STRUCTDB\AGRO2009 or C:\TurboMass\STRUCTDB\AGRO2009, respectively. The structure files for the VG formats are installed below the path specified to install the mass spectrum database files. To access the AGRO2009 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:

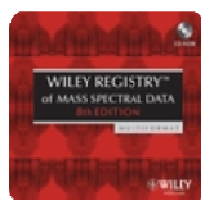
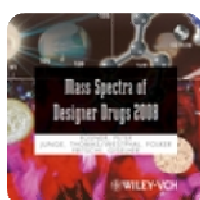
To access the AGRO2009 chemical structure database select File/Structures... from the Search Library module in your spectral software package. In the file browser window coming up select the STRUCT.DB file from the directory where the AGRO2009 chemical structure database files were copied into.



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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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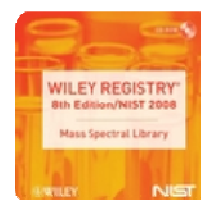
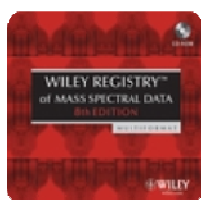
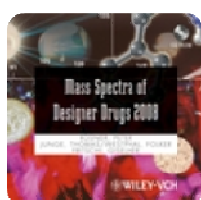


Appendix A: CAS Registry Numbers and Structure Pointers (CAS Registry Number-like IDs)

For linking MS records to the respective structure records in the structure add-on for Agilent Chemstation, PerkinElmer TurboMass, Waters Masslynx and VG Labbase/Masslab, the IDs in the two lists given below are used. Due to the nature of the linking mechanism, these ID values are stored in the CAS Registry Number data field. Please note that the ID values in the second list don't actually represent real CAS Registry numbers and are used here only for referring to the structure record in a separate database file.

The CAS Registry Number-like IDs used were created as 9-digit numbers with a leading '999' (Agilent Chemstation) or '996' (PerkinElmer TurboMass, Waters Masslynx, VG Labbase/Masslab) to make them distinguishable to real CAS Registry numbers (no real CAS Registry Number starting with '999' or '996' appears in the Pesticides 2009 library). The greatest real CAS Registry number within the Pesticides 2009 Mass Spectral Library is '112748-69-3', thus all structure pointer IDs listed below are greater than this CAS Registry number.

Given below are two lists detailing the 'real' CAS Registry Numbers used in the Pesticides 2009 Mass Spectral Library and the 'CAS Registry Number-like' identifiers created to refer to the chemical structure records.

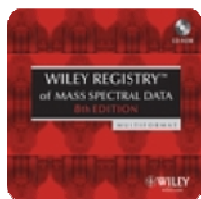
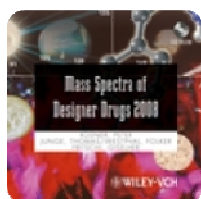


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'Real' CAS Registry Numbers used in the Mass Spectra of Pesticides 2009 Library (duplicate entries removed from the list below):

| | | | | | | |
|---------|---------|----------|----------|----------|----------|-----------|
| 50-29-3 | 83-26-1 | 95-50-1 | 108-68-9 | 133-06-2 | 510-15-6 | 709-98-8 |
| 50-30-6 | 83-74-9 | 95-51-2 | 108-80-5 | 133-07-3 | 518-20-7 | 731-27-1 |
| 50-65-7 | 83-79-4 | 95-55-6 | 108-90-7 | 133-32-4 | 526-75-0 | 732-11-6 |
| 50-79-3 | 84-61-7 | 95-57-8 | 110-91-8 | 133-90-4 | 527-20-8 | 741-58-2 |
| 50-84-0 | 84-62-8 | 95-65-8 | 111-92-2 | 134-62-3 | 532-27-4 | 756-79-6 |
| 51-03-6 | 84-65-1 | 95-69-2 | 113-48-4 | 136-45-8 | 533-23-3 | 759-94-4 |
| 51-44-5 | 84-66-2 | 95-76-1 | 114-26-1 | 137-26-8 | 533-74-4 | 767-00-0 |
| 52-51-7 | 84-69-5 | 95-82-9 | 115-26-4 | 137-30-4 | 534-52-1 | 786-19-6 |
| 52-85-7 | 84-74-2 | 95-87-4 | 115-32-2 | 139-40-2 | 535-89-7 | 830-96-6 |
| 53-19-0 | 84-76-4 | 95-94-3 | 115-90-2 | 139-66-2 | 541-73-1 | 834-12-8 |
| 54-11-5 | 84-77-5 | 95-95-4 | 115-93-5 | 140-57-8 | 553-26-4 | 841-06-5 |
| 55-38-9 | 85-41-6 | 96-12-8 | 115-96-8 | 141-66-2 | 554-00-7 | 879-39-0 |
| 56-25-7 | 85-44-9 | 96-31-1 | 116-06-3 | 142-28-9 | 555-37-3 | 886-50-0 |
| 56-35-9 | 85-68-7 | 96-45-7 | 116-29-0 | 143-50-0 | 556-22-9 | 900-95-8 |
| 56-38-2 | 86-50-0 | 97-00-7 | 117-18-0 | 144-49-0 | 556-61-6 | 919-76-6 |
| 56-72-4 | 86-86-2 | 97-16-5 | 117-26-0 | 145-73-3 | 563-12-2 | 919-86-8 |
| 57-06-7 | 86-87-3 | 97-17-6 | 117-52-2 | 148-79-8 | 576-24-9 | 933-75-5 |
| 57-15-8 | 86-88-4 | 97-50-7 | 117-79-3 | 150-50-5 | 576-26-1 | 933-78-8 |
| 57-24-9 | 87-40-1 | 98-82-8 | 117-80-6 | 150-68-5 | 576-55-6 | 934-32-7 |
| 58-89-9 | 87-51-4 | 99-30-9 | 117-81-7 | 152-18-1 | 579-66-8 | 944-22-9 |
| 60-51-5 | 87-61-6 | 99-54-7 | 118-69-4 | 297-97-2 | 583-78-8 | 945-51-7 |
| 60-57-1 | 87-65-0 | 99-88-7 | 118-74-1 | 298-00-0 | 584-79-2 | 950-35-6 |
| 61-82-5 | 87-68-3 | 100-02-7 | 118-75-2 | 298-02-2 | 587-85-9 | 950-37-8 |
| 62-38-4 | 87-82-1 | 100-56-1 | 118-96-7 | 298-03-3 | 591-20-8 | 957-51-7 |
| 62-73-7 | 87-86-5 | 101-05-3 | 120-32-1 | 298-04-4 | 591-27-5 | 959-98-8 |
| 63-25-2 | 88-75-5 | 101-21-3 | 120-36-5 | 299-84-3 | 598-99-2 | 960-25-8 |
| 63-74-1 | 88-82-4 | 101-27-9 | 120-80-9 | 299-86-5 | 599-70-2 | 973-21-7 |
| 66-81-9 | 88-85-7 | 101-42-8 | 120-82-1 | 300-76-5 | 606-20-2 | 1007-28-9 |
| 70-30-4 | 89-98-5 | 101-76-8 | 120-83-2 | 301-12-2 | 608-27-5 | 1014-69-3 |
| 72-20-8 | 90-00-6 | 103-17-3 | 121-14-2 | 309-00-2 | 608-31-1 | 1014-70-6 |
| 72-43-5 | 90-15-3 | 103-33-3 | 121-20-0 | 311-45-5 | 608-93-5 | 1022-22-6 |
| 72-54-8 | 90-43-7 | 103-71-9 | 121-29-9 | 314-40-9 | 611-19-8 | 1022-46-4 |
| 72-55-9 | 90-97-1 | 104-12-1 | 121-75-5 | 315-18-4 | 611-92-7 | 1031-07-8 |
| 72-56-0 | 90-98-2 | 105-67-9 | 122-14-5 | 319-84-6 | 618-88-2 | 1031-47-6 |
| 75-99-0 | 91-16-7 | 106-40-1 | 122-34-9 | 319-85-7 | 620-17-7 | 1076-38-6 |
| 76-03-9 | 91-53-2 | 106-43-4 | 122-39-4 | 321-54-0 | 623-12-1 | 1085-98-9 |
| 76-06-2 | 92-52-4 | 106-44-5 | 122-42-9 | 327-98-0 | 626-43-7 | 1113-02-6 |
| 76-44-8 | 92-84-2 | 106-46-7 | 122-88-3 | 330-54-1 | 626-67-5 | 1114-71-2 |
| 76-87-9 | 93-65-2 | 106-47-8 | 123-07-9 | 330-55-2 | 629-19-6 | 1129-41-5 |
| 78-87-5 | 93-71-0 | 106-48-9 | 123-30-8 | 333-41-5 | 634-66-2 | 1134-23-2 |
| 79-43-6 | 93-72-1 | 106-50-3 | 123-33-1 | 366-18-7 | 634-67-3 | 1172-63-0 |
| 80-06-8 | 93-75-4 | 106-93-4 | 126-15-8 | 402-45-9 | 634-83-3 | 1194-65-6 |
| 80-33-1 | 93-76-5 | 107-07-3 | 126-68-1 | 420-04-2 | 634-90-2 | 1262-21-1 |
| 80-38-6 | 93-79-8 | 107-49-3 | 126-75-0 | 462-08-8 | 636-30-6 | 1319-80-8 |
| 81-81-2 | 94-74-6 | 107-99-3 | 127-63-9 | 470-90-6 | 639-58-7 | 1420-06-0 |
| 81-82-3 | 94-75-7 | 108-39-4 | 127-90-2 | 485-31-4 | 640-15-3 | 1420-07-1 |
| 82-38-2 | 94-81-5 | 108-41-8 | 131-09-9 | 486-25-9 | 640-19-7 | 1563-38-8 |
| 82-66-6 | 94-99-5 | 108-42-9 | 131-11-3 | 500-28-7 | 644-64-4 | 1563-66-2 |
| 82-68-8 | 95-06-7 | 108-43-0 | 131-16-8 | 504-24-5 | 671-04-5 | 1570-64-5 |
| 83-05-6 | 95-49-8 | 108-62-3 | 131-17-9 | 504-29-0 | 697-82-5 | 1582-09-8 |



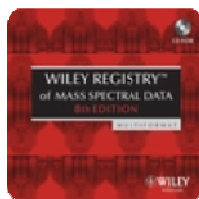
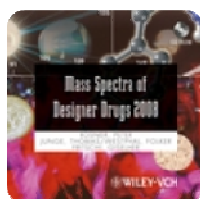
Wiley-Blackwell Data Collections



| | | | | | | |
|-----------|-----------|------------|------------|------------|------------|-------------|
| 1593-77-7 | 2164-17-2 | 3689-24-5 | 13071-79-9 | 22212-55-1 | 33693-04-8 | 55219-65-3 |
| 1596-84-5 | 2212-67-1 | 3691-35-8 | 13171-21-6 | 22224-92-6 | 33719-74-3 | 55283-68-6 |
| 1610-17-9 | 2227-13-6 | 3734-48-3 | 13181-17-4 | 22248-79-9 | 33820-53-0 | 55335-06-3 |
| 1610-18-0 | 2234-13-1 | 3735-01-1 | 13194-48-4 | 22259-30-9 | 34014-18-1 | 55511-98-3 |
| 1634-78-2 | 2275-18-5 | 3766-60-7 | 13290-96-5 | 22781-23-3 | 34123-59-6 | 55512-33-9 |
| 1646-88-4 | 2275-23-2 | 3766-81-2 | 13457-18-6 | 22936-75-0 | 34462-96-9 | 56073-07-5 |
| 1689-83-4 | 2282-34-0 | 3861-47-0 | 13593-03-8 | 22936-86-3 | 34622-58-7 | 57018-04-9 |
| 1689-84-5 | 2303-16-4 | 3868-61-9 | 13684-56-5 | 23103-98-2 | 34643-46-4 | 57052-04-7 |
| 1698-60-8 | 2303-17-5 | 3878-19-1 | 13684-63-4 | 23135-22-0 | 34681-10-2 | 57153-17-0 |
| 1702-17-6 | 2307-68-8 | 3988-03-2 | 13798-23-7 | 23505-41-1 | 34681-24-8 | 57153-18-1 |
| 1713-15-1 | 2310-17-0 | 4147-51-7 | 14214-32-5 | 23560-59-0 | 34883-39-1 | 57369-32-1 |
| 1715-40-8 | 2312-35-8 | 4163-78-4 | 14255-72-2 | 23564-05-8 | 34883-41-5 | 57646-30-7 |
| 1746-81-2 | 2314-09-2 | 4234-79-1 | 14255-88-0 | 23564-06-9 | 35065-27-1 | 57837-19-1 |
| 1757-18-2 | 2385-85-5 | 4301-50-2 | 14324-55-1 | 23844-56-6 | 35065-29-3 | 58002-19-0 |
| 1836-75-5 | 2416-94-6 | 4396-19-4 | 14426-42-7 | 23947-60-6 | 35256-85-0 | 58877-92-2 |
| 1861-32-1 | 2425-06-1 | 4466-14-2 | 14437-17-3 | 23950-58-5 | 35367-38-5 | 59682-52-9 |
| 1861-40-1 | 2524-09-6 | 4658-28-0 | 14484-64-1 | 24017-47-8 | 35400-43-2 | 59756-60-4 |
| 1889-58-3 | 2439-01-2 | 4726-14-1 | 14816-18-3 | 24579-73-5 | 35554-44-0 | 60168-88-9 |
| 1896-62-4 | 2487-01-6 | 4824-78-6 | 14816-20-7 | 24602-86-6 | 35575-96-3 | 60207-90-1 |
| 1897-45-6 | 2524-09-6 | 4841-20-7 | 15299-99-7 | 24691-76-7 | 35693-99-3 | 60207-93-4 |
| 1912-24-9 | 2536-31-4 | 4849-32-5 | 15310-01-7 | 24691-80-3 | 35694-06-5 | 60568-05-0 |
| 1912-26-1 | 2540-82-1 | 4901-51-3 | 15457-05-3 | 24934-91-6 | 36734-19-7 | 61213-25-0 |
| 1918-00-9 | 2550-75-6 | 5131-24-8 | 15545-48-9 | 25057-89-0 | 37680-73-2 | 62610-77-9 |
| 1918-02-1 | 2581-34-2 | 5221-53-4 | 15879-93-3 | 25168-26-7 | 37893-02-0 | 62924-70-3 |
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| 1918-16-7 | 2597-03-7 | 5296-64-0 | 16596-04-6 | 25900-20-3 | 39184-59-3 | 65907-30-4 |
| 1918-18-9 | 2631-37-0 | 5598-13-0 | 16605-91-7 | 26002-80-2 | 39196-18-4 | 66063-05-6 |
| 1928-37-6 | 2631-40-5 | 5707-69-7 | 16655-82-6 | 26225-79-6 | 39515-41-8 | 66215-27-8 |
| 1928-38-7 | 2635-10-1 | 5836-10-2 | 16672-87-0 | 26259-45-0 | 39807-19-7 | 66246-88-6 |
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| 1984-59-4 | 2876-78-0 | 6923-22-4 | 17700-09-3 | 29185-21-5 | 42576-02-3 | 73250-68-7 |
| 1984-65-2 | 2921-88-2 | 6988-21-2 | 17781-15-6 | 29232-93-7 | 42874-01-1 | 74051-80-2 |
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| 2157-19-9 | 3397-62-4 | 10605-21-7 | 21267-72-1 | 33213-65-9 | 52756-25-9 | |
| 2163-68-0 | 3424-82-6 | 12771-68-5 | 21609-90-5 | 33245-39-5 | 52918-63-5 | |
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CAS Registry Numbers-like IDs used in the Mass Spectra of Pesticides 2009 Library:

For Agilent Chemstation:

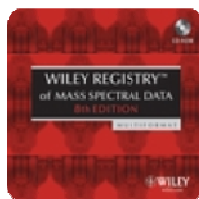
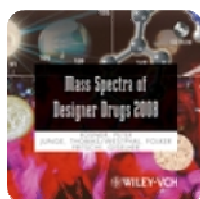
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For PerkinElmer TurboMass, Waters Masslynx and VG Labbase/Masslab:

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Wiley-Blackwell Data Collections
Hoboken • Weinheim • Chichester



Wiley-Blackwell Data Collections



| | | | | | | |
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