Agilent G6854 MassHunter Personal Pesticide Database

Quick Start Guide

Where to find more information

Use the online Help for in-depth information not given in this *Quick Start Guide*. Display online Help in one of two ways:

- Select **Contents**, **Index**, or **Search** from the PCDL software **Help** menu.
- Press the **F1** key to get more information about a window, tab, or dialog box.

Agilent Technologies

What is MassHunter Personal Pesticide Database?

MassHunter Personal Pesticide Database consists of an accurate mass compound database of pesticides and MassHunter Personal Compound Database and Library software.

Database refers to a compound databass that can be searched using accurate mass and optional retention time. Databases also include information such as formula, structure, and links to public databases, for each compound.

Library refers to a compound database that also contain MS/MS spectra for some or all compounds. Library compounds can contain multiple spectra, acquired with different instrument conditions, such as different collision energy values.

MassHunter Personal Compound Database and Library (PCDL) software lets you:

- Search or browse MS/MS spectra in libraries.
- Search for compounds in both databases and libraries, using text, formula, accurate mass, and retention time (optional or required). The use of retention time increases the compound identification specificity.
- Create and edit custom databases and libraries, including adding proprietary compounds, retention times, and MS/MS spectra.
- Import mass lists from Agilent MassHunter Mass Profiler, GeneSpring MS, and Qualitative Analysis software.
- Load spectra from either a **.CEF** file or by copy-and-pasting mass spectra from MassHunter Qualitative Analysis software.
- Do private, on-site searches, which keep intellectual property safe.
- Link to websites for more information on many compounds.

MassHunter Personal Pesticide Database also lets you do automated or manual searches from MassHunter Qualitative Analysis software as described on .

Compound names in the database
Many compounds are commonly known as their salts. The mass spectrometer, however, detects the anion or cation portion of the salt, rather than the neutral salt. Database entries contain the familiar compound names, but the empirical formulae reflect the interesting (cation or anion) portion of the molecule rather than the formula of the neutral compound salt. For example, the full name Vecuronium bromide is used for identification in the database, even though the mass/formula only includes the Vecuronium part of the compound.

Installation

If the MassHunter Personal Pesticide Database is not already installed on your system, install it as follows.

1 Insert the MassHunter Personal Pesticide Database disk into the disk drive.

2 Click the Windows **Start** button and select **Run**.

3 Type **x:\setup**, where **x** is the letter of the disk drive, and click **OK**.

4 Follow the instructions on the screen.

The compound database of pesticides (**Pesticides.cdb**) and MassHunter Personal Compound Database and Library (PCDL) software are installed.

To remove the software

Use the **Add/Remove** window of the Control Panel.

Doing this removes the MassHunter Personal Compound Database and Library (PCDL) software and master databases that have been installed, such as **Pesticides.cdb**, but does *not* remove custom databases you have created.

Startup

1 Select **Programs > Agilent > MassHunter Workstation > Personal Compound Database and Library** from the Windows Start menu, as shown below, to start the PCDL software.
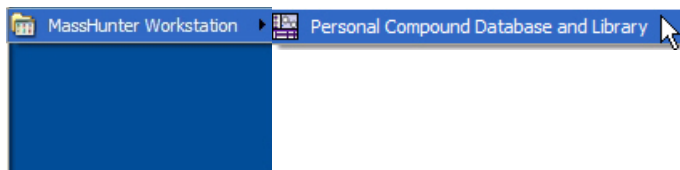
The database or library that was last used is displayed as the default database or library to open when you start the PCDL software.

2 To open a different database or library, see
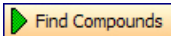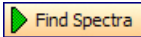
Main Window

The MassHunter Personal Compound Database and Library (PCDL) software main window has the following areas and controls.

Toolbar

The following items are available on the PCDL software toolbar:

Button	Equivalent Menu Item	Comments
Find Compounds	Database/Library > Find Compounds	Available only when the Single Search or Batch Search tabs are displayed. Same as pressing the **F5** key.
Find Spectra	Database/Library > Find Spectra	Available only when the Spectral Search or Browse Spectra tabs are displayed. Same as pressing the **F5** key.
🖨	File > Print Results	
💾	File > Export Results	For use with Batch Summary Results only.
📄	File > New Database/Library	
📂	File > Open Database/Library	
❓	Help > Contents	

Menus

The following menus are available in PCDL software:

File menu

New Database/Library   Lets you create a custom database or library that can be edited and personalized for your lab. This is done by creating a copy of an existing database or library with a new name that can be edited. See "To create a custom database or library" on page 14.

Open Database/Library   Lets you open a different database or library.

Backup Database/Library   Lets you copy the database or library for archive purposes.

Import Compounds   Lets you select a file that contains compounds to add to a custom database if editing is enabled. If you start with an empty database, then you are essentially creating a custom database from the imported compounds.

Export Results   Lets you export batch summary results for use with other programs, such as spreadsheets and word processors.

Print Results   Lets you print search results and structures.

Exit   Closes the PCDL software window.

Edit menu

These menu items are for use with custom databases with editing enabled only and are only available when the Edit Compounds tab is displayed.

Add New Compound   Creates a new compound in the database with a mass of 0 named "New Compound". The new compound is displayed at the end of the Results table. Enter information such as RT, Formula, Name, and Structure for the new compound in the Edit Compounds tab.

Save As New Compound   Creates a new compound in the database using the current values of the edit fields on the Edit Compounds tab. The new compound is displayed at the end of the Results table.

Update Selected Compound   Updates the information for the selected compound in the database. The updated information is reflected in the Results table.

Delete Selected Compound   Removes the selected lines of the Results table, which removes the selected compounds from the database. Use **Ctrl+click** or **Shift+click** to select multiple lines.

View menu

Add/Remove Compound Columns   Opens the Add/Remove Columns dialog box, which lets you specify what information is displayed in the Compound Results table.

Restore Default Compound Columns   Displays the columns in the Compound Results table as they were originally set in the software.

Structure Details   Opens the Structure Details dialog box, which displays the current structure in a larger size for easier viewing.

Database/Library menu

Find Compounds   Searches the database for compounds that match criteria specified on the Single Search tab or Batch Search tab. Only available when either the Single Search tab or Batch Search tab is displayed.

Find Spectra   Searches the library for spectra that match criteria specified on the Spectral Search tab or Browse Spectra tab. Only available when either the Spectral Search tab or Browse Spectra tab is displayed.

Allow Editing   A toggle that enables or disables editing operations to a custom database. *A master database cannot be edited.*

Database/Library Information   Lets you view information about the current database and edit the description for custom databases with editing enabled.

Links menu

Lets you access websites for information on compounds or metabolites. The links displayed depend on the type of the current database or library as follows:

Links for a General database or library

- PubChem (National Center for Biotechnology Information)
- ChemSpider (structure-based chemistry information)

Links for a Metabolomics database or library

- Agilent Metabolomics
- Agilent Metabolomics Lab
- PubChem (National Center for Biotechnology Information)
- ChemSpider
- METLIN (Scripps Center for Mass Spectrometry)
- KEGG (Kyoto Encyclopedia of Genes and Genomes)
- HMP (Human Metabolome database)
- Lipid MAPS (LIPID Metabolites And Pathways Strategy)

Links for a Forensics database or library

- PubChem (National Center for Biotechnology Information)
- ChemSpider
- Chem Industry
- TOXNET
- ChemBioFinder
- NIST Chemistry WebBook
- IPCS INTOX Databank
- SOFT
- TIAFT
- AAFS
- Related Forensics Websites

Links for a Pesticides database or library

- PubChem (National Center for Biotechnology Information)
- ChemSpider
- Chem Industry
- Compendium of Pesticides
- EPA - Pesticides (Environmental Protection Agency)
- NPIC (National Pesticide Information Center)
- NIH NLM (National Institute of Health - National Library of Medicine)
- TOXNET
- PAN Database
- WHO - Pesticides (World Health Organization)

Help menu

Contents, Index, and Search   Opens the online Help window for PCDL software, with the appropriate tab displayed.

View EULA   Displays the license agreement for PCDL software in a Notepad window.

About   Displays the version and build number of the PCDL software.

Compound Tabs

The following tabs are available for searching, viewing, and editing *compounds*:

Single Search tab

Lets you search for compounds in the database. Search results are displayed in the Compound Results table in the lower part of the window. See "To find compounds" on page 17.

Batch Search tab

Lets you search for compounds in the database by specifying a mass list and optional retention times. Search results are displayed in the Compound Results table in the lower part of the window. See "To find compounds from a mass list" on page 21.

Batch Summary tab

Shows a summary view of all Best fit hits from a Batch Search. Results can be exported for use with other applications. You can also add comments and update retention times for custom databases with editing enabled. See "To view batch summary results" on page 24.

Edit Compounds tab

For custom databases that allow editing, you can use this tab to edit information for compounds and to add new compounds. Before editing existing compounds, do a Single or Batch search, so that the compounds to be modified are present in the Compound Results table. See "To edit compounds in custom database" on page 27.

Compound Results

Compound search results are displayed in the lower part of several tabs in the PCDL software window. The way the results are displayed can be changed as described in "To change how data is displayed in results tables" on page 19.

Clicking on a row of the table displays structure information about that compound in the **Structures** area, if the structure is available in the database.

You can also select compounds in the results table for editing on the Edit Compounds and Edit Spectra tabs (*custom databases with editing enabled only*). See "To edit compounds in custom database" on page 27.

Structures

Structure tab   This area on the right side of compound-related tabs displays structure information for the compound currently selected in the Compound Results table, if it is available in the database. Clicking the 🔍 button opens the Structure Details dialog box and displays a larger image of the structure.

MOL Text tab   Displays the text version of the structure. If the current database is a custom database with editing enabled, you can copy text from a molecular drawing tool that is capable of generating MOL file text and paste it into this area to update the structure of the selected compound. Or you can use the 📂 button in the Structure area to load a structure from a **.MOL** file.

Spectral Tabs

The following tabs are available for searching, viewing, and editing *spectra*:

Spectral Search Tab

Lets you load spectra from a **.CEF** file or copy-and-paste spectra from Qualitative Analysis and search for the spectra in the current library.

Browse Spectra Tab

Lets you search the current library for spectra that match certain parameters, such as mass, collision energy, ion polarity, and ionization mode. Use the default search parameters to view all spectra in the library.

You can also view spectral information for compounds retrieved from the Single Search tab or Batch Search tab by clicking on the compound of interest in the compound results table in the lower part of the tab.

Spectral results are displayed in the Spectral Information Table in the middle part of the tab.

Edit Spectra Tab

You can use this tab to add, delete, and edit spectra in a custom library, if editing is enabled for the library. Before editing, you must do a Single or Batch search, so that some compounds are present in the compound results table in the lower part of the tab.

Spectral Plot Window

This area of the spectra-related tabs lets you view selected spectra in graphic format and as a list of masses and relative abundances.

Getting Started

The following topics will help you get started with Agilent PCDL software. This guide and the online Help explain these activities.

Database operations

The following database or library operations are described in the following pages:

- "To open a database or library" (*below*)
- "To back up a database or library" (*below*)
- "To view database or library information" on page 13
- "To create a custom database or library" on page 14
- "To import compounds to a custom database" on page 14

To open a database or library

The database or library that was last used is displayed as the default database or library to open when you start PCDL software application. Use this procedure to open a *different* database or library.

1 Open the Open Database/Library dialog box in *either* of the following ways:

- Select **Open Database/Library** from the File menu.
- Click the ![folder icon] button on the toolbar.

2 Select the file of interest (**.cdb** extension) and click the **Open** button. The following files are supplied with the software:

- **databases\Pesticides.cdb** - Pesticides master database.
- **databases\Sulfas.cdb** - a small example master database.
- **databases\Empty.cdb** - an empty master database, which can be used to create a custom database for importing compounds. To create a database and import compounds, see "To create a custom database or library" on page 14 and "To import compounds to a custom database" on page 14.
- **Library\SulfasLib.cdb** - a small example master library.
- **Library\EmptyLib.cdb** - an empty master library, which can be used to create a custom library.

NOTE Master databases and libraries can't be edited, but they can be used to create custom databases that can be edited. See "To create a custom database or library" on page 14.

To back up a database or library

1 Select **Backup Database/Library** from the File menu.

2 Select a folder for the backup file or accept the default folder, which is:
MassHunter\Library\Archive

3 Type in a file name for the backup file or accept the default file name, which is in the form:
<dbname>.<yyyy.mm.dd>.cdb

where **dbname** is the name of the current database or library, **yyyy** is the current year, **mm** is the current month, and **dd** is the current day of the month.

4 Click the **Save** button. A backup copy of the database or library is created using the specified file name and location.

To view database or library information

1 Select **Database/Library Information** from the Database/Library menu.

2 View the following information about the database or library:

- File name
- # Compounds (entries) in the database or library
- **Master** or **User**
- Type: **General**, **Metabolomics**, **Pesticides**, or **Forensics**
- Edit allowed (**Yes** or **No**)
- Last modified timestamp
- Version number
- Description - the description can be edited if the current database or library is a custom database or library with editing enabled.

3 Click the **Apply** button if you modified the description or changed the database type.

4 Click the **Close** button to close the Database/Library Information dialog box.

To create a custom database or library

1 Select **New Database/Library** from the File menu or click the ☐ button on the toolbar.

2 Do the following steps on the New Database/Library dialog box:

   a Select a starting database or library for the new database or library. Database files are stored in the **\databases** folder. The default path is **\Library**, which contains spectral library files.

   b Select the database or library type for the new database or library from the following choices: **General**, **Metabolomics**, **Pesticides**, or **Forensics**.

   c Type in a name for the new database or library file.

   d Enter a description for the new database or library.

   e Click the **Create** button to create the new database or library.

   The new database or library becomes the current working database or library and is automatically enabled for editing.

To import compounds to a custom database

Use the following procedure to import compounds into a custom database or to create a custom database from a compound list created by another application. If you start with an empty database, then you are essentially creating a custom database from the imported compounds.

1 Prepare the import file. The format required for the import file is described in the online Help. The **.CSV** or **.TXT** file can be created in *any* of the following ways:

   • Exported from PCDL software as described in

   • Exported from another application such as Agilent Mass Profiler or GeneSpring MS software.

   • Manually in Excel.

2 Open the custom database of interest or create a new database as described in

3 Enable editing on this database by marking **Allow Editing** on the Database/Library menu.

4 Select **Import Compounds** from the File menu.

5 Select the **.CSV** or **.TXT** file prepared in Step 1 that contains the compounds of interest, then click the **Open** button.

6 To view the new compounds in the database, do a search on the Single Search tab with no criteria or criteria that you know will find the

compounds of interest. The compounds will be listed in the Compound Results table in the lower part of the window.

NOTE   The mass is calculated from the formula, unless the difference is > 0.0001 Da. In that case, the Mass and Formula values will be as read from the input file, and those compounds will be added to the log file described in Step 7. The information in the log file can be used to determine the correct Formula or Mass. Errors can occur when 1) the mass value was the mass from the spectrum and not a neutral mass, or 2) the formula contained the adduct (such as Cl).

7 Compounds that were not imported due to problems with the input file are saved in the file **<ImportFileName>-ImportLog.csv**, where **<ImportFileName>** is the name of the import file selected in Step 5. Edit this log file to fix the problems, then import the corrected file.

8 (*Optional*) See "To edit compounds in custom database" on page 27 if you want to change information for the imported compounds.

Searching a PCDL-format database in Qualitative Analysis

Use the following procedures to search a PCDL-format database with MassHunter Workstation Software–Qualitative Analysis program. These steps apply to version B.03.01 of Qualitative Analysis and may be slightly different in later revisions.

To use a PCDL-format database to identify compounds in Qualitative Analysis

Use this procedure to identify compounds with a PCDL-format database:

1 Open the data file of interest in Qualitative Analysis.
2 Find compounds as described in Qualitative Analysis online Help.
3 Select the compounds to search in the Compound List window or Data Navigator.
4 Set the database search criteria in the **Identify Compounds > Search Database** section of Method Editor:

   a On the **Search Criteria** tab, select **Mass** as the Values to match option.

   b On the **Database** tab, click the Browse [...] button to open the Open Database File dialog box.

   • Select File Type **.cdb** to see a list of PCDL-format databases.

   • Select the database of interest.

5 Initiate the search and review the results in the DB Search Results window.

To use a PCDL-format database to identify spectrum peaks in Qualitative Analysis

Use this procedure to identify spectrum peaks with a PCDL-format database:

1 Open the data file of interest in Qualitative Analysis.
2 Extract a mass spectrum or extract a peak spectrum as described in Qualitative Analysis online Help.
3 If not already set, set the database search criteria in the **Identify Compounds > Search Database** section of Method Editor as described in Step 4 above.
4 Initiate the search by right-clicking on the spectrum and selecting **Search Database for Spectrum Peaks** from the shortcut menu (or in other ways described in Qualitative Analysis online Help).

The database is searched for the masses in the spectrum. If hits are found, information such as masses, formulas, and compound names is displayed in the DB Search Results window.

5 Review the results in the DB Search Results window.

Searching a database in PCDL software

Searching a compound database for compounds matching certain criteria can be broken into the following activities, which are described in the following pages:

- "To find compounds" (*below*)
- "To view compound search results" on page 19
- "To change how data is displayed in results tables" on page 19
- "To print compound results" on page 20

To find compounds

1 If the database you want to search is not already open, open it in either of the following ways:

- Select **Open Database/Library** from the File menu, *or*
- Click the ![folder icon] button on the toolbar.

2 Click on the **Single Search** tab.

3 To return the contents of the entire database, leave the search fields blank and skip to Step 6. Otherwise, set the desired mass search criteria:

a **Mass** and **Mass tolerance** in **ppm** or **mDa**

b **Type of mass** (**[M+H]+**, **Neutral**, or **[M‑H]‑**)

- Select **[M+H]+** mass type if you are searching for an observed positive ion in the database. The neutral mass value will be automatically calculated, assuming the ion was a positive protonated ion.

  If **Include cations** is selected in Step 3c, the neutral mass of a cation is calculated. Only those compounds that have been defined as cations in the database will be compared to the calculated neutral mass of a cation.

- Select **Neutral** if the mass is the calculated neutral mass value, usually a value that was calculated by Molecular Feature Extraction (MFE) software. *Do not select this value for a mass observed in a spectrum.* Ions observed in a spectrum have a charge and need to be converted to neutral to work with the database. For observed ions use either the **[M+H]+** or **[M‑H]‑** selection.

  If **Neutral** is selected, you can choose **Include anions** or **Include cations** for the **Ion search mode** setting in Step 3c.

- Select **[M-H]-** mass type if you are searching for an observed negative ion in the database. The neutral mass value will be automatically calculated, assuming the ion was a negative deprotonated ion.

    If **Include anions** is selected in Step 3c, the neutral mass of an anion is calculated. Only those compounds that have been defined as anions in the database will be compared to the calculated neutral mass of an anion.

  c **Ion search mode**:
  - **Include neutrals** is normally always selected. Clear it if you want to search ions only.
  - If you selected **Neutral** for the mass type in Step 3b, then select **Include anions** *or* **Include cations** if you also want to consider those chemicals that don't pick up or lose a proton to ionize. Searching *both* modes will return false matches.
  - Choose **Include anions** if the data was acquired in *negative* ion mode.
  - Choose **Include cations** if the data was acquired in *positive* ion mode.

4 When searching a master database or a custom database without retention time data, be sure to *clear* the **Require** checkbox for **Retention time**. When searching a database that contains retention time information for compounds, enter a retention time and RT tolerance if you want to consider retention times in the search.

5 If desired, enter a **Formula**, **Name**, **CAS** ID, or **ChemSpider** ID to find compounds based on these fields. You can also enter text in the **Notes** field to search for a text string, such as "antidiabetic".

The following additional search fields are available for Metabolomics databases only: **METLIN**, **KEGG**, **HMP**, and **LMP** IDs.

6 Initiate the search in any of the following ways:
  - Click the **Find Compounds** button on the toolbar,
  - Select **Find Compounds** from the Database menu, *or*
  - Press the **F5** key.

7 View search results in the Compound Results table at the bottom of the window. For more information, see "To view compound search results" on page 19 and "To change how data is displayed in results tables" on page 19.

To view compound search results

1 Do a search on the Single Search tab as described in "To find compounds" on page 17.

2 View search results in the Compound Results table at the bottom of the window. You can change how compound results are displayed as described in "To change how data is displayed in results tables" on page 19.

3 Click on a compound in the Results table to view its structure information in the Structures area on the right side of the window, if the structure is available in the database.

4 Click on the **Edit Compounds** tab to edit information for custom databases that allow editing, as described in "To edit compounds in custom database" on page 27.

5 To print results, see "To print compound results" on page 20.

6 If any of the compound results contain mass spectra, you can view them as described in "To view spectra for a compound" on page 31.

To change how data is displayed in results tables

1 To sort the table by the entries in a column, click the heading for the column of interest.

2 To change the order of the columns of information in the table, drag a column heading to a different position. Repeat this until the desired order is achieved.

3 To resize a column to fit the information contained in it, double-click on the right column divider in the heading of the column of interest.

4 To resize a column to a specific width, drag the separator between the column headings to the right or left until the column is the desired width.

5 To change which columns of information are displayed in the table:

a Right-click in the table and select **Add/Remove Columns** from the shortcut menu to open the Add/Remove Columns dialog box.

b Move the items of information that you want to display from the **Available columns** list to the **Show these columns** list using the **Add ->** button or by double-clicking on them.

c Remove any unwanted items of information from the **Show these columns** list using the **<- Remove** button or by double-clicking on them.

d Click **OK**.

The results table will be updated to reflect the selected columns of information.

To print compound results

Results can be printed from the Single Search, Batch Search, Batch Summary, and Edit Compounds tabs.

1 If you want to print only certain compounds, highlight those rows in the Compound Results table using **Ctrl+click** or **Shift+click**.

2 Open the Print Results dialog box in *any* of the following ways:

- Select **Print Results** from the File menu.
- Click the 🖨 button on the toolbar.
- Right-click in the results table and select **Print Results** from the shortcut menu.

3 Select desired report options from the following:

- **Printer** (destination)
- **Print Preview** if you want to view the report on the screen first.
- **Fit to page** to size the report to fit the width of the page.
- **Orientation** (**Landscape** or **Portrait**). The default is Landscape, as it allows more columns of information.

4 Select the desired report content options from the following:

- **All rows** or **Only highlighted rows** of the results table
- **Include search parameters**
- **Include unmatched masses**
- **Print structures** and the size (**240 x 160**, **360 x 240**, or **540 x 360**)

5 Click **OK** to generate the report.

If you selected **Print Preview** in Step 3, review the report in the Print preview pane. Click the 🖨 button on the toolbar to print the report.

NOTE For Single Search, only the first 30 compound results will be printed.

Doing a batch search

Searching a database for compounds based on a mass list can be broken into the following activities, which are described in the following pages:

- "To find compounds from a mass list" (below)
- "To view batch search results" on page 23
- "To view batch summary results" on page 24
- "To export batch summary results" on page 25

To find compounds from a mass list

1 If the database you want to search is not already open, open it in *either* of the following ways:
- Select **Open Database/Library** from the File menu.
- Click the ![folder] button on the toolbar.

2 Click on the **Batch Search** tab.

3 Enter a mass list in *one* of the following ways:
- Click the **File** button to the left of the mass list table to open a mass list file output by MassHunter Qualitative Analysis (.**csv** or .**txt** file), Mass Profiler (.**xls** file), or GeneSpring MS (.**txt** file).
- Copy and paste a compound list from MassHunter Qualitative Analysis.
- Type in masses and retention times directly into the table.

4 Select or enter the **Type of mass** (normally **Neutral** for Batch Search) and **Mass tolerance**, in **ppm** or **mDa**.

5 Select **Ion search mode** options as follows:
- **Include neutrals** is normally always selected.
- Select **Include anions** and/or **Include cations** if you also want to consider those few chemicals that don't pick up or lose a proton to ionize.

6 Select one of the following options for **Retention times**:

Option	Meaning	Application
Ignore	Don't consider retention time even if it is present in the list	When searching the sample master database or any custom database *without* retention time data.

Optional	Use retention time information to rank a compound higher if its retention time matches with the observed retention time.	When searching a database that contains retention time information for *some* compounds.
Required	Consider only compounds that match the specified retention time range.	When searching a database that contains retention times for some compounds and both mass and RT criteria must be met.

7 Initiate the search in *any* of the following ways:

- Click the **Find Compounds** button on the toolbar.
- Select **Find Compounds** from the Database/Library menu.
- Press the **F5** key.

8 When the search is complete, the number of hits for each mass appears in the **Hits** column of the mass list, and the list is automatically sorted to show the masses with the most hits at the top of the list. To sort the list by a different criterion, click the heading for the column of interest (**Mass** or **RT**).

Masses with conflicting hits are shown in red text in the Mass List table.

9 Click on a row in the Mass List table to display the compounds found for that mass in the Compound Results table in the lower part of the window. For more information on viewing batch search results, see "To view batch search results" on page 23.

10 Select and view the best compound hit for each mass as described in "To view batch summary results" on page 24.

To view batch search results

1 Do a search on the Batch Search tab as described in "To find compounds from a mass list" on page 21.

2 When the search is complete, the number of hits for each mass appears in the **Hits** column of the mass list, and the list is automatically sorted to show the masses with the most hits at the top of the list. To sort the list by a different criterion, click the heading for the column of interest (**Mass** or **RT**). Masses with conflicting hits are shown in red text in the Mass List table.

3 Click on a row in the Mass List table to display the compounds found for that mass in the Search Results table in the lower part of the window.

Tip For ease of reviewing results, use the **F4** key to scroll down the Mass List and the **Shift+F4** keys to scroll back up. The information in the Results table will be updated as you scroll through the mass list.

4 (*Optional*) Change how the batch search results are displayed as described in "To change how data is displayed in results tables" on page 19.

5 See "To view batch summary results" on page 24 for information on selecting and viewing the best compound hit for each mass.

6 Click on a compound in the Compound Results table to view its structure information in the Structures area on the right side of the window, if the structure is available in the database.

7 Click on the **Edit Compounds** tab to edit information for custom databases that allow editing, as described in "To edit compounds in custom database" on page 27.

8 To print batch results, see "To print compound results" on page 20.

9 If any of the compound results contain mass spectra, you can view them as described in "To view spectra for a compound" on page 31.

To view batch summary results

1 Do a search on the Batch Search tab as described in "To find compounds from a mass list" on page 21.

2 Click on a row in the Mass List table to display the compounds found for that mass in the Batch Search Results table in the lower part of the window. Masses with conflicting hits are shown in red text in the Mass List table.

3 Review the entries marked in the **Best** column for each mass and if necessary, edit the Batch Search Results table to select the best compound hit by marking the desired row (compound). You can also *clear* the box for the selected hit to ignore all the results for that compound.

4 Click the **Batch Summary** tab to view only the best hits from the Batch Search Results table. Compounds with conflicting mass hits are shown in red text in the results table.

5 (*Optional*) Change how the batch summary results are displayed as described in "To change how data is displayed in results tables" on page 19.

6 Click on a compound in the results table to view its structure information in the Structures area on the right side of the window, if the structure is available in the database.

7 Click on the **Edit Compounds** tab to edit information for custom databases that allow editing, as described in "To edit compounds in custom database" on page 27.

8 To export batch summary results, see "To export batch summary results" on page 25.

9 To print batch summary results, see "To print compound results" on page 20.

10 (*Optional*) For a custom database with editing enabled, you can update retention times in the database for the compounds shown in the Batch Summary Results table. See "To update retention time data" on page 26.

To export batch summary results

1 Do a batch search as described in "To find compounds from a mass list" on page 21.

2 Select and view the best compound hit for each mass as described in "To view batch summary results" on page 24, or clear the box for the selected hit to ignore all the results for that compound.

3 (*Optional*) Change the display of data in the Batch Summary tab as described in "To change how data is displayed in results tables" on page 19.

4 Open the Export Results dialog box in *any* of the following ways:

- Select **Export Results** from the File menu.
- Click the 🖫 button on the toolbar.
- Right-click in the results table and select **Export Results** from the shortcut menu in the Batch Summary results table.

5 Click the **Select** button if you wish to specify a different file name, location, or file type for the export file. Otherwise the following default file name, location, and format is used:

- If the mass list was opened from a file, the export file name is: **<massListFileName>-<timestampInSecs>.txt**
- If you entered the mass list manually, the export file name is: **MassList-<timestampInSecs>.txt**
- The default location for the export file is **MassHunter\PCDL\Results**.
- The default output file format is **.TXT** (tab-separated values), but you can select **.CSV** (comma-separated values) instead.

6 Select one or more of the following types of information to include in the report: **Search parameters**, **Results**, and **Unmatched masses** (available only if the **Results** checkbox is marked).

7 Mark the **Open results file after exporting** option to open the batch summary results file automatically in the associated application.

8 Click **OK** to output the results.

9 The results will open in the associated application such as Excel if you selected the **Open results file** option in Step 7. Otherwise open the exported results file in your application of choice at a later time.

NOTE When a **.csv** file is opened in Excel, the Text Import Wizard may be displayed automatically. If so, follow the prompts to specify the proper delimiter for your file, e.g. comma or tab.

If the wizard is *not* displayed automatically, all the values for each row may appear in the first column. To split the text into columns, select the first column (A), then start the wizard by selecting **Text to Columns** on the Data tab, in the Data Tools group.

Editing a custom database

Compound information in a custom database can be edited in the following ways:

-
-

To update retention time data

This procedure applies to custom databases only.

1 Open the custom database of interest. Be sure that editing is enabled by marking **Allow Editing** on the Database/Library menu.

2 Click on the **Batch Search** tab.

3 Enter a mass list in *one* of the following ways:

- Click the **File** button to the left of the mass list table to open a mass list file output by MassHunter Workstation Qualitative Analysis (**.csv** or **.txt** file), Mass Profiler (**.xls** file), or GeneSpring MS (**.txt** file).
- Copy and paste a compound list from Qualitative Analysis.
- Type in masses and retention times directly into the table.

NOTE   Every mass in the mass list must have a retention time value for this procedure.

---

4 Select *one* of the following options for **Retention times**:

- **Ignore** - Use this option to search a database with no retention time information or retention times that may be outside the tolerance window.
- **Optional** - Use this option to search a database that either has no retention time information or has retention times missing for some compounds that you now want to update.
- **Required** - Use this option if you only want to identify and update those compounds that already have retention time information in the database. Specify an **RT tolerance** value in minutes as well.

5 Set other search criteria if desired as described in

6 Initiate the search in *any* of the following ways:

- Click the **Find Compounds** button on the toolbar.
- Select **Find Compounds** from the Database/Library menu.

- Press the **F5** key.

7 When the search is complete, the number of hits for each mass appears in the **Hits** column of the mass list, and the list is automatically sorted to show the masses with the most hits at the top of the list. To sort the list by a different criterion, click the heading for the column of interest (**Mass** or **RT**).

Masses with conflicting hits are shown in red text in the Mass List table.

8 Click on a row in the Mass List table to display the compounds found for that mass in the Search Results table in the lower part of the window. For more information on viewing batch search results, see "To view batch search results" on page 23.

9 Select and view the best compound hit for each mass as described in "To view batch summary results" on page 24 or clear the box for the selected hit to ignore that compound.

NOTE   All conflicting results must be resolved before retention time data can be updated.

10 Click the **Apply Retention Times** button to apply retention times from the Mass List in the Batch Search tab for each of the compounds listed in the Batch Summary table.

To edit compounds in custom database

Use this procedure to edit information for compounds, to add a new compound, or to remove a compound.

1 Open the custom database of interest.

2 Enable editing by marking **Allow Editing** on the Database/Library menu.

3 Do a search using *either* of the following:
- "To find compounds" on page 17.
- "To find compounds from a mass list" on page 21.

4 When the search is complete, click the **Edit Compounds** tab.

5 To update information for a particular compound:

a Select the compound of interest by clicking on it in the Search Results table. Information for the selected compound is displayed in the **Edit Compounds** tab.

b Update information on the left side of the Edit Compounds tab, such as Name, Mass, RT, Formula, CAS or ChemSpider ID, and Ion type.

c Update structure information if desired in either of the following ways:

- Click on the MOL Text tab and paste in MOL file text that you have copied from a molecular drawing tool (**Ctrl+V**), *or*

- Click the [ ] button in the Molecule area to open a **.MOL** file.

d Click the **Update Selected** button. The information for the compound is updated in the database and the information you entered in Step 5b is reflected in the Results table.

6 To add a new compound to the database:

a Click the **Add New** button. A new compound is created in the database with a mass of 0 named "New Compound" and the new compound is displayed at the end of the Results table.

b Enter or change information for the new compound as described in Step 5 above.

c Click the **Update Selected** button. The information you entered for the new compound is updated in the database and the information is reflected in the Results table.

Alternate method to add a new compound

Enter information for a new compound on the left side of the Edit Compounds tab, such as Name, Mass, RT, Formula, CAS ID, and Ion type, then click the **Save As New** button. A new compound is created in the database using the specified values. The new compound is displayed at the end of the Results table.

7 To remove a compound from the database:

a Select the compound of interest by clicking on it in the Search Results table. Use **Ctrl+click** or **Shift+click** to select multiple compounds for deletion.

b Click the **Delete Selected** button.

Spectral searching and editing

Searching and editing mass spectra in a spectral library is broken down into the following tasks:

- "To import spectra from a .CEF file" - *below*
- "To copy spectra from MassHunter Qualitative Analysis" - *below*
- "To paste spectra into PCDL" on page 30
- "To search a spectral library" on page 30
- "To browse spectra in the library" on page 31
- "To view spectra for a compound" on page 31
- "To add, move, or remove spectra in a custom library" on page 32
- "To clean up noisy spectra" on page 33

To import spectra from a .CEF file

Use this procedure to load spectra into PCDL software that have been output to a **.CEF** file from another program such as MassHunter Qualitative Analysis software.

1 Click to display the **Spectral Search** or **Edit Spectra** tab.

2 Click the **Load Spectra** button ⬚.

3 Select the **.CEF** file of interest and click the **Open** button.

If Profile spectra or non-MS/MS spectra are contained in the file, a message is displayed saying that they have been skipped. Only centroided MS/MS spectra are loaded for use in PCDL software.

The spectra appear in the Acquired spectra table. See the following topics for further use of imported spectra:

- "To search a spectral library" on page 30
- "To add, move, or remove spectra in a custom library" on page 32
- "To clean up noisy spectra" on page 33

To copy spectra from MassHunter Qualitative Analysis

1 Open the data file of interest in MassHunter Qualitative Analysis software.

2 Run **Find by Targeted MS/MS** or **Find by Auto MS/MS**, depending on how the data was acquired.

3 Expand the compounds of interest in Data Navigator to see the spectral results.

4 Select the product ion spectra of interest.

5 If the data was acquired in Profile mode, right-click and select **Convert Profile to Centroid and Replace** from the shortcut menu.

6 Right-click the MS Spectrum Results window and select **Copy to Clipboard**.

All spectra displayed in the MS Spectrum Results window are copied, not just the highlighted ones.

To paste spectra into PCDL

1 Copy spectra from MassHunter Qualitative Analysis as described in "To copy spectra from MassHunter Qualitative Analysis" on page 29.

2 Click to display the **Spectral Search** or **Edit Spectra** tab.

3 Right-click in the **Acquired spectra** table and select **Paste Spectra**.

If Profile spectra or non-MS/MS spectra were copied from MassHunter Qualitative Analysis, a message is displayed saying that they have been skipped. Only centroided MS/MS spectra are pasted into PCDL software. The spectra are listed in the Acquired spectra table.

NOTE Spectra *cannot* be pasted into the Library spectra table.
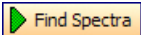
To search a spectral library

1 If the library you want to search is not already open, open it by clicking **Open Database/Library** from the File menu or the 📂 button on the toolbar.

2 Import spectra as described in "To import spectra from a .CEF file" or "To copy spectra from MassHunter Qualitative Analysis" on the previous page.

3 Click to select the spectrum to search from the **Acquired spectra** table on the **Spectral Search** tab.

4 Use the default search parameters or set any of the following search parameters: **Search type**, **Filters**, or **Tolerances**. These parameters are described in online Help.

5 Click ▶ Find Spectra to start the search.

The library search results are displayed in the Spectral Results table in the lower part of the tab. If desired, the spectral results display can be changed as described in To change how data is displayed in results tables.

6 Click on a row of the results table to view the mass spectrum plot for the selected compound in the Spectral Plot Window to the right of the table.

7 Click the **Mass Lists** tab in the Spectral Plot window to view a list of masses and abundance values for the selected compound.

To browse spectra in the library

Use the following procedure to search the current library for spectra that match certain parameters, such as mass, collision energy, ion polarity, and ionization mode.

1 Click the **Browse Spectra** tab.

2 Use the default search parameters to return the contents of the entire library and skip to Step 3. Otherwise, set the desired search criteria: **Mass**, **Collision energy**, **Ion polarity**, and **Ionization mode**. These parameters are described in online Help.

3 Click ▶ Find Spectra to start the search.

The library search results are displayed in the Spectral Results table in the middle of the tab. If desired, the spectral results display can be changed as described in "To change how data is displayed in results tables" on page 19.

4 Click on a row of the results table to view the mass spectrum plot for the selected spectrum in the Spectral Plot Window to the right of the table.

5 Click the **Mass Lists** tab in the Spectral Plot window to view a list of masses and abundance values for the selected spectrum.

To view spectra for a compound

1 Do a compound search using *either* of the following:

- "To find compounds" on page 17.
- "To find compounds from a mass list" on page 21.

2 When the compound search is complete, click the **Browse Spectra** tab.

The compound search results are displayed in the Compound Results table in the lower part of the tab.

3 Click on a compound of interest in the Compound Results table. The library spectra associated with the selected compound are displayed in the Spectral Results table in the middle of the tab. In this case, the search parameters set in the top of the tab are ignored.

4 Click on a row of the Spectral Results table to view the mass spectrum plot for the selected spectrum in the Spectral Plot Window to the right of the table.

5 Click the **Mass Lists** tab in the Spectral Plot window to view a list of masses and abundance values for the selected spectrum.

6 Repeat Steps 3 - 5 for other compounds of interest.

To add, move, or remove spectra in a custom library

1 Enable editing of the current library by marking **Allow Editing** on the Database/Library menu.

2 Do a compound search using *either* of the following:

 • "To find compounds" on page 17.

 • "To find compounds from a mass list" on page 21.

3 When the compound search is complete, click the **Edit Spectra** tab.

 The compound search results are displayed in the Compound Results table in the lower part of the tab.

4 Click on a compound you want to view or modify in the Compound Results table. The library spectra associated with the selected compound are displayed in the Library spectra table in the middle of the tab.

5 Load spectra into the Acquired spectra table at the top of the tab in either of the following ways:

 • From **.CEF** file as described in "To import spectra from a .CEF file" on page 29, *or*

 • From Qualitative Analysis, as described in "To copy spectra from MassHunter Qualitative Analysis" and "To paste spectra into PCDL" on page 30.

6 To add spectra to the library compound selected in Step 4:

 a Click to select the spectrum of interest in the Acquired Spectra table. Multiple spectra can be selected using **Ctrl+click** or **Shift+click**.

 b Click the **Add Spectra** button. The Library spectra table will be updated to show the new list of spectra for the compound.

7 To delete spectra from the library compound selected in Step 4:

 a Click to select the spectrum of interest in the Library Spectra table. Multiple spectra can be selected using **Ctrl+click** or **Shift+click**.

 b Click the **Delete Spectra** button. The Library spectra table will be updated to show the revised list of spectra for the compound.

8 To move spectra between compounds:

a Click to select the compound to copy spectra from in the **Compound Results** table in the lower part of the tab.

The spectra for that compound are displayed in the Library spectra table in the middle of the tab.

b Click to select the spectra of interest in the **Library spectra** table, then right‑click in the table and select **Copy Spectra** from the shortcut menu. Use **Ctrl-click** or **Shift-click** before copying if you want to select multiple spectra.

c Right‑click in the **Acquired spectra** table in the upper part of the tab and select **Paste Spectra** from the shortcut menu.

The spectra are added to the Acquired spectra table.

d Click to select the compound to copy the spectra to in the Compound Results table in the lower part of the tab.

e Click the **Add Spectra** button.

The Library spectra table will be updated to show the revised list of spectra for the compound.

To clean up noisy spectra

Use this procedure to remove small noise peaks from spectra before or after you add them to a custom library.

1 Select the spectrum of interest in either the **Acquired spectra** or **Library spectra** table on the **Edit Spectra** tab.

2 Click the **Mass Lists** tab in the Spectral Plot window. By default, the masses are sorted in descending order by relative abundance value. Click the **Rel Abund** column header if you want the lowest relative abundance values (likely noise peaks) to appear at the top of the table.

3 Select the masses to delete by clicking on them in the **Acquired masses** or **Library masses** list. Use **Ctrl-click** or **Shift-click** to select multiple masses.

4 Right‑click in the **Acquired masses** or **Library masses** list and select **Delete Masses** from the shortcut menu.

5 Update the library as follows, depending on whether the spectrum modified in Step 4 was an **Acquired** or **Library** spectrum.

• Click the **Add Spectra** button to add an **Acquired** spectrum to the selected library compound.

• Click the **Update Spectra** button to update the selected library compound with a modified **Library** spectrum.

Familiarization Exercises

These exercises will help you learn to use the PCDL software:
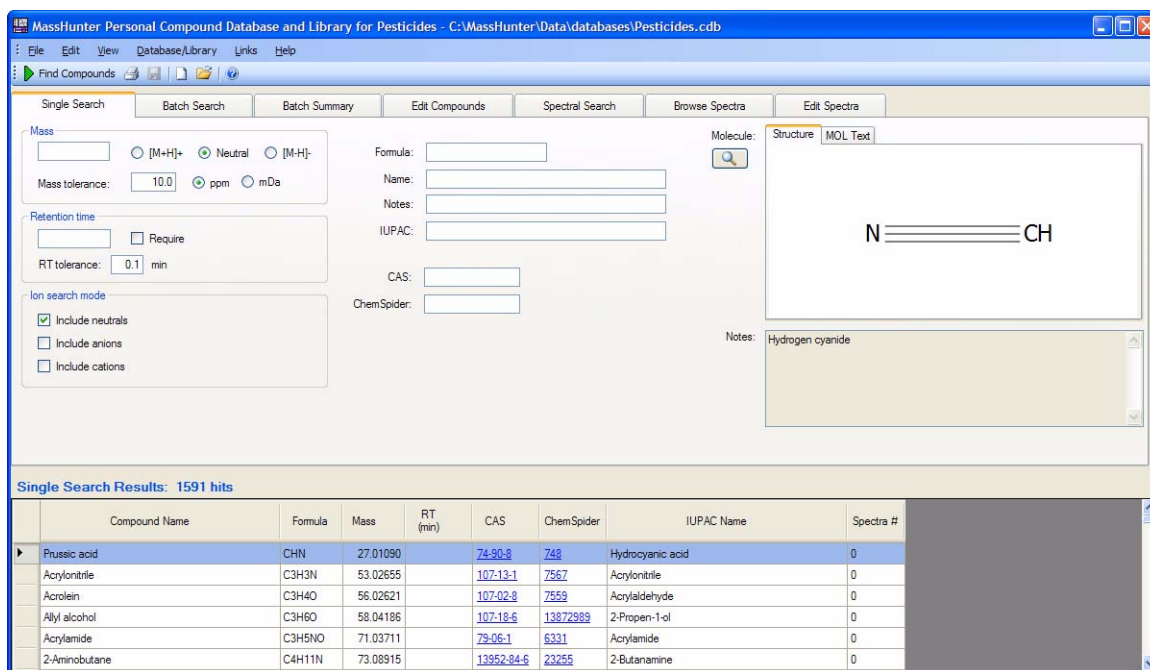
Spectral library operations:

Exercise 1. Search for compounds in a database

In this exercise, you will search for compounds in an example database and review the search results.

Steps	Detailed Instructions	Comments
1 Open the master Pesticide database.	**a** Select **Open Database/Library** from the File menu, *or* click the 📁 button on the toolbar. **b** Select the **databases\Pesticides.cdb** file, and click the **Open** button.	Skip this step if the Pesticides database is already open.
2 Click on the **Single Search** tab.		
3 Leave the search fields blank.	Be sure that the **Require** checkbox for Retention time is *cleared*, since the example Pesticides database does *not* contain retention time information.	This will return all compounds in the database. See "To find compounds" on page 17 for a discussion of search parameters to narrow your search.
4 Begin searching.	Click the **Find Compounds** button on the toolbar.	Alternate methods: • Select **Find Compounds** from the Database/Library menu. • Press the **F5** key.
5 Review the search results in the table in the lower half of the tab.	See Figure 1 on page 37.	The results are sorted from low mass to high mass.

Steps	Detailed Instructions	Comments
6 View structure information for a selected compound.	Click on a compound in the Compound Results table. Its structure is displayed in the Structures area on the right side of the window.	• Clicking the [🔍] button displays a larger image of the structure. • Clicking the **MOL Text** tab displays the text version of the structure.
7 Sort the table by name.	Click the heading of the **Compound Name** column. Click it again to sort by name in the opposite order.	Clicking on any column heading will sort the table according to the values in that column.
8 Reorder the columns in the table.	**a** Drag a column heading to a different position. **b** Repeat until the desired order is achieved.	
9 Resize a column.	You can resize columns in either of the following ways: • Double-click on the right column divider in the heading of the column of interest to resize the column to fit the information contained in it. • Drag the separator between column headings to the right or left until the column of interest is the desired width.	
10 Change which columns of information are displayed in the table.	**a** Right-click in the table and select **Add/Remove Columns** from the shortcut menu. **b** Move the items of information that you want to display from the **Available columns** list into the **Show these columns** list using the **Add->** button. **c** Move the items of information that *you don't want to display* out of the **Show these columns** list into the **Available columns** list using the **<-Remove** button. **d** Click **OK**.	Alternate Methods: • You can also open the Add/Remove Columns dialog box by selecting **Add/Remove Compound Columns** from the View menu. • You can move individual items between the two lists by double-clicking them. Note that the original column layout can be restored at anytime by selecting **Restore Default Compound Columns** from the View menu.

Steps	Detailed Instructions	Comments
11 Print results.	**a** Click the 🖨 button on the toolbar to open the Print Results dialog box. **b** Select print options. For a discussion of print options, see "To print compound results" on page 20. **c** Click **OK**. If you selected the Print Preview option, review the report in the Print Preview window, then click the 🖨 button to print it.	To print only selected results, highlight those rows in the Compound Results table using **Ctrl+click** or **Shift+click**, then select **Only highlighted rows** as one of the print options in Step c.

Figure 1   Results of Single Search for Pesticides

Exercise 2. Batch search from a mass list

In this exercise, you will search the master Pesticides database using an imported mass list.

Steps	Detailed Instructions	Comments
1 Open the master Pesticides database.	**a** Select **Open Database/Library** from the File menu, *or* click the 🗁 button on the toolbar. **b** Select the **databases\Pesticides.cdb** file, and click the **Open** button.	Skip this step if the master Pesticides database is already open, as it is after Exercise 2.
2 Click on the **Batch Search** tab.		
3 Open a mass list.	**a** Click the **File** button to the left of the mass list table. **b** Select the **pest_compounds.txt** mass list file in the **PCDL\Mass List Files** folder. **c** Click the **Open** button.	• Mass lists can also be copy-and-pasted into PCDL software from MassHunter Qualitative Analysis. • See online Help in MassHunter Qualitative Analysis for instructions on how to output a mass list.
4 Set the batch search parameters.	In this case the following default search parameters can be used for the search: • **Neutral Masses** option marked. • **Mass tolerance** 10 ppm. • **Optional** for **Retention times** marked. • Only the **Include neutrals** option marked for **Ion search mode**.	The Pesticides database does *not* include retention times.
5 Begin searching.	Click the **Find Compounds** button on the toolbar.	You can also start the search in *either* of the following ways: • Select **Find Compounds** from the Database/Library menu. • Press the **F5** key.
6 Review search results.	When the search is complete, the number of hits for each mass appears in the **Hits** column of the mass list, and the list is automatically sorted to show the masses with the most hits at the top of the list. See Figure 2 on page 40.	• To sort the mass list by a different criterion, click the heading for the column of interest. • Masses with conflicting hits are shown in red text in the Mass List table.

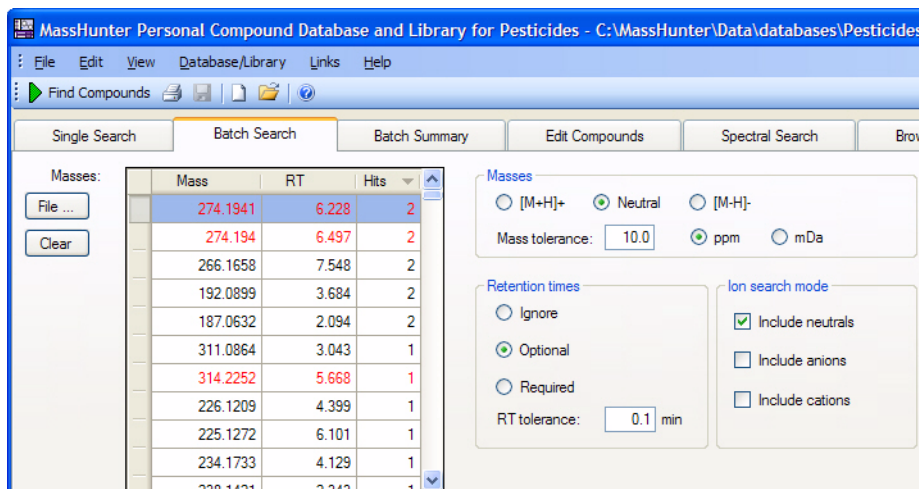| Steps	Detailed Instructions	Comments
7 View hits for selected masses.	Click on a row in the Mass List table to display the compounds found for that mass in the Batch Search Results table in the lower part of the window.	For ease of reviewing results, use the **F4** key to scroll down the Mass List and the **Shift**+**F4** keys to scroll back up. The information in the results table will be updated as you scroll through the mass list. The batch search results table can be resorted as described in "To change how data is displayed in results tables" on page 19.
8 Select the best compound hit for each mass.	Mark the **Best** column for the row (compound) you believe is the best compound hit for each mass. In many cases, this will be the one already selected by the software.	You can also clear the box for the selected hit to ignore that mass.
9 View the best hit results.	Click the **Batch Summary tab**. The Best hit for each mass is shown in the Batch Summary table in the lower part of the window. See Figure 3 on page 40.	Compounds with conflicting mass hits are shown in red text in the results table. The batch summary results table can be resorted as described in "To change how data is displayed in results tables" on page 19.
10 Export batch summary results.	**a** Click the ⊟ button on the toolbar to open the Export Results dialog box. **b** Select the following options: **Search parameters**, **Results**, and **Unmatched masses**. **c** Mark the **Open results file after exporting** option. **d** Click **OK** to output the results. The results will open in the associated application such as Excel. The following export file is created in the **PCDL\Results** folder: **pest_compounds-<timestamp>.txt**	You can also open the Export Results dialog box in either of the following ways: • Select **Export Results** from the File menu. • Right-click in the Batch Summary results table and select **Export Results** from the shortcut menu. You can select a different file name, location or type as described in "To export batch summary results" on page 25.

Figure 2   Results of Batch Search - Mass List
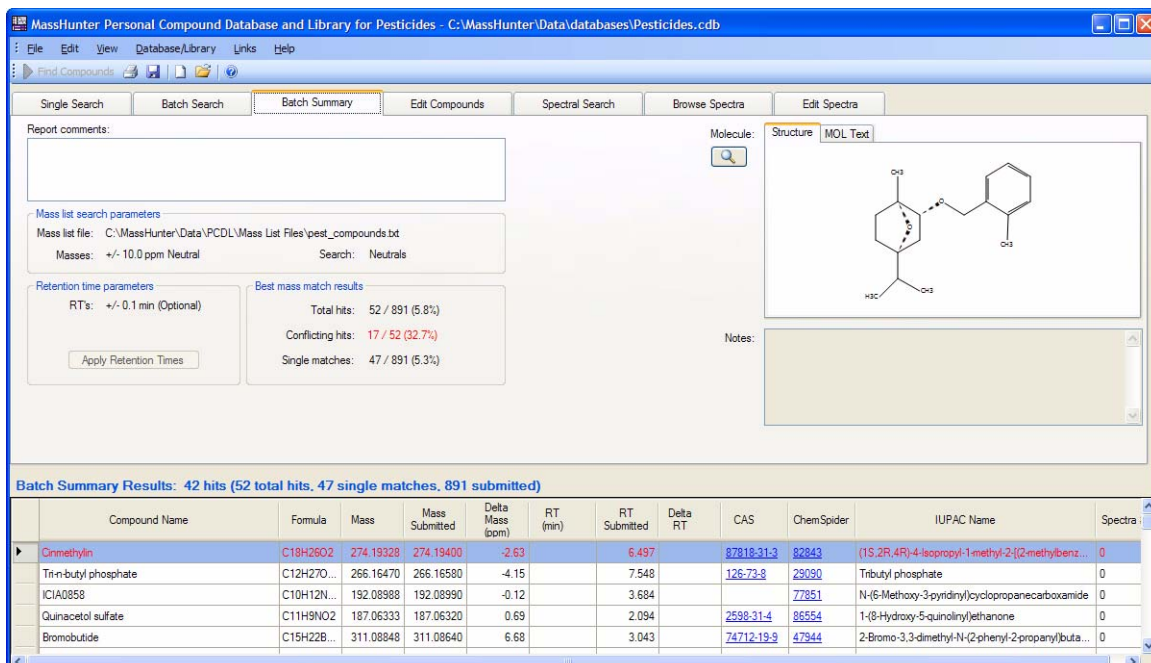

Figure 3   Batch Summary Results

Exercise 3. Create a custom database

In this exercise, you will create a custom database that is a subset of the example Pesticides database.

Steps	Detailed Instructions	Comments
1 Open the New Database/Library dialog box.	Select **New Database/Library** from the File menu or click the ☐ button on the toolbar.	
2 Create the new database.	**a** Browse to **\databases** as the Database/library path, since the default path is **\Library**. **b** Select **Pesticides** as the starting database. **c** Select **Pesticides** as the database type. **d** Type in a name for the new database, such as **Pest_Subset**. **e** Enter a description for the new database. **f** Click the **Create** button to create the new database.	• The new database becomes the current working database and is automatically enabled for editing. • The new custom database will contain all compounds and spectra from the starting database.
3 Edit the database.	See "Exercise 4. Edit compounds" on page 42.	

Exercise 4. Edit compounds
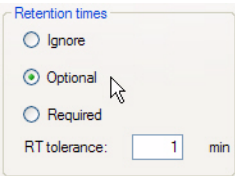
In this exercise, you will edit the custom database that you created in Exercise 3.

Steps	Detailed Instructions	Comments
1 Open the custom database you created in Exercise 3, if it is not already open.	**a** Select **Open Database/Library** from the File menu, *or* click the 🗁 button on the toolbar. **b** Select the **databases\Pest_Subset.cdb** file, and click the **Open** button.	Skip this step if the custom database is already open, as it will be if you just completed Exercise 3.
2 Enable editing for this database.	**a** Open the **Database/Library** menu. **b** Mark **Allow Editing** if it is not currently marked.	A new database or library is automatically enabled for editing when it is created.
3 Do a search.	**a** Click the **Single Search** tab. **b** Click the **Find Compounds** button on the toolbar to start the search. The search results appear in the table in the lower half of the window.	This search returns all neutral mass compounds in the database.
4 Click the **Edit Compounds** tab.		
5 Update information for a particular compound.	**a** Select the compound of interest by clicking on it in the Compound Results table. **b** Update information on the left side of the Edit Compounds tab, such as Mass, RT, Formula, Name, CAS ID, and Ion type. **c** Click the **Update Selected** button to apply the changes to the database.	Information for the selected compound is displayed in the Edit Compounds tab. The updated information will be changed in the database and reflected in the results table.
6 Update structure information for a particular compound.	**a** Select the compound of interest by clicking on it in the Compound Results table. **b** Click the 🗁 button in the Molecule area to open a **.MOL** file. **c** Click the **Update Selected** button. The information you entered will be changed in the library.	You can also update structure information for a selected compound by clicking on the **MOL Text** tab and pasting in MOL file text that you copied from a molecular drawing tool (**Ctrl+V**).

Steps	Detailed Instructions	Comments
7 Add a new compound to the database.	**a** Click the **Add New** button. A new compound is created in the database with a mass of 0 named "New Compound", and the new compound is displayed at the end of the Compound Results table. **b** Enter or change information for the new compound as described in Step 5 above. **c** Click the **Update Selected** button. The information you entered for the new compound is updated in the database and the information is reflected in the results table.	**Alternate method:** **a** Enter information for a new compound on the left side of the Edit Compounds tab, such as Mass, RT, Formula, Name, and Ion type. **b** Click the **Save As New** button. A new compound is created in the library using the specified values. The new compound is displayed at the end of the results table.
8 Remove a compound from the database.	**a** Select the compound of interest by clicking on it in the Compound Results table. **b** Click the **Delete Selected** button.	The selected compound is removed from the library.
9 Add retention times to the database as described in Exercise 5.		

Exercise 5. Add retention times to a database

In this exercise, you will add retention times to the custom database created in Exercise 3.

Steps	Detailed Instructions	Comments
1 Open the custom database you created in Exercise 3 and edited in Exercise 4, if it is not already open.	**a** Select **Open Database/Library** from the File menu, *or* click the 📂 toolbar button. **b** Select the **databases\Pest_Subset.cdb** file, and click the **Open** button.	
2 Enable editing for this database.	**a** Open the **Database/Library** menu. **b** Mark **Allow Editing** if it is not currently marked.	A new database or library is automatically enabled for editing when it is created.
3 Click the **Batch Search** tab.		
4 Open a mass list file that contains retention time information for the masses.	**a** Click the **File** button to the left of the mass list table. **b** Select **pest_compounds.txt** in the **PCDL\Mass List Files** folder. **c** Click the **Open** button.	Each mass in the mass list must have an associated retention time value.
5 Set the search parameters.	**a** Set the **Mass tolerance** to 10 ppm. **b** Mark **Retention times Optional**. **c** Set the **RT tolerance** to 1 minute as shown below:	
6 Start the search.	Click the **Find Compounds** toolbar button. The number of hits for each mass appears in the **Hits** column of the mass list. Masses with conflicting hits are shown in red text in the Mass List. See Figure 4.	To sort the list by a different criterion, click the heading for the column of interest.

Steps	Detailed Instructions	Comments
7 View hits for selected masses.	Click on a row in the Mass List table to display the compounds found for that mass in the Batch Search Results table in the lower part of the window.	For ease of reviewing results, use the **F4** key to scroll down the Mass List and the **Shift**+**F4** keys to scroll back up. The information in the results table will be updated as you scroll through the mass list. The batch search results table can be resorted as described in "To change how data is displayed in results tables" on page 19.
8 Select the best compound hit for each mass.	Mark the **Best** column for the row (compound) you believe is the best compound hit for each mass. In many cases, this will be the one already selected by the software.	You can also clear the box for the selected hit to ignore that mass.
9 Click the **Batch Summary** tab.	See Figure 5.	
10 Update retention times in the database from the current mass list.	Click the **Apply Retention Times** button. Note that this button is unavailable until all conflicting hits are resolved as described in Step 8.	Retention time information is updated in the database for each of the compounds listed in the Batch Summary table. See Figure 6.

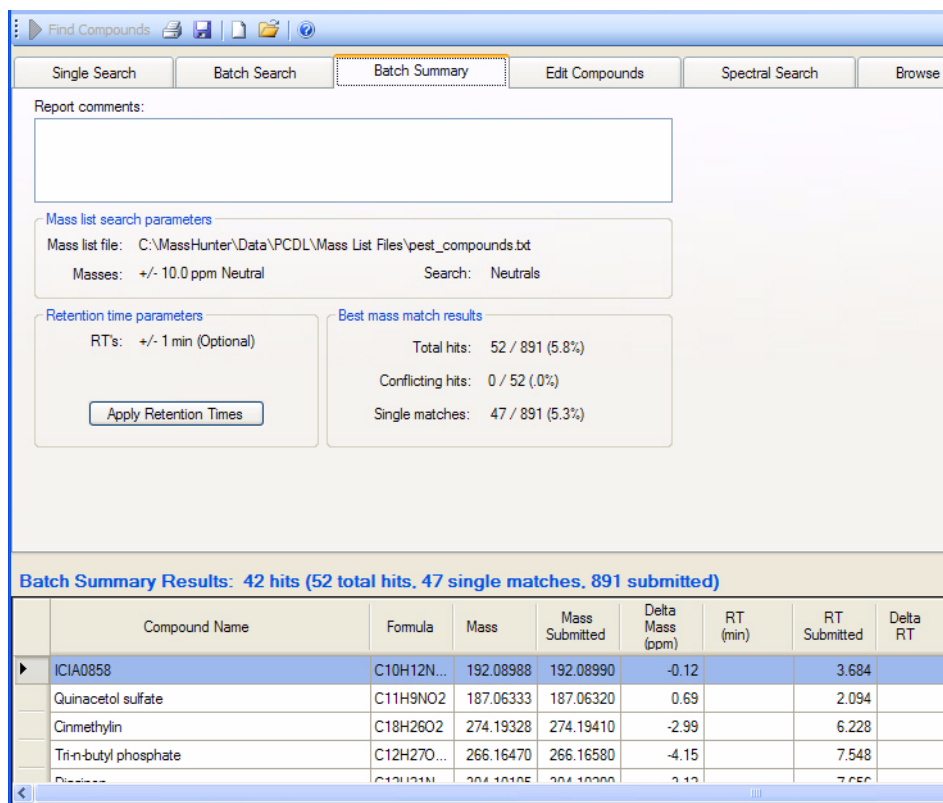**Figure 4**   Batch Search Results with Retention Time Optional

Figure 5 Batch Summary Results with Retention Time Optional (before updating)
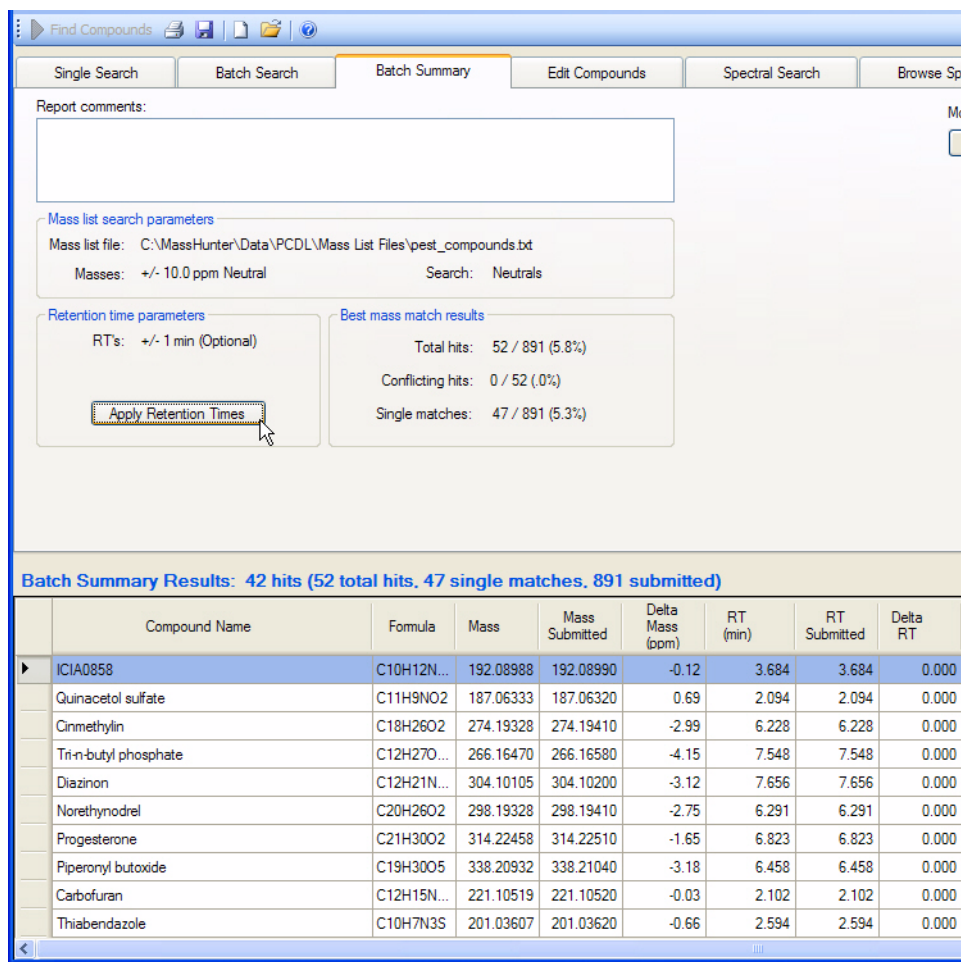
Figure 6   Batch Summary Results with Retention Times Updated

Exercise 6. Search a spectral library

In this exercise, you will load spectra from a **.CEF** file and search for spectra in an example library.

Steps	Detailed Instructions	Comments
1 Open the example SulfasLib library.	**a** Select **Open Database/Library** from the File menu, *or* click the 📂 button on the toolbar. **b** Select the **Library\SulfasLib.cdb** file, and click the **Open** button.	
2 Import spectra.	**a** Click the 📄 button on the **Spectral Search** tab. **b** Select the **Sulfas.cef** file in the **Example Data** folder on the MassHunter Personal Pesticide Database installation disk. **c** Click the **Open** button. **d** When the message "Any profile or non-MS/MS spectra were skipped" appears, click **OK**.	• See online Help in MassHunter Qualitative Analysis for instructions on how to output spectra to a **.cef** file. • This message appears when the import file contains Profile spectra or non-MS/MS spectra, as is the case in the example **.cef** file. Only centroided MS/MS spectra are imported for use in PCDL software.
	The imported spectra appear in the Acquired spectra table in the upper part of the tab.	Often the **Compound Name** field will be blank. Compound Name is shown only if the compound was identified in MassHunter Qualitative Analysis before the .cef file is exported.
3 Select the spectrum to search.	Click on the **Sulfamethazine** row in the Acquired spectra table that has **Collision Energy** value of **0**.	
4 Set search parameters.	*Clear* the check mark for the **Collision energy Filter**.	Use default values for the other search parameters.
5 Start searching.	Click the **Find Spectra** button on the toolbar.	You can also start the search in *either* of the following ways: • Select **Find Spectra** from the Database/Library menu. • Press the **F5** key.

| Steps	Detailed Instructions	Comments
6 View search results.	The library search results are displayed in the Library spectra table in the lower part of the tab. In this case, two library spectra are returned by the search, as shown in Figure 7 below.	If desired, the spectral results display can be changed as described in "To change how data is displayed in results tables" on page 19.
7 Select a different results spectra.	Click on a different row of the Library spectra table.	Notice that the lower spectrum in the **Graphics** tab of the Spectral Plot Window to the right of the table is updated.
8 View the mass list.	Click the **Mass Lists** tab in the Spectral Plot window.	
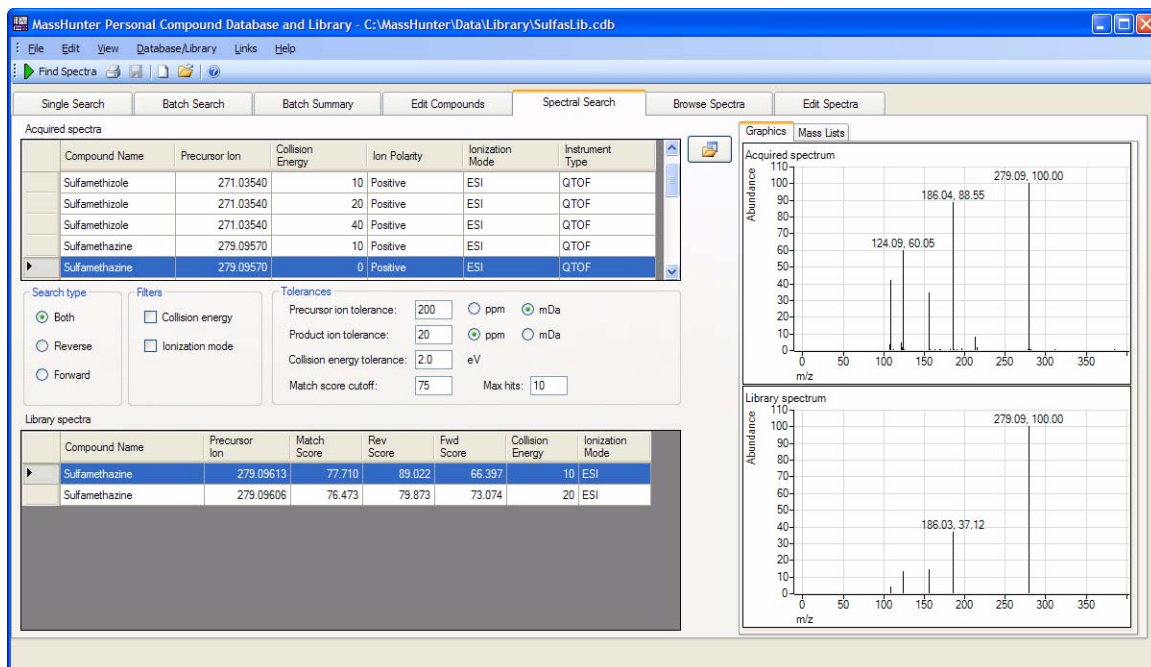
Figure 7   Spectral Search Results

Exercise 7. Browse spectra in the library

In this exercise, you will search an example library for spectra that match certain parameters, such as mass, collision energy, ion polarity, and ionization mode.

Steps	Detailed Instructions	Comments
1 Open the example SulfasLib library.	**a** Select **Open Database/Library** from the File menu, *or* click the 📂 button on the toolbar. **b** Select the **Library\SulfasLib.cdb** file, and click the **Open** button.	Skip this step if the SulfasLib library is already open, as it will be after Exercise 6.
2 Display the Browse Spectra tab.	Click to display the **Browse Spectra** tab.	
3 View all compounds in the library.	**a** Use the default search parameters: • **Precursor Ion Mass** and **Collision energy** blank • **Ion polarity (**Any) • **Ionization mode** (Any) **b** Click the **Find Spectra** button on the toolbar to start the search.	
4 View spectral information.	View **Compound Name**, **Precursor Ion**, **Collision Energy**, **Ion Polarity**, **Ionization Mode**, and **Instrument type** in the Spectral Search Results table in the middle of the tab. See Figure 8 on page 52.	
5 View the mass spectrum plot for one of the spectra.	**a** Click on a row of the results table to select a spectrum. **b** Click the **Graphic** tab in the spectral plot window to the right of the table.	
6 View the mass list for the selected spectra.	Click the **Mass List** tab in the spectral plot window.	
7 Filter spectra by Precursor ion mass.	**a** Set the Precursor ion mass to **279.09**. **b** Click the **Find Spectra** button on the toolbar to start the search.	Note that only the three Sulfamethazine spectra are returned.

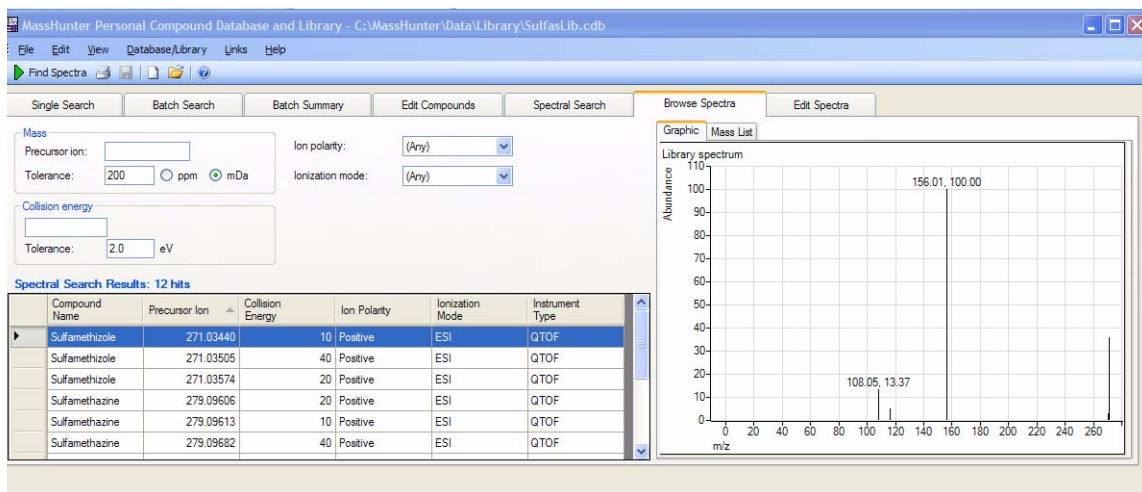| Steps	Detailed Instructions	Comments
8 Reset the default search parameters.	**a** Right click in the upper part of the Browse Spectra tab and select **Reset Search Fields** from the shortcut menu.	
9 Filter spectra by Collision energy voltage.	**a** Set the Collision energy to **40**. **b** Click the **Find Spectra** button on the toolbar to start the search.	Note that the four spectra are returned by the search that have Collision Energy values of 40,

Figure 8　　Browsing Spectra Results

Exercise 8. View spectra for compounds

In this exercise, you will view mass spectra for the compounds in an example library.

Steps	Detailed Instructions	Comments
1 Open the example SulfasLib library.	**a** Select **Open Database/Library** from the File menu, *or* click the ![icon] button on the toolbar. **b** Select the **Library\SulfasLib.cdb** file, and click the **Open** button.	Skip this step if the SulfasLib library is already open, as it will be after Exercise 7.
2 Click on the **Single Search** tab.		
3 Leave the search fields blank.	Be sure that the **Require** checkbox for Retention time is *cleared*, since the example library does *not* contain retention time information.	This will return all compounds in the database. See "To find compounds" on page 17 for a discussion of search parameters to narrow your search.
4 Begin searching.	Click the **Find Compounds** button on the toolbar.	Alternate methods: • Select **Find Compounds** from the Database/Library menu. • Press the **F5** key.
5 Display the Browse Spectra tab.	Click to display the **Browse Spectra** tab.	This procedure can also be performed from the **Edit Spectra** tab.
6 Select Sulfamethizole from the Single Search Results table.	Click on the **Sulfamethizole** row of the Single Search Results table.	The Single Search Results table is in the lower part of the tab and should contain the compound results from Exercise 1.
7 View the spectral information for Sulfamethizole.	View **Compound Name**, **Precursor Ion**, **Collision Energy**, **Ion Polarity**, **Ionization Mode**, and **Instrument type** in the spectral information table.	The spectral information table is in the middle of the tab.
8 View the mass spectrum plot for Sulfamethizole.	Click the **Graphic** tab in the spectral plot window. See Figure 9 on page 54.	The spectral plot window is on the right side of the tab.
9 View the mass list for Sulfamethizole.	Click the **Mass List** tab in the spectral plot window.	

| Steps	Detailed Instructions	Comments
10 View information for another Sulfamethizole spectrum.	**a** Click on a different row of the spectral information table. **b** View the mass spectrum and mass list for this spectrum in the Spectral Plot Window as described in Steps 8 and 9.	Different mass spectra were obtained for Sulfamethizole by acquiring data with three different Collision Energy values: 10, 20, and 40.
11 View spectral information for a different compound.	Click on the **Sulfamethazine** row of the Single Search Results table in the lower part of the tab.	View the spectral information for this compound as described in Step 7.
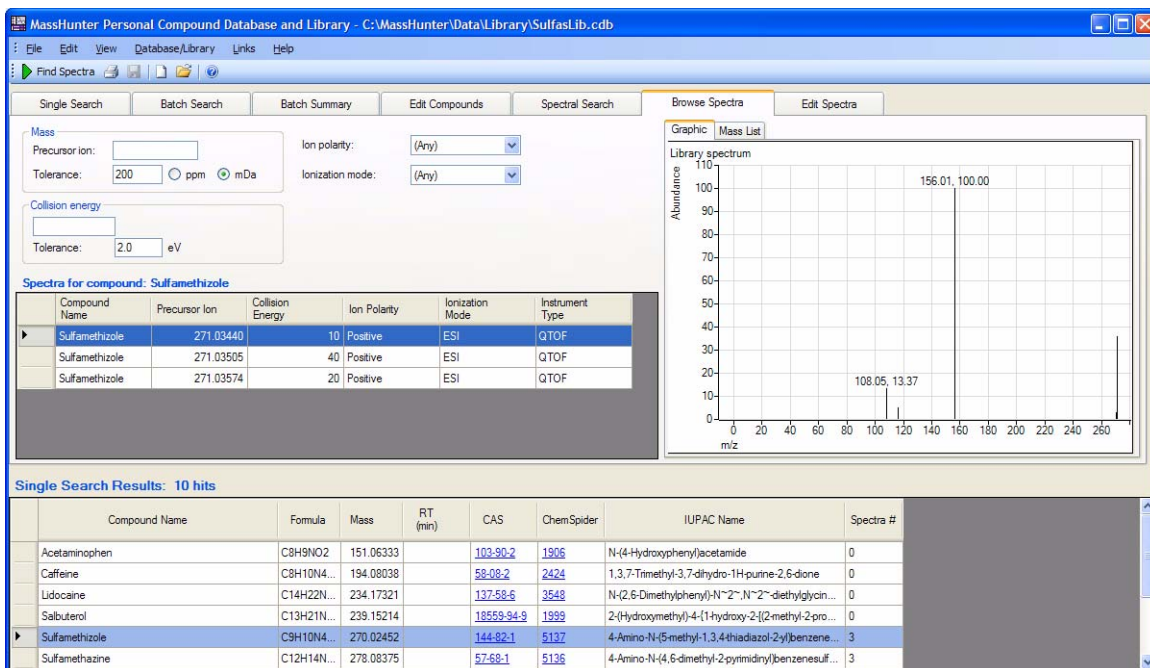
Figure 9   Viewing spectral information for Single Search results

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In this Book

This *Quick Start Guide* describes how to install and use the MassHunter Personal Pesticide Database.

It also includes familiarization exercises to help you get started with PCDL software.

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