MassHunter Personal Compound Database and Library Manager

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 MassHunter PCDL Manager **Help** menu.
- Press the **F1** key to get more information about a window, tab, or dialog box.

Agilent Technologies

What is MassHunter Personal Compound Database and Library Manager?

The MassHunter Personal Compound Database and Library Manager lets you manage content in personal compound databases (PCDs) and personal compound databases and libraries (PCDLs).

You can use the Agilent Personal Compound Database and Library Manager to add, remove and edit the compounds in your PCD/PCDL to meet the specific needs of your laboratory and your analyses. You can add retention times to your customized PCD/PCDL based on standards and/or retention times for compounds you analyze. You can also add your own spectra to your customized PCDL, in addition to those provided in the master PCDL.

With MassHunter Qualitative Analysis B.07.00, you can run a database search to identify compounds, and then send the MS/MS spectra to your customized PCDL. You can also filter spectral noise and correct the product ions to their theoretical accurate mass.

You will use the MassHunter Qualitative Analysis program to do automated or manual searches of a PCD or PCDL to identify compounds and spectrum peaks in your data files, as described in "Searching a PCDL in Qualitative Analysis" on page 24.

MassHunter PCDL Manager lets you

- Search for compounds in both PCDs and PCDLs, using text, formula, accurate mass, and retention time (optional or required). The use of retention time increases the compound identification specificity.
- Search or browse MS/MS spectra in PCDLs.
- Create and edit custom PCDs and PCDLs, including adding proprietary compounds, retention times, and theoretically corrected MS/MS and GC/MS spectra.
- Import mass lists with retention time in the form of a .txt or .csv file.
- Send spectra to your customized PCDL directly from the Qualitative Analysis program to create your own custom library. Choose from options to filter spectral noise and/or to correct the product ions to their theoretical accurate mass.
- Load spectra from either a **.CEF** file or by copy-and-pasting mass spectra from MassHunter Qualitative Analysis software and search for those spectra in the current PCDL.

- Do private, on-site searches, which keep intellectual property safe.
- Link to websites for more information on compounds.

Terminology Note

A ***PCD*** is an accurate mass compound database with or without retention times.

A ***PCDL*** is an accurate mass compound database with optional retention time, which also contains one or more MS/MS accurate mass spectra, also referred to as a spectral library.

Compound names

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. PCD and PCDL entries may contain the familiar compound names, but the empirical formulae reflect the detectable cation or anion portion of the molecule, rather than the formula of the neutral compound salt. For example, the full name Vecuronium bromide may be used for identification in the PCDL, even though the mass/formula only includes the Vecuronium cation.

Installation

If the MassHunter Personal Compound Database and Library Manager is not already installed on your system, install it as follows.

1 Insert the MassHunter Personal Compound Database and Library Manager disk into the disk drive.

2 From the installation disk, double-click **PCDLSetup.exe**.

3 Follow the instructions on the screen.

The MassHunter PCDL Manager is installed, along with the following **.cdb** files:

- **PCDL\Sulfas_AM_PCDL.cdb** - a small example master PCDL, which can be used to create a custom PCDL for importing compounds.
- **PCDL\Empty.cdb** - an empty master PCDL.

To create a PCDL and import compounds, see "To create a custom PCDL" on page 16 and "To import compounds to a custom PCDL" on page 17.

To remove MassHunter PCDL Manager

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

Doing this removes the PCDL Manager and master PCDs and PCDLs that have been installed, but does *not* remove custom PCDs and PCDLs you have created.

Startup

1 Select **Programs > Agilent > MassHunter Workstation > PCDL Manager** from the Windows Start menu to start the MassHunter PCDL Manager.

The PCDL that was last used is displayed as the default PCDL to open when you start the MassHunter PCDL Manager.

2 To open a different PCDL, see "To open a PCDL" on page 13.

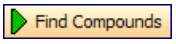
Main Window

The PCDL Manager main window has the following areas and controls.

- "Toolbar"(below)
- "Menus" on page 6
- "Compound Tabs" on page 8
- "Spectral Tabs" on page 10

Toolbar

The following items are available on the MassHunter PCDL Manager toolbar:

Button	Equivalent Menu Item	Comments
	PCDL > Find Compounds	Available only when the Single Search or Batch Search tabs are displayed. Same as pressing the **F5** key.
	PCDL > 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 PCDL	
	File > Open PCDL	
	View > Autosize Columns	
	View > Hide Empty Columns	
	Help > Contents	

Menus

The following menus are available in MassHunter PCDL Manager:

File menu

New PCDL Lets you create a custom PCDL that can be edited and personalized for your lab. This is done by creating a copy of an existing PCDL with a new name that can be edited. See "To create a custom PCDL" on page 16.

Open PCDL Lets you open a different PCDL.

Backup PCDL Lets you copy the PCDL for archive purposes.

Create Subset PCDL Lets you create a new PCDL from an input file, which is a subset of the currently loaded PCDL.

Import Compounds Lets you select a file that contains compounds to add to a custom PCDL if editing is enabled. If you start with an empty PCDL, then you are essentially creating a custom PCDL 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 MassHunter PCDL Manager window.

Edit menu

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

Add New Compound Creates a new compound in the PCDL. It has a mass of 0 and is 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 PCDL 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 PCDL. 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 PCDL. 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.

Autosize Columns Changes the width of each column in the compound and spectra tables so that the data is visible within its column. All columns in the table are resized except for Compound Name, IUPAC Name, and Notes. Columns are automatically resized if necessary, when you edit content on the Edit Compounds tab or the Edit Spectra tab. You may still need to scroll after using this command.

Hide Empty Columns Automatically hides columns in compound and spectra tables that do not have any content. You can display that column again when you click **Add/Remove Compound Columns**.

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

PCDL menu

Find Compounds Searches the PCDL 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. You can also press the **F5** key.

Find Spectra Searches the PCDL 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. You can also press the **F5** key.

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

Convert PCDL Opens the **Convert PCDL** dialog box. You need to convert a PCDL which was developed with an older version of PCDL to the format which is used with PCDL version B.07.00. Once you convert a PCDL to version B.07.00, you cannot use that PCDL in a version of Qualitative Analysis that is before B.07.00.

NOTE If you open an older PCDL, the program will automatically ask if you want to update to the newer format now. A copy of the original PCDL is archived in the \MassHunter\PCDL\Archive folder.

PCDL Information Opens the **PCDL Information** dialog box. You can view information about the current PCDL and edit the description for custom PCDs or PCDLs with editing enabled.

Links menu

Lets you access websites such as PubChem and ChemSpider for additional information on compounds or metabolites. The links displayed depend on the type of the current PCDL.

Help menu

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

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

About Displays the version and build number of the MassHunter PCDL Manager.

Compound Tabs

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

Single Search tab

Lets you search for compounds in the PCDL. Search results are displayed in the Compound Results table. See "To find compounds" on page 27.

Batch Search tab

Lets you search for compounds in the PCDL by specifying a mass list and optional retention times. Search results are displayed in the Compound Results table. See "To find compounds from a mass list" on page 34.

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 PCDs or PCDLs with editing enabled. See "To view batch summary results" on page 37.

Edit Compounds tab

For custom PCDs or PCDLs 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 a custom PCDL" on page 42.

Compound Results

Compound search results are displayed in the lower part of several tabs in the MassHunter PCDL Manager window. See "To change how data is displayed in results tables" on page 29 for more information on displaying search results.

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

You can also select compounds in the results table for editing on the Edit Compounds and Edit Spectra tabs (*custom PCDs or PCDLs with editing enabled only*). See "To edit compounds in a custom PCDL" on page 42.

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 PCDL. Clicking the  button opens the Structure Details dialog box and displays a larger image of the structure. Both MOL structures and glycan structures are supported.

If the structure attached to the currently selected compound is a glycan format, then the glycan cartoon is displayed in the Structures tab. Right-clicking on a glycan drawing lets you change the display settings, such as Show Linkage and Switch Direction.

MOL Text tab Displays the text version of the structure. If the current PCDL is a custom PCDL with editing enabled, you can copy text from a molecular drawing tool that is capable of generating MOL file text or a glycan structure 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**, **.kcf**, **.linucs**, or **.glycoct_condensed** 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 PCDL.

Browse Spectra Tab

Lets you search the current PCDL 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 PCDL.

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 PCDL, if editing is enabled for the PCDL. 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.

Clicking the Precursor Ion or Ion Species column for a particular spectrum brings up the Edit Species menu.

NOTE It is strongly recommended to use the Send Spectra to PCDL feature in MassHunter Qualitative Analysis to import spectra to a PCDL when creating your own custom library. This feature allows you to filter spectral noise, set a pass/fail base peak height filter, and correct the product ions to their theoretical accurate mass.

Graphic tab

This area of the spectra-related tabs lets you view selected spectra in graphic format. You can see the Acquired spectrum and the Library spectrum.

Mass List tab

This tab shows you the mass list for the current spectra that is displayed in the Graphic tab. The mass list consists of a list of masses and relative abundances

Getting Started

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

PCDL operations

The following PCDL operations are described in the following pages:

To open a PCDL

The PCDL that was last used is displayed as the default PCDL to open when you start MassHunter PCDL Manager. Do this step to open a *different* PCDL.

1 Open the Open PCDL dialog box in *either* of the following ways:
   - Click **Open PCDL** from the File menu, *or*
   - Click  on the toolbar.
2 Select the file of interest (**.cdb** extension) and click **Open**.
3 If the PCDL that you selected is from a previous version of PCDL Manager, then you are prompted to update the database to the new format. Click **Yes** to continue. If you click **No**, then you won't be able to edit, append or create subsets of the database in the older format.

NOTE Master PCDs and PCDLs cannot be edited, but they can be used to create custom PCDs or PCDLs that can be edited. See "To create a custom PCDL" on page 16.

To convert a PCDL

PCDLs from previous versions of MassHunter PCDL can be converted for use in MassHunter PCDL B.07.00 and later.

1. Click **Convert PCDL** from the **PCDL** menu to open the **Convert PCDL** dialog box.
2. Select the PCDL database that you want to convert (.CDB file extension) and click the **Convert** Button. The database is converted to the latest schema, and the name of the converted library is the same name. An archive of the PCDL is saved in the **Archive** folder before it is converted.

To back up a PCDL

1. Click **Backup PCDL** from the File menu.
2. Select a folder for the backup file or accept the default folder, which is:

   MassHunter\PCDL\Archive
3. Type in a file name for the backup file or accept the default file name, which is in the form:

   <name>.<yyyy.mm.dd>.cdb

   where **name** is the name of the current PCDL, **yyyy** is the current year, **mm** is the current month, and **dd** is the current day of the month.
4. Click **Save**.
   A backup copy of the PCDL is created using the specified file name and location.

To view PCDL information

1. Click **PCDL Information** from the PCDL menu.
2. View the following information about the PCDL:
   - File name
   - **# Compounds** (entries)
   - **Master** or **User**
   - **Type**: **General**, **Metabolomics**, **Pesticides**, **Forensics**, or **Glycans**
   - **Edit allowed**: **Yes** or **No**
   - **Last modified** timestamp
   - **Version** number
   - **Description**: the description can be edited if the current PCDL is a custom PCDL with editing enabled.
3. If you modified the **Description** or changed the database **Type**, click **Apply**.
4. Click **Close** to close the PCDL Information dialog box.

To view more information

1. Open the **Links** menu.
2. Click the web link of interest. The available links will vary depending on the type of the current PCDL: **General**, **Metabolomics**, **Pesticides**, **Forensics**, or **Glycans**.

   The selected web page will open in your Internet browser window.

To create a custom PCDL

1 Click **New PCDL** from the File menu or click  on the toolbar.

Tip You can also create a custom PCDL by creating a subset of an existing PCDL in either of the following ways:

- "To create a subset PCDL from an input file" on page 18
- "To create a subset PCDL from selected compounds" on page 32

2 Do the following steps on the New PCDL dialog box:

a Select a starting file for the new PCDL. The default path is **\MassHunter\PCDL**. The following files are supplied with the software and can be used to create custom PCDLs that you can edit and customize:

- **PCDL\Empty.cdb** - an empty master PCDL
- **PCDL\Sulfas_AM_PCDL.cdb** - a small example master PCDL. If you start with this PCDL, you will need to remove the example entries in this PCDL before using it.

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

c Type a name for the new PCDL.

d Enter a description for the new PCDL.

e Click **Create** to create the new PCDL.

The new PCDL becomes the current working PCDL and is automatically enabled for editing.

3 You can add compounds to the new PCDL in either of the following ways:

- "To import compounds to a custom PCDL" on page 17
- "To append compounds to a PCDL" on page 33
- "To send spectra from Qualitative Analysis" on page 19

To import compounds to a custom PCDL

Use the following procedure to import compounds into a custom PCDL or to create a custom PCDL from a compound list created by another application. If you start with an empty PCDL, then you are essentially creating a custom PCDL 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 MassHunter PCDL Manager as described in "To export batch summary results" on page 38.
   - Exported from another application such as Agilent Qualitative Analysis, Mass Profiler, or GeneSpring MS software.
   - Manually in Excel.
2. Open the custom PCDL of interest or create a new PCDL as described in "To create a custom PCDL" on page 16.
3. Enable editing on this PCDL by clicking **Allow Editing** on the PCDL menu. If it has a check mark next to this command, you can edit this PCDL.
4. Click **Import Compounds** from the File menu.
5. Select the **.CSV** or **.TXT** file prepared in Step 1 that contains the compounds of interest, and then click **Open**.
6. To view the new compounds in the PCDL, 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.
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. Examine this log file to determine how to fix the problems, and then import the corrected file.

NOTE

During import, the mass is calculated from the formula and that value is used for the PCDL. If the difference between the calculated value and the mass contained in the import file is > 0.0001 Da, then that compound is added to the log file. Common problems that result in mass errors are 1) the mass value is the mass from the spectrum and not a neutral mass, and 2) the formula contains the adduct (such as Cl). The information in the log file can be used to determine the correct Formula or Mass.

8. (*Optional*) See "To edit compounds in a custom PCDL" on page 42 if you want to change information for the imported compounds.

To create a subset PCDL from an input file

You use the following procedure to create a custom subset PCDL starting from the PCDL currently open in PCDL Manager. You can use a Master PCDL or a Custom PCDL as the starting template. You can use this procedure to create a small customizable subset of one of the Agilent Master PCDLs.

1. Prepare the input file in the proper format, as described in online Help.
2. Open the desired starting PCDL from which you want to create the subset PCDL.
3. Click **File > Create Subset PCDL** to open the **Create Subset PCDL** dialog box.
4. Select the input file prepared in Step 1.
5. Select the PCDL type (General, Metabolomics, Pesticides, Forensics, or Glycans).
6. Type in a name for the subset PCDL.
7. Select whether or not to include mass spectra.
8. Type in a description for the subset PCDL.
9. Click **Create**.

   The subset PCDL is created and a message is displayed that tells the number of compounds that were copied into the new subset PCDL.

   A log file is created that has a list of the compounds that were not found. The log file is created in the same directory as the subset PCDL and with the same name, i.e. **<name>.log**.
10. When a message is displayed to ask if you want to load the new subset PCDL, click **Yes** to load it or **No** to continue working with the current PCDL.

To send spectra from Qualitative Analysis

You use this procedure to send spectra, that have been identified in MassHunter Qualitative Analysis, for use in PCDL Manager. These actions are performed in the Qualitative Analysis program.

NOTE We strongly recommend that only the lowest monoisotopic ion is selected as the precursor ion for use in MS/MS library creation. The quadrupole resolution during acquisition must be set to narrow for this purpose. Doing this ensures the best possible match to the MS/MS fragmentation library when dealing with complex mixtures.

1. Open the MassHunter Qualitative Analysis program.
2. Create the spectrum that you want to send to a PCDL library. See "To extract spectra in Qualitative Analysis to send to PCDL" on page 21.

NOTE Using a large PCDL such as METLIN as a **Formula source** for identification when extracting spectra will result in multiple hits for each compound which will need to be manually sorted to identify the correct compound.

3. Open the **Send Spectra to PCDL** dialog box.
   - Right-click the spectrum in the MS Spectrum Results window and click **Send Spectra to PCDL**.
   - Select the spectrum. Then, click **Spectra > Send Spectra to PCDL**.
4. Select the **Library path**. The spectra are added to the selected PCDL.
5. (optional) Mark the **Minimum base peak height** check box. If you mark this check box, you can enter the minimum base peak counts that are needed to add the spectrum to the library. A default value of 1000 counts has been used and is recommended. You can change this value if necessary to achieve desired results. This option allows you to set a pass/fail criteria based on base peak height to ensure good ion statistics in the spectral library.
6. Click one of the **Annotation filter** options. You can click either **Formula annotated peaks (excludes unknowns) if present else all peaks** or **All peaks**. When **Formula annotated peaks (excludes unknowns) if present else all peaks** is selected, the program checks that the m/z fragment ions observed are

consistent with the assigned precursor ion species and assigns the fragment ion species as an annotation above each fragment ion peak.

7 Click one of the **m/z selection options**. You can click either **Calculated m/z if present else observed m/z** or **Observed m/z**.

8 Click one of the **Conflict resolution** options. If the spectrum already exists in the library, you can either **Send and replace the spectrum in library** or **Skip sending this spectrum**.

If profile or LC/MS spectra are contained in the file, a message is displayed saying that they have been skipped. Only identified, centroided MS/MS and GC/MS spectra are loaded for use in PCDL Manager.

The spectra appear in the library spectra table.

To send theoretically mass corrected spectra to a PCDL

The following options have been set as defaults in the Send Spectra to PCDL tab in the LibrarySearch-Default.m method. These options need to be re-selected if another method file is used.

- Minimum base peak height
- Formula annotated peaks (excludes unknowns) if present, else all data
- Calculated m/z if present else observed m/z

Before sending the spectra to the PCDL, manually inspect each spectrum and ensure that all peaks have been annotated. Annotated peaks are green and have the formula annotated above each peak. You may need to expand the x-axis to view the annotation. In the case that the spectrum itself is green, please click **Edit > Choose Defined Color** and choose a different color.

Any un-annotated peaks indicate the following:

1 An impurity ion which cannot be present according to the assigned precursor ion species empirical formula

2 A higher m/z isotope which can be seen when the quadrupole resolution has not been set to narrow during data acquisition.

When pure single compound standards have been used along with a quadrupole resolution set to narrow during acquisition but un-annotated peaks are still seen, please retune and calibrate the instrument before reacquiring data.

To extract spectra in Qualitative Analysis to send to PCDL

This topic describes how to extract the spectra. To send the spectra to PCDL, see "To send spectra from Qualitative Analysis" on page 19.

1 Open the LibrarySearching-Default.m method.
   a Click Method > Open.
   b Select this method
   c Click Open.
2 Set up Find Compounds by Formula parameters.

To extract MS/MS spectra and identify compounds, use Find Compounds by Formula and extract MS/MS spectra

   a In the Method Explorer window, click the **Find Compounds by Formula > Options** tab.
   b Click the **Results** tab.
   c Mark the **Extract MS/MS spectrum** check box.
   d Click the **Separate MS/MS spectrum per CE** button.
   e Click the **Formula Source** tab and select a PCDL database/library that contains the compounds of interest.

NOTE Using a large PCDL such as METLIN as a **Formula source** will result in multiple hits for each compound which will need to be manually sorted to identify the correct compound.

To extract GC/MS spectra and identify compounds, use Find Compounds by Formula

   a In the Method Explorer window, click the **Find Compounds by Formula > Options** section.
   b Click the **Formula Source** tab and select a PCDL **Database/Library** containing the compounds of interest.

NOTE Using a large PCDL such as METLIN as a **Formula source** will result in multiple hits for each compound which will need to be manually sorted to identify the correct compound.

3 Setup Generate Formulas parameters.

To Assign correct possible ion species

a In the Method Explorer, click the **Identify Compounds > Generate Formulas** section.

b Click the **Allowed Species** tab.

c Mark all desired ion species under **Charge carrier to be assumed if not known**.

d Verify that appropriate elements and limits are set under **Elements and Limits**.

NOTE For general LC and GC/MS spectrometry, the default value of **MS ion electron state** should be set to **Allow both even and odd**.

NOTE The following defaults are set in the LibrarySearching-Default.m method. Please verify these options if you are using another method.

Add fragment annotation.

a Click the **Fragment Formulas** tab.

b Mark **Annotate fragment spectrum peaks with formulas**.

NOTE When **Formula annotate peaks with formulas** is marked, the program checks that the *m/z* fragment ions observed are consistent with the assigned precursor ion species and assigns the fragmented ion species as an annotation above each fragment ion peak.

Set spectral noise filters.

a Click the **Fragment Formulas** tab.

b Mark **Absolute height** and type `10` for the **counts**.

c Mark **Relative height** and type `1` for the **% of largest peak**.

NOTE The above filters can be adjusted to achieve desired results.

NOTE For large molecules and/or molecules which have a high degree of fragmentation, you may need to set the **Maximum number of peaks** to a value that is higher than 250. This value is set on the Fragment Formulas tab.

4 Run the Find Compounds by Formula algorithm. Click **Find > Find Compounds by Formula**.

5 Verify that the compounds are identified properly, and inspect the degree of spectral annotation.

Annotated peaks are green and have the formula annotated above each peak. You may need to expand the x-axis to view the annotation. In the case that the spectrum itself is green, please click **Edit > Choose Defined Color** and choose a different color.

Any un-annotated peaks indicate the following:

1 An impurity ion which cannot be present according to the assigned precursor ion species empirical formula

2 A higher m/z isotope which can be seen when the quadrupole resolution has not been set to narrow during data acquisition.

NOTE Spectra acquired for library creation must have the quadrupole resolution set to narrow during acquisition. However, spectra acquired for library matching purposes can be routinely acquired with a lower resolution with the consequence that higher m/z isotopes will appear in the sample spectrum but not the library spectrum and will lower the forward score.

NOTE When acquiring spectra for library creation and pure single compound standards have been used along with a quadrupole resolution set to narrow during acquisition but un-annotated peaks are still seen, please tune and calibrate the instrument again before re-acquiring data.

Searching a PCDL in Qualitative Analysis

A mass-only search can be done on an ion in a spectrum or a compound. AMRT search can only be done on a compound. MS/MS library search can be done on an MS/MS spectra or a compound with MS/MS spectra. GC/MS library search can be done on GC/MS spectra or a compound with GC/MS spectra.

Use the following procedures to search a PCDL with MassHunter Workstation Software Qualitative Analysis program. These steps apply to version B.07.00 of Qualitative Analysis and may be slightly different in later revisions.

To use a PCDL to identify ions in a spectrum in Qualitative Analysis

Do this step to identify ions in a spectrum with a PCDL:

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. Set the 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.
   c. Select **PCDL Files (.cdb)** as the file type to see a list of PCDLs.
   d. Select the PCDL of interest and click **Open**.
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 PCDL 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 Spectrum Identification Results window.

To use a PCDL to identify compounds by mass or mass and retention time in Qualitative Analysis

Do this step to identify compounds with a PCDL:

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 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.
   c. Select **PCDL Files (.cdb)** as the file type to see a list of PCDLs.
   d. Select the PCDL of interest and click **Open**.
5. Initiate the search and review the results in the Compound Identification Results window.

To search an accurate mass library for spectra in Qualitative Analysis

Do this step to identify spectrum peaks with a PCDL:

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. Set the search criteria in the **Identify Compounds > Search Library** section of Method Editor:
4. On the **Libraries** tab, click the **Add Library** button to open the **Open Library File** dialog box. Select ,**cdb** as the **Files of type** to see a list of PCDLs. Select a library and then click **Open** to select the PCDL of interest.
5. Initiate the search in one of the following ways:
   - Click **Identify > Search Library for Spectra**
   - Click **Search Library for Spectra** on the Data Navigator Spectra shortcut menu
   - Click **Search Library for Spectra** in the MS Spectrum Results shortcut menu
   - Click **Search Library for Spectra** in the Actions menu

6 Review the results in the Spectrum Identification Results window, the Structure Viewer window, and the Spectral Difference Results window.

To search an accurate mass library for compounds in Qualitative Analysis

Do this task to identify compounds with a PCDL.

1 Open the data file of interest in Qualitative Analysis.

2 Find compounds using one of the Find Compounds with MS/MS extraction algorithms as described in Qualitative Analysis online Help.

3 Select the compounds to search in the Compound List window or Data Navigator.

4 Set the search criteria in the **Identify Compounds > Search Library** section of Method Editor.

5 On the **Libraries** tab, click the **Add Library** button to open the **Open Library File** dialog box. Select ,**cdb** as the **Files of type** to see a list of PCDLs. Select a library and then click **Open** to select the PCDL of interest.

6 Initiate the search in one of the following ways:

- Click **Identify > Search Library for Compounds**
- Click **Search Library for Compounds** in the Data Navigator Compounds shortcut menu
- Click **Search Library for Compounds** in the Compound List shortcut menu
- Click **Search Library for Compounds** in the Actions menu

7 Review the results in the Compound Identification Results window.

Searching a PCDL in MassHunter PCDL Manager

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

To find compounds

1. If the PCDL you want to search is not already open, click **Open PCDL** from the File menu or click  on the toolbar to open it.
2. Click the **Single Search** tab.
3. To return the contents of the entire PCDL, leave the search parameters 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 compound 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.
   - Select **Neutral** mass type if the mass is the calculated neutral mass value, usually a value that was calculated by Molecular Feature Extraction (MFE). *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 PCDL. For observed ions use either the **[M+H]+** or **[M-H]-** selection.
   - Select **[M-H]-** mass type if you are searching for an observed negative ion in the compound 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.

c Mark the options under **Ion search mode**:

- **Include neutrals** is typically marked. Clear it if you want to search anions and cations only.
- Mark **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 may return false matches.
- Mark **Include anions** if the data was acquired in *negative* ion mode.
- Mark **Include cations** if the data was acquired in *positive* ion mode.

4 Enter Retention time parameters, keeping the following guidelines in mind:

- When searching a PCDL *without* retention time data, be sure to *clear* the **Require** checkbox for **Retention time**.
- When searching a PCDL 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**, **IUPAC**, **CAS**, 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 PCDs or PCDLs only: **METLIN**, **KEGG**, **HMP**, and **LMP** IDs.

6 Start the search in any of the following ways:

- Click **Find Compounds** on the toolbar,
- Click **Find Compounds** on the PCDL 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 29 and “To change how data is displayed in results tables” on page 29.

To view compound search results

1. Do a search on the Single Search tab as described in "To find compounds" on page 27.
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 29.
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 PCDL.
4. To edit information for custom PCDs or PCDLs that allow editing, click the **Edit Compounds** tab, as described in "To edit compounds in a custom PCDL" on page 42.
5. If any of the compound results contain mass spectra, you can view them as described in "To view spectra for a compound" on page 47.

See Also

If desired, the following additional actions can be performed on the current compound results.

- "To print compound results" on page 31.
- "To create a subset PCDL from selected compounds" on page 32.
- "To append compounds to a PCDL" on page 33.

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. Click **View > Autosize Columns** to resize the widths of columns to the width of the widest content in any cell of the column. All columns in the table are resized except for **Compound Name**, **IUPAC Name**, and **Notes**.

NOTE Autosizing large CDBs can take a very long time. For example, any of the master METLIN cdb files can take 30 to 90 minutes to complete the procedure, depending on cdb size and computer model.

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

- **a** Right-click the table and click **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 by clicking **Add ->** or by double-clicking on them.
- **c** Remove any unwanted items of information from the **Show these columns** list by clicking **<- Remove** or by double-clicking on them.
- **d** Click **OK**.
- **e** Click **View > Hide Empty Columns** to automatically hide columns that do not have any content.

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

To print compound results

The **Print/Copy in Summary Format** check box changes the format and number of compounds printed. The **Print/Copy in Summary Format** check box is located above the compound results table.

If you clear the **Print/Copy in Summary Format** check box, then up to the first 30 compound entities selected are printed with all of the columns displayed in the Results table.

If you mark the **Print/Copy in Summary** check box, then all compounds selected or all compounds are printed. They are printed in the following summary format:

- **Compound Name**
- **Formula**
- **Mass**
- **RT** (min)
- One External ID
- **Agilent ID** and **METLIN ID**

1. If you want to print only certain compounds, highlight those rows in the Compound Results table using **Ctrl+click** or **Shift+click**.
2. (optional) Mark the **Print/Copy in Summary Format** check box above the compound results table.
3. Open the **Print Results** dialog box in *any* of the following ways:
   - Select **Print Results** from the File menu.
   - Click  on the toolbar.
   - Right-click the results table and click **Print Results** from the shortcut menu.
4. 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.
5. 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**)
6. Click **OK** to generate the report.

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

NOTE For Single Search results, only the first 30 compound results will be printed as displayed in the results table. To print all compounds selected in summary format, mark the **Print/Copy in Summary Format** check box.

To create a subset PCDL from selected compounds

1. Do either of the following searches to display compound information in the Results table:
   - "To find compounds" on page 27
   - "To find compounds from a mass list" on page 34
2. To select the compounds of interest, highlight those rows in the table.
3. To open the Create Subset PCDL dialog box, right-click the table, and then click **Create Subset PCDL** from the shortcut menu.
4. Enter the following information on the **Create Subset PCDL** dialog box:
   - Select the type: **General**, **Metabolomics**, **Pesticides**, **Forensics**, or **Glycans**. The type affects which user interface options are available when the PCDL is opened in PCDL Manager.
   - Type in a name for the subset PCDL.
   - Mark whether or not to include spectra for compounds if present in the PCDL.
   - Enter a description for the subset PCDL.
5. Click **Create**.
   The subset PCDL is created and a message is displayed that tells the number of compounds that were copied into the new subset PCDL.
6. When a message is displayed to ask if you want to load the new subset PCDL, click **Yes** to load it or **No** to continue working with the current PCDL.
7. You can append additional compounds to the subset database as described in "To append compounds to a PCDL" on page 33.

To append compounds to a PCDL

1. Do either of the following searches to display compound information in the Results table:
   - "To find compounds" on page 27
   - "To find compounds from a mass list" on page 34
2. To select the compounds of interest, highlight those rows in the table.
3. To open the Append to PCDL dialog box, right-click the table, and then click **Append to PCDL** from the shortcut menu.
4. Enter the following information on the **Append to PCDL** dialog box:
   - Select the path for the PCDL you want to append to or accept the default path displayed.
   - Select the PCDL to append the compounds to.
   - Mark whether or not to include spectra for compounds if present in the PCDL.
5. Click **Append**.

   The compounds are appended to the selected PCDL and a message is displayed that tells the number of compounds that were added.
6. When a message is displayed to ask if you want to load the PCDL, click **Yes** to load it or **No** to continue working with the current PCDL.

Doing a batch search

Searching a PCDL 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

1. If the PCDL you want to search is not already open, open it in *either* of the following ways:
   - Select **Open PCDL** from the File menu.
   - Click  on the toolbar.
2. Click 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 masses and retention times directly into the table.
4. Select or enter the **Type of mass** (typically **Neutral** for Batch Search) and **Mass tolerance**, in **ppm** or **mDa**.
5. Mark the **Ion search mode** check boxes as follows:
   - **Include neutrals** is typically marked.
   - Mark **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. Click 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 PCDL or any custom PCDL *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 PCDL that contains retention time information for *some* compounds.
Required	Consider only compounds that match the specified retention time range.	When searching a PCDL 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 **Find Compounds** on the toolbar.
- Click **Find Compounds** from the PCDL 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 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 36.

10 Select and view the best compound hit for each mass as described in "To view batch summary results" on page 37.

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 34.
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 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 29.
5. See "To view batch summary results" on page 37 for information on selecting and viewing the best compound hit for each mass.
6. Click 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 PCDL.
7. Click the **Edit Compounds** tab to edit information for custom PCDs or PCDLs that allow editing, as described in "To edit compounds in a custom PCDL" on page 42.
8. If any of the compound results contain mass spectra, you can view them as described in "To view spectra for a compound" on page 47.

See Also If desired, the following additional actions can be performed on the current compound results.

- "To print compound results" on page 31.
- "To create a subset PCDL from selected compounds" on page 32.
- "To append compounds to a PCDL" on page 33.

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 34.
2. Click 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 29.
6. Click 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 PCDL.
7. Click the **Edit Compounds** tab to edit information for custom PCDs or PCDLs that allow editing, as described in "To edit compounds in a custom PCDL" on page 42.
8. To export batch summary results, see "To export batch summary results" on page 38.
9. To print batch summary results, see "To print compound results" on page 31.
10. (*Optional*) For a custom PCDL with editing enabled, you can update retention times in the PCDL for the compounds shown in the Batch Summary Results table. See "To update retention time data" on page 40.

To export batch summary results

1. Do a batch search as described in "To find compounds from a mass list" on page 34.
2. Select and view the best compound hit for each mass as described in "To view batch summary results" on page 37, 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 29.
4. Open the **Export Results** dialog box in *any* of the following ways:
   - Click **Export Results** from the File menu.
   - Click  on the toolbar.
   - Right-click the results table and click **Export Results** from the shortcut menu in the Batch Summary results table.
5. Click **Select** 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 are 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 PCDL

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

- "To update retention time data" on page 40
- "To edit compounds in a custom PCDL" on page 42

To update retention time data

This procedure applies to custom PCDs or PCDLs only.

1. Open the custom PCDL of interest. Be sure that editing is enabled by marking **Allow Editing** on the PCDL menu.
2. Click 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 PCDL with no retention time information or retention times that may be outside the tolerance window.
   - **Optional** - Use this option to search a PCDL 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 PCDL. Specify an **RT tolerance** value in minutes as well.
5. Set other search criteria if desired as described in "To find compounds from a mass list" on page 34.
6. Initiate the search in *any* of the following ways:
   - Click **Find Compounds** on the toolbar.

- Click **Find Compounds** from the PCDL 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 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 36.

9 Select and view the best compound hit for each mass as described in "To view batch summary results" on page 37 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 **Apply Retention Times** 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 a custom PCDL

Do this step to edit information for compounds, to add a new compound, or to remove a compound.

1 Open the custom PCDL of interest.

2 Enable editing by marking **Allow Editing** on the PCDL menu.

3 Do a search using *either* of the following:

- "To find compounds" on page 27.
- "To find compounds from a mass list" on page 34.

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

NOTE

If the mol file does not contain a structure with the same molecular formula as in the Formula box, a warning appears stating that the structure's formula and thus Mass differs from that in the Formula box. You can click Yes to apply the structure's formula, and the current information in the Formula and Mass boxes is automatically edited.

If you click No, the mol file is updated, but the compound information is not changed.

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

6 To add a new compound to the PCDL:

a Click **Add New**. A new compound is created in the PCDL 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 **Update Selected**. The information you entered for the new compound is updated in the PCDL and the information is reflected in the Results table.

NOTE If you select another compound entry before clicking **Update Selected**, all entered information is lost.

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 **Save As New**. A new compound is created in the PCDL using the specified values. The new compound is displayed at the end of the Results table.

7 To remove a compound from the PCDL:

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

b Click **Delete Selected**.

Spectral searching and editing

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

To import spectra from a .CEF file

Do this step to load spectra into MassHunter PCDL Manager 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 **Load Spectra**  .
3. Select the **.CEF** file of interest and click **Open**.

   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 MassHunter PCDL Manager.

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

   - "To search spectra in a PCDL" on page 46
   - "To add, move, or remove spectra in a custom PCDL" on page 48
   - "To clean up noisy spectra" on page 50

To copy spectra from MassHunter Qualitative Analysis

1. Open the data file of interest in MassHunter Qualitative Analysis software.
2. Find compounds. You can use one of the following algorithms:
   - **Find by Targeted MS/MS**, depending on how the data was acquired.
   - **Find by Auto MS/MS**, depending on how the data was acquired.
   - **Find by Formula**, as long as the **Extract MS/MS spectra** check box is marked
   - **Find by Molecular Feature**, as long as the **Extract MS/MS spectra** check box is marked.
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 click **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. It may be simpler to only display one spectra at a time.

NOTE It is also possible to copy spectra from one compound or from one PCDL to another. Multiple windows of PCDL Manager, including multiple windows of the same PCDL file, can be open at the same time.

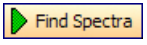
To paste spectra into MassHunter PCDL Manager

1. Copy spectra from MassHunter Qualitative Analysis as described in "To copy spectra from MassHunter Qualitative Analysis" on page 45.
2. Click to display the **Spectral Search** or **Edit Spectra** tab as appropriate.
3. Right-click the **Acquired spectra** table and click **Paste Spectra**.

   If profile spectra or LC/MS spectra were copied from MassHunter Qualitative Analysis, a message is displayed saying that they have been skipped. Only centroided MS/MS and GC/MS spectra are pasted into MassHunter PCDL Manager. The spectra are listed in the Acquired spectra table.

NOTE Spectra *cannot* be pasted into the Library spectra table.

To search spectra in a PCDL

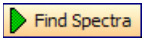
1. If the PCDL you want to search is not already open, open it by clicking **Open PCDL** from the File menu or  on the toolbar.
2. Import spectra as described in "To import spectra from a .CEF file" or "To copy spectra from MassHunter Qualitative Analysis" on the previous page.
3. Click to select the 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 

to start the search.

   The 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 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 relative abundance values for the selected spectrum.

To browse spectra in the PCDL

Use the following procedure to search the current PCDL 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 PCDL 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 

to start the search.

   The PCDL 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 29.
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 27.
   - "To find compounds from a mass list" on page 34.
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 a compound of interest in the Compound Results table. The PCDL 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 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 relative abundance values for the selected spectrum.
6. Repeat step 3 through step 5 for other compounds of interest.

To change ion species for a compound

1. View spectral information for compounds in the spectral tables on the Edit Spectra tab.
2. Double-click the Ion Species cell in the row for the compound of interest to open the Edit Species dialog box.
3. The following information is displayed but cannot be edited: Compound Name, Compound Mass, and Ionization Mode.
4. If desired, change the value for the **Precursor Ion**.
5. Select an Ion Species for the compound.
6. Click **OK** to close the **Ion Species** dialog box.
7. Repeat steps 2 to step 6 for other compounds of interest.

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

NOTE The information about the spectra such as collision energy, ion polarity, ionization mode, and instrument type *cannot* be edited. The acquisition parameters used for data acquisition are stored with the spectra in the PCDL. The Ion species and Precursor Ion values can be edited and allow you to choose the correct ion species from a pull down context sensitive menu or directly type in the ion species.

NOTE Agilent strongly recommends to use the Send Spectra to PCDL feature in MassHunter Qualitative Analysis to import spectra to a PCDL when you create a custom library. The spectra are loaded directly into the library table. This function allows you to filter spectral noise, set a pass/fail base peak height filter and correct the product ions to their theoretical accurate mass.

1. Enable editing of the current PCDL by marking **Allow Editing** on the PCDL menu.
2. Do a compound search using *either* of the following:
   - "To find compounds" on page 27.
   - "To find compounds from a mass list" on page 34.
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 a compound you want to view or modify in the Compound Results table. The spectra associated with the selected compound are displayed in the Library spectra table in the middle of the tab.

5 To view more of the table, drag the vertical blue line that divides the screen.

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

- From a **.CEF** file as described in "To import spectra from a .CEF file" on page 44, *or*
- From Qualitative Analysis, as described in "To copy spectra from MassHunter Qualitative Analysis" and "To paste spectra into MassHunter PCDL Manager" on page 46.

7 To add spectra to the 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 **Add Spectra**. The Library spectra table will be updated to show the new list of spectra for the compound.

c Click each spectrum to edit the **Ion Species**.

8 To delete spectra from the 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 **Delete Spectra**. The Library spectra table will be updated to show the revised list of spectra for the compound.

9 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 **Add Spectra**.

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

To clean up noisy spectra

Do this step to remove small noise peaks from spectra before or after you add them to a custom PCDL, if you used the import from cef file or copied spectra from MassHunter Qualitative Analysis. Using the **Send Spectra to PCDL** feature in MassHunter Qualitative Analysis eliminates the need for this step.

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 PCDL as follows, depending on whether the spectrum modified in Step 4 was an **Acquired** or **Library** spectrum.
   - Click **Add Spectra** to add an Acquired spectrum to the selected library compound.
   - Click **Update Spectra** to update the selected library compound with a modified Library spectrum.

Familiarization Exercises

These exercises will help you learn to use the MassHunter Personal Compound Database and Library Manager:

Custom PCDL operations:

Exercise 1. Search for compounds

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

Steps	Detailed Instructions	Comments
1 Open the example PCDL.	**a** Click **Open PCDL** from the File menu, *or* click the  button on the toolbar. **b** Select the **Sulfas_AM_PCDL.cdb** file, and click the **Open** button.	Skip this step if the Sulfas PCDL is already open.
2 Click the **Single Search** tab.		
3 Leave the search parameters blank.	• Verify that the **Require** checkbox for Retention time is *cleared*, since the example Sulfas PCDL does *not* contain retention time information.	This will return all compounds in the PCDL. See "To find compounds" on page 27 for a discussion of search parameters to narrow your search.
4 Begin searching.	• Click the **Find Compounds** button on the toolbar.	Alternate methods: • Click **Find Compounds** from the PCDL menu. • Press the **F5** key.

Steps	Detailed Instructions	Comments
5 Review the search results in the table in the lower half of the tab.	• See Figure 1 on page 54.	The results are sorted from low mass to high mass.
6 View structure information for a selected compound.	• Click a compound in the Compound Results table. Its structure is displayed in the **Structure** 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.	• Double-click the right column divider in the heading of the column of interest to resize the column to fit the information contained in it.	Alternate Method: • Drag the separator between column headings to the right or left until the column of interest is the desired width. • Click **View > Autosize Columns**.
10 Change which columns of information are displayed in the table.	**a** Right-click the table and click **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 by clicking 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 clicking **Restore Default Compound Columns** from the View menu.

Steps	Detailed Instructions	Comments
11 Create a subset PCDL from selected compounds.	**a** To select the compounds of interest, highlight those rows in the table. **b** Right-click the table, and then click **Create Subset PCDL**. **c** Enter the information on the **Create Subset PCDL** dialog box. **d** Click **Create**. **e** Click **No** when asked whether or not to load the new PCDL.	• For more information, see "To create a subset PCDL from selected compounds" on page 32. • You can also append selected results to an existing PCDL as described in "To append compounds to a PCDL" on page 33.
12 Print results.	**a** Mark or clear the **Print/Copy in Summary Format** check box. **b** Click the  button on the toolbar to open the Print Results dialog box. **c** Select print options. For a discussion of print options, see "To print compound results" on page 31. **d** Click **OK**. If you selected the Print Preview option, review the report in the Print Preview window, then click the  button to print it.	• If you mark the **Print/Copy in Summary Format** check box, then all compounds with only certain columns are printed. See "To print compound results" on page 31. • If you clear this check box, then all columns shown in the results table are printed for the first 30 selected compounds. • 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.

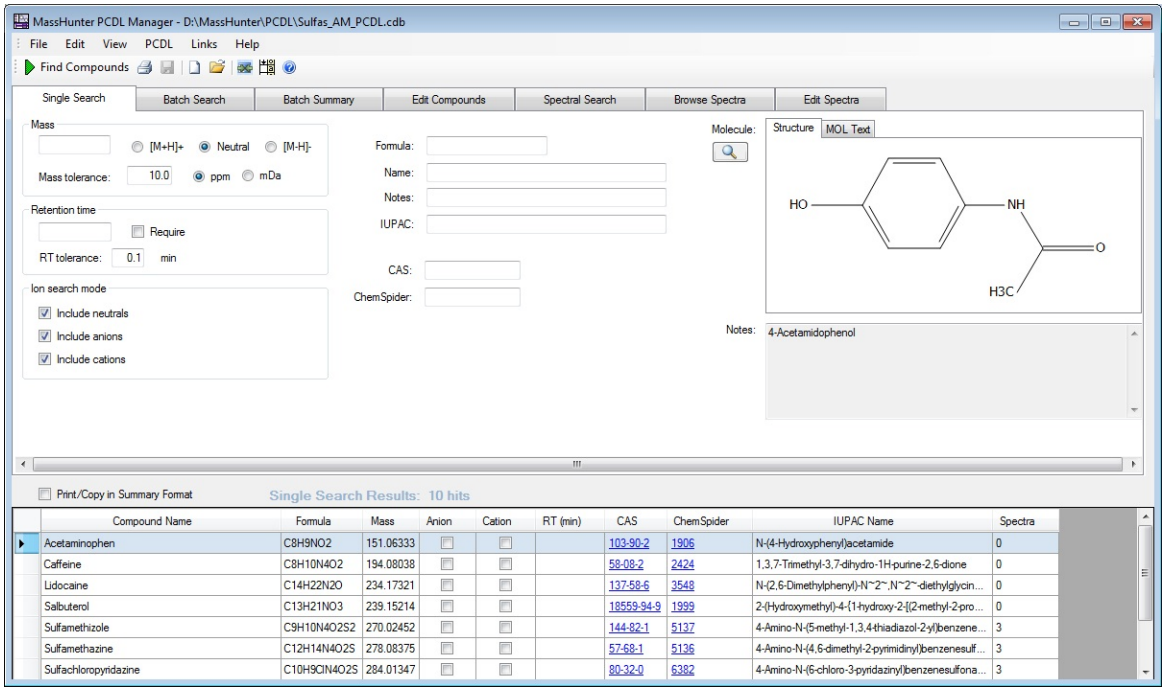


Figure 1 Results of Single Search for Compounds

Exercise 2. View spectra for compounds

In this exercise, you will view mass spectra for the compounds retrieved in the Single Search done in Exercise 1.

Steps	Detailed Instructions	Comments
1 Display the Browse Spectra tab.	Click to display the **Browse Spectra** tab.	This procedure can also be performed from the **Edit Spectra** tab.
2 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.
3 View the spectral information for Sulfamethizole.	View **Compound Name**, **Ion Species**, **Precursor Ion**, **CE (V)**, **Polarity**, **Ionization**, and **Instrument** in the spectral information table.	The spectral information table is in the middle of the tab.
4 View the mass spectrum plot for Sulfamethizole.	Click the **Graphic** tab in the spectral plot window. See Figure 2 on page 56.	The spectral plot window is on the right side of the tab.
5 View the mass list for Sulfamethizole.	Click the **Mass List** tab in the spectral plot window.	
6 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 4 and 5.	Different mass spectra were obtained for Sulfamethizole by acquiring data with three different Collision Energy values: 10, 20, and 40.
7 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 3.

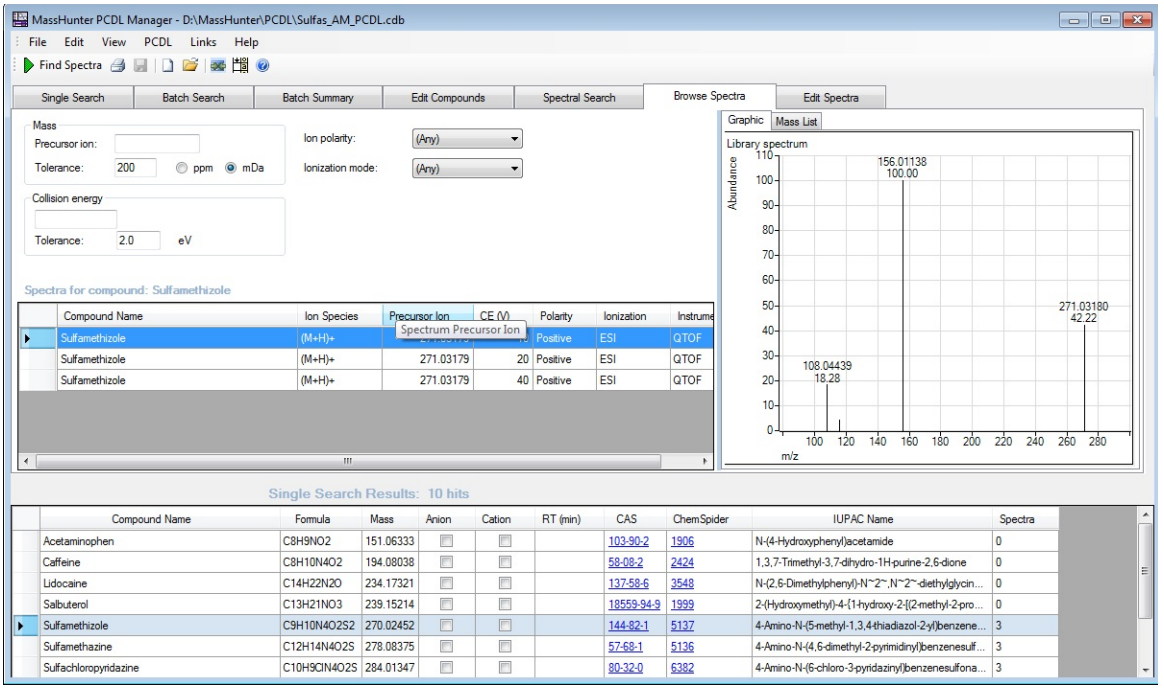


Figure 2 Viewing Browse Spectra tab

Exercise 3. Batch search from a mass list

In this exercise, you will search an example PCDL using an imported mass list.

Steps	Detailed Instructions	Comments
1 Open the example PCDL.	**a** Select **Open PCDL** from the File menu, *or* click the  button on the toolbar. **b** Select the **Sulfas_AM_PCDL.cdb** file, and click the **Open** button.	Skip this step if the Sulfas PCDL is already open, as it is after Exercise 2.
2 Click 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 **sulfa_compounds.txt** mass list file in the **MassHunter\PCDL\Mass List Files** folder. **c** Click the **Open** button.	• Mass lists can also be copy-and-pasted into PCDL Manager 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.	**a** 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** clicked. • Only the **Include neutrals** option marked for **Ion search mode**.	The example PCDL does *not* include retention times.
5 Begin searching.	Click the **Find Compounds** button on the toolbar.	Alternate methods: • Select **Find Compounds** from the PCDL 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. • The list is automatically sorted to show the masses with the most hits at the top of the list. See Figure 3 on page 59.	• 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.
7 (Optional) Create a subset PCDL from selected compounds or append selected compounds to an existing PCDL.	• See "To create a subset PCDL from selected compounds" on page 32.	• See "To append compounds to a PCDL" on page 33.

Steps	Detailed Instructions	Comments
8 View hits for selected masses.	Click 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 29.
9 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.
10 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 4 on page 59.	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 29.
11 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 **MassHunter\PCDL\Results** folder: **sulfa_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 38.

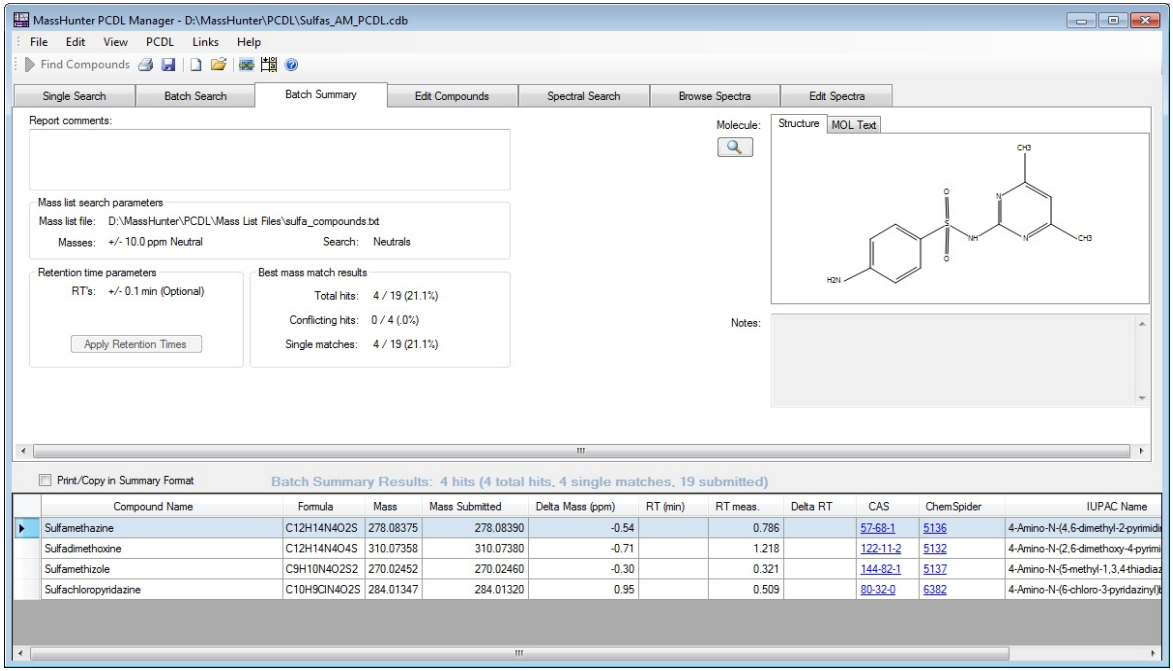


Figure 4 Batch Summary Results

Exercise 4. Search a spectral library

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

Steps	Detailed Instructions	Comments
1 Open the example PCDL.	**a** Select **Open PCDL** from the File menu, *or* click the  button on the toolbar. **b** Select the **Sulfas_AM_PCDL.cdb** file, and click the **Open** button.	Skip this step if the Sulfas PCDL is already open, as it will be after Exercise 3.
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 PCDL installation disk. **c** Click the **Open** button.	• See online help in MassHunter Qualitative Analysis for instructions on how to output spectra to a **.CEF** file. • When MS spectra are loaded into the Spectral Search tab, the **Precursor Ion** value is empty.
	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 **Sulfamethizole** row in the Acquired spectra table that has **Collision Energy** value of **12**.	
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 PCDL menu. • Press the **F5** key.
6 View search results.	The search results are displayed in the Library spectra table in the lower part of the tab. See Figure 5 on page 61.	If desired, the spectral results display can be changed as described in "To change how data is displayed in results tables" on page 29.
7 View the mass list.	• Click the **Mass Lists** tab in the Spectral Plot window.	

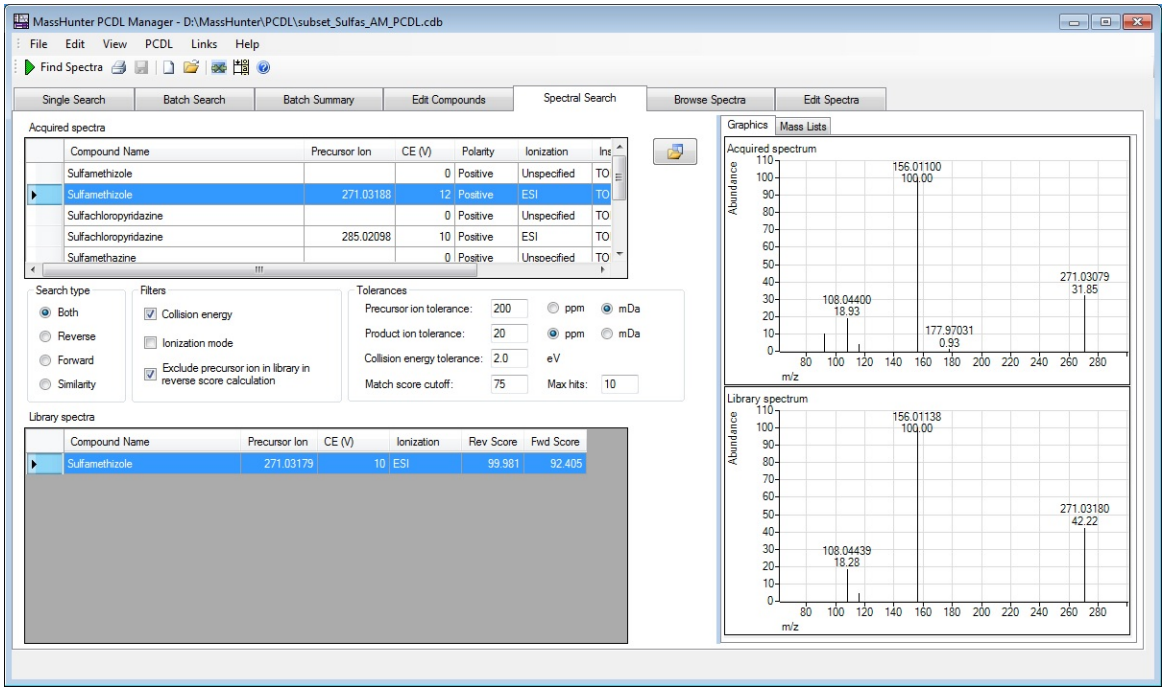


Figure 5 Spectral Search results

Exercise 5. Browse spectra in the PCDL

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

Steps	Detailed Instructions	Comments
1 Open the example PCDL.	**a** Select **Open PCDL** from the File menu, *or* click the  button on the toolbar. **b** Select the **Sulfas_AM_PCDL.cdb** file, and click the **Open** button.	Skip this step if the Sulfas PCDL is already open, as it will be after Exercise 4.
2 Display the Browse Spectra tab.	Click to display the **Browse Spectra** tab.	
3 View all compounds in the PCDL.	**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**, **Ion Species**, **Precursor Ion**, **CE(V)**, **Polarity**, **Ionization**, and **Instrument** in the Spectral Search Results table in the middle of the tab. See Figure 6 on page 63.	
5 View the mass spectrum plot for one of the spectra.	**a** Click 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,

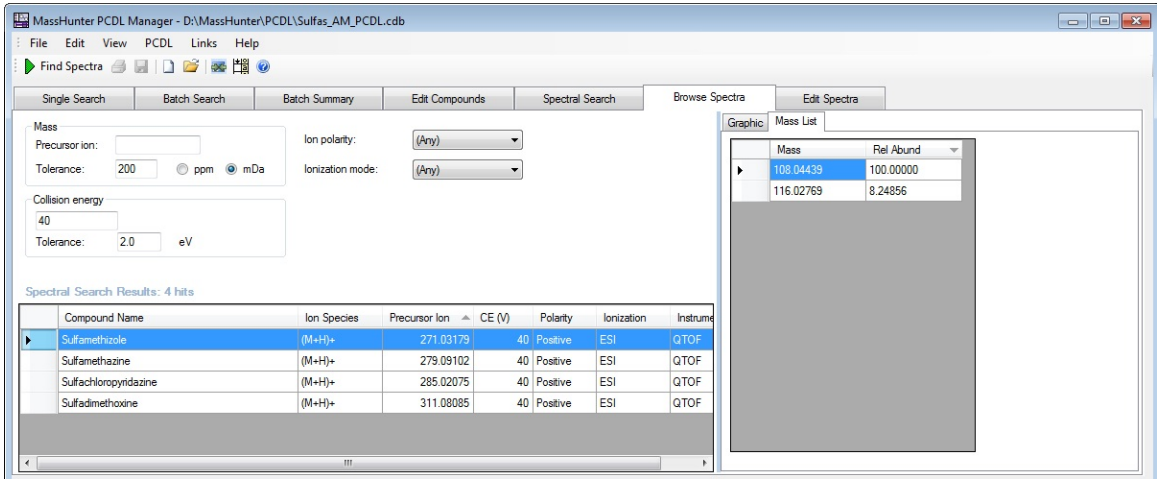


Figure 6 Browsing Spectra Results

Exercise 6. Create a custom PCDL

In this exercise, you will create a custom PCDL from the example Sulfas PCDL.

Steps	Detailed Instructions	Comments
1 Open the New PCDL dialog box.	• Click **New PCDL** from the File menu or click the  button on the toolbar.	Alternate method: You can also create custom PCDLs as described in the following topics: • "To create a subset PCDL from an input file" on page 18 • "To create a subset PCDL from selected compounds" on page 32
2 Create the new PCDL.	**a** Select **Sulfas_AM_PCDL** as the starting PCDL. **b** Select **General** as the PCDL type. **c** Type in a name for the new PCDL, such as **Sulfas_AM_Custom**. **d** Enter a description for the new PCDL. **e** Click the **Create** button to create the new PCDL.	• The new PCDL becomes the current working PCDL and is automatically enabled for editing. • The new custom PCDL will contain all compounds and spectra from the starting PCDL.
3 Edit the PCDL.	See "Exercise 7. Edit compounds".	

Exercise 7. Edit compounds

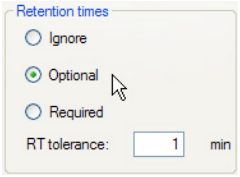
In this exercise, you will edit the custom PCDL that you created in Exercise 6.

Steps	Detailed Instructions	Comments
1 Open the custom PCDL you created in Exercise 6, if it is not already open.	**a** Select **Open PCDL** from the File menu, *or* click the  button on the toolbar. **b** Select the **Sulfas_AM_Custom.cdb** file, and click the **Open** button.	Skip this step if the custom PCDL is already open, as it will be if you just completed Exercise 6.
2 Enable editing for this PCDL.	**a** Open the **PCDL** menu. **b** Mark **Allow Editing** if it is not currently marked.	A new PCDL 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 PCDL.
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 PCDL.	Information for the selected compound is displayed in the Edit Compounds tab. The updated information will be changed in the PCDL 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 Structures area to open a **.MOL** file. **c** Click the **Update Selected** button. The information you entered will be changed in the PCDL.	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 PCDL.	**a** Click the **Add New** button. A new compound is created in the PCDL 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 PCDL 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 PCDL using the specified values. The new compound is displayed at the end of the results table.
8 Remove a compound from the PCDL.	**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 PCDL.
9 Add retention times to the PCDL as described in Exercise 8.		

Exercise 8. Add retention times to a PCDL

In this exercise, you will add retention times to the custom PCDL created in Exercise 6.

Steps	Detailed Instructions	Comments
1 Open the custom PCDL you created in Exercise 6 and edited in Exercise 7, if it is not already open.	**a** Select **Open PCDL** from the File menu, *or* click the  toolbar button. **b** Select the **Sulfas_AM_Custom.cdb** file, and click the **Open** button.	None of the compounds in this example PCDL have retention times.
2 Enable editing for this PCDL.	**a** Open the **PCDL** menu. **b** Mark **Allow Editing** if it is not currently marked.	A new PCDL 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 **sulfa_compounds.txt** in the **MassHunter\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 100 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. In this example, hits were found for four masses, which appear at the top of the mass list. See Figure 7.	To sort the list by a different criterion, click the heading for the column of interest.

Steps	Detailed Instructions	Comments
7 Resolve conflicting hits.	Masses with conflicting hits are shown in red text in the Mass List table.	This example has no conflicting hits so you can skip this step.
8 Click the **Batch Summary** tab.	See Figure 8.	
9 Update retention times in the PCDL 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 7.	Retention time information is updated in the PCDL for each of the compounds listed in the Batch Summary table. See Figure 9.

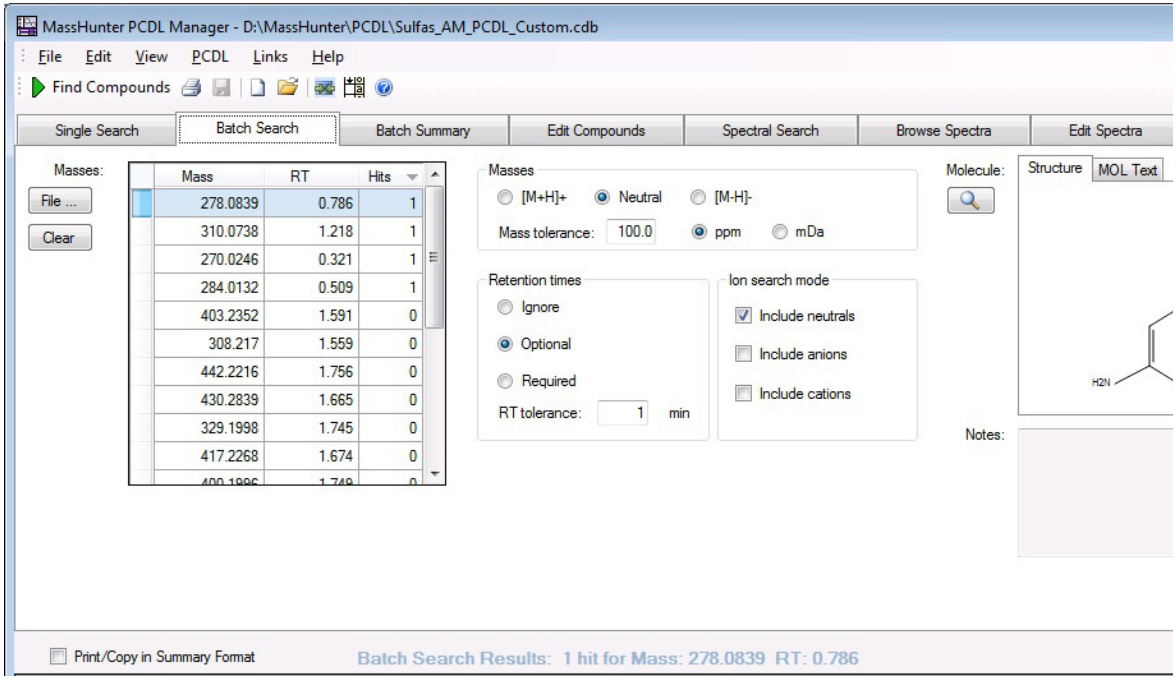


Figure 7 Batch Search Results with Retention Time Optional

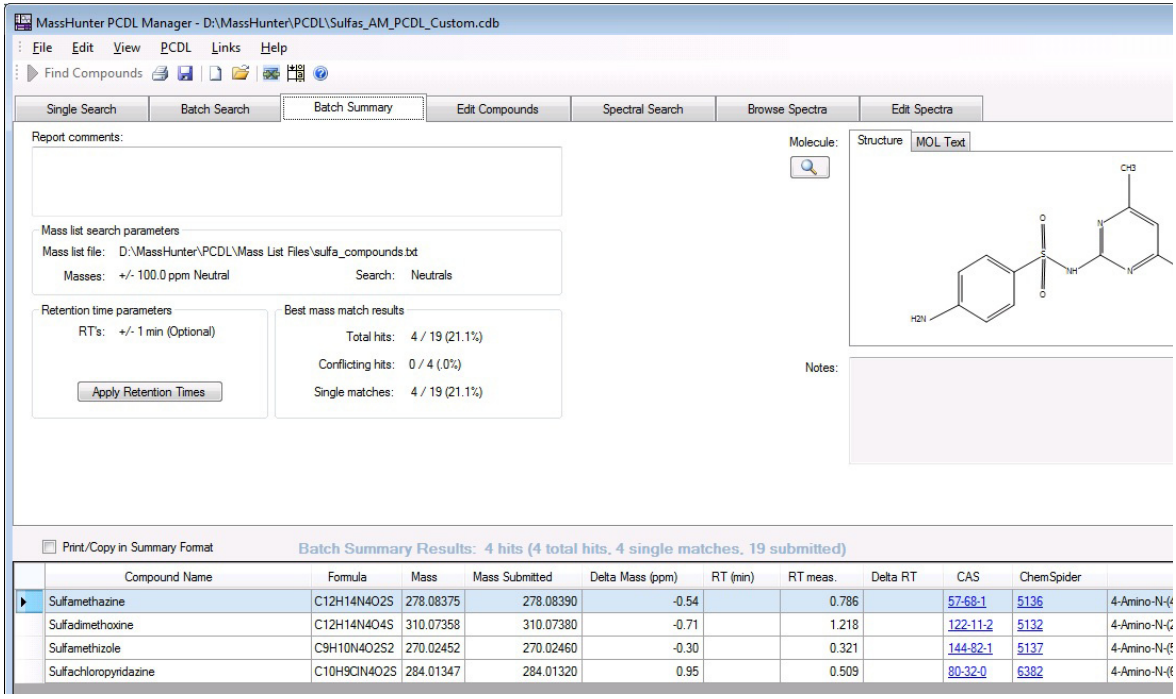


Figure 8 Batch Summary Results with Retention Time Optional (before updating)

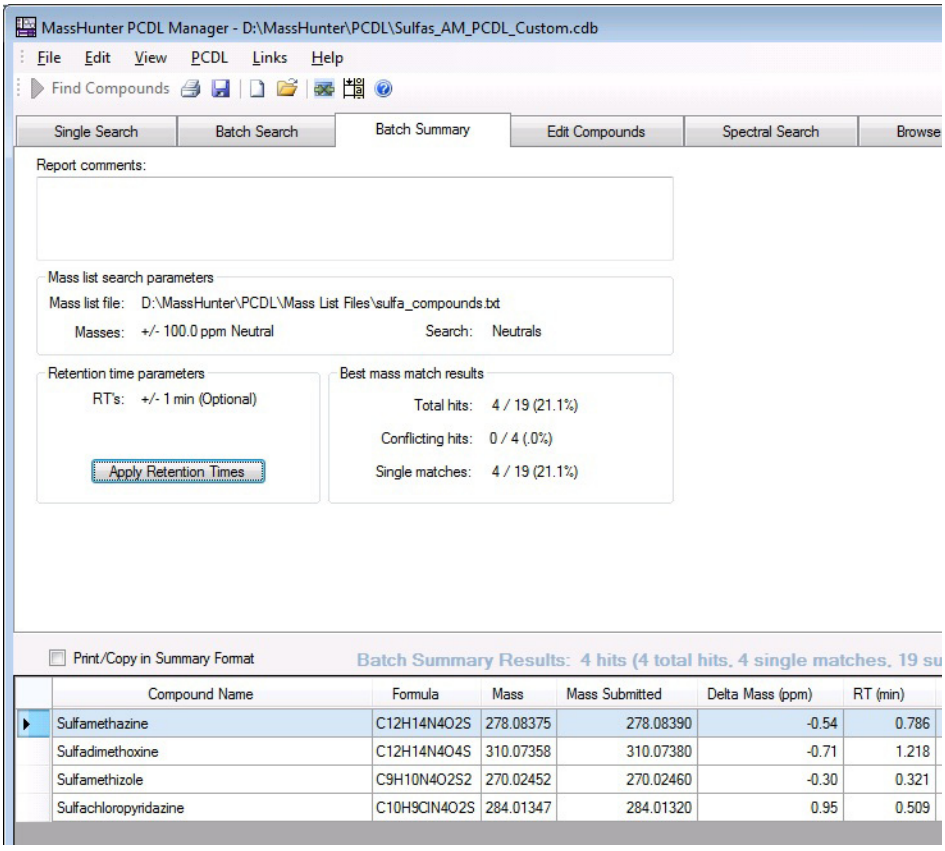


Figure 9 Batch Summary Results with Retention Times Updated

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In this Book

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

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

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