

# MassHunter Personal Compound Database and Library Manager

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### 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 will use the MassHunter Workstation Software-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 “[Searching a PCDL in Qualitative Analysis](#)” on page 16.

### 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.
- Search and store MS/MS centroid spectra acquired on a Q-TOF instrument.
- Create and edit custom PCDs and PCDLs, including adding proprietary compounds, retention times, and MS/MS spectra.
- Import mass lists with retention time in the form of a .txt or .csv file.
- 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 **setup.exe**.  
If the operating system is Windows 7, right-click **setup.exe** and select **Run as Administrator**.
- 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.
- **PCDL\Empty.cdb** - an empty master PCDL, which can be used to create a custom PCDL for importing compounds. To create a PCDL and import compounds, see [“To create a custom PCDL”](#) on page 13 and [“To import compounds to a custom PCDL”](#) on page 14.

### 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 11.

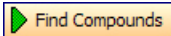
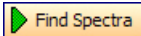





## Main Window

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

- “[Toolbar](#)”(below)
- “[Menus](#)” on page 5
- “[Compound Tabs](#)” on page 7
- “[Spectral Tabs](#)” on page 9

### 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.<br>Same as pressing the <b>F5</b> key.     |
|    | PCDL > Find Spectra   | Available only when the Spectral Search or Browse Spectra tabs are displayed.<br>Same as pressing the <b>F5</b> key. |
|    | File > Print Results  |  |
|   | File > Export Results | For use with Batch Summary Results only.   |
|  | File > New PCDL       |  |
|  | File > Open PCDL      |  |
|  | 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 13.

**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.

**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.

**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.

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

**PCDL Information** Lets you 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 19.

### 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 26.

### 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 29.

### 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 32.


### 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 21 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 32.

### 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.

### Spectral Plot Window

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

# Getting Started

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

- [“PCDL operations”](#) on page 11
- [“Searching a PCDL in Qualitative Analysis”](#) on page 16
- [“Searching a PCDL in MassHunter PCDL Manager”](#) on page 19
- [“Doing a batch search”](#) on page 26
- [“Editing a custom PCDL”](#) on page 31
- [“Spectral searching and editing”](#) on page 34

## PCDL operations


The following PCDL operations are described in the following pages:

- “[To open a PCDL](#)” on page 11
- “[To back up a PCDL](#)” on page 12
- “[To view PCDL information](#)” on page 12
- “[To view more information](#)” on page 12
- “[To create a custom PCDL](#)” on page 13
- “[To import compounds to a custom PCDL](#)” on page 14
- “[To create a subset PCDL from an input file](#)” on page 15

### 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:

- Select **Open PCDL** from the File menu, *or*
- Click  on the toolbar.

**2** Select the file of interest (.cdb extension) and click **Open**.

#### 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 13.

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## 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 15
- “[To create a subset PCDL from selected compounds](#)” on page 24

- 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\Sulfas\_AM\_PCDL.cdb** - a small example master PCDL
    - **PCDL\Empty.cdb** - an empty master PCDL
  - b Select the PCDL type for the new PCDL from the following choices: **General**, **Metabolomics**, **Pesticides**, **Forensics**, or **Glycans**.
  - c Type in 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 14
  - “[To append compounds to a PCDL](#)” on page 25

## 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 30.
  - 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 13.
- 3 Enable editing on this PCDL by marking **Allow Editing** on the PCDL menu.
- 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, 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. Edit this log file to fix the problems, 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 32 if you want to change information for the imported compounds.

## To create a subset PCDL from an input file

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

## Searching a PCDL in Qualitative Analysis

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

Use the following procedures to search a PCDL with MassHunter Workstation Software–Qualitative Analysis program. These steps apply to version B.04.00 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 If not already set, set the search criteria in the **Identify Compounds > Search Database** section of Method Editor as described in Step 4 above.
- 4 Initiate the search by right-clicking on the spectrum and selecting **Search Database for Spectrum Peaks** from the shortcut menu (or in other ways described in Qualitative Analysis online Help).

The 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 AMRT 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.
    - Select File Type **.cdb** to see a list of PCDLs.
    - Select the PCDL of interest.
- 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 Accurate Mass Library** section of Method Editor:
- 4 On the **Settings** tab, click the Browse [...] button to open the Open Library File dialog box. Select File Type **.cdb** to see a list of PCDLs, then click 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
- 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 step to identify compounds with a PCDL:


- 1 Open the data file of interest in Qualitative Analysis.
- 2 Find compounds using the Auto MS/MS, Targeted MS/MS or Molecular Feature with MS/MS extraction algorithm 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 Accurate Mass Library** section of Method Editor:
- 5 On the **Settings** tab, click the Browse [...] button to open the Open Library File dialog box. Select File Type **.cdb** to see a list of PCDLs, then click 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
- 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” (*below*)
- “To view compound search results” on page 21
- “To change how data is displayed in results tables” on page 21
- “To print compound results” on page 23
- “To create a subset PCDL from selected compounds” on page 24
- “To append compounds to a PCDL” on page 25

### 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 on the **Single Search** tab.
- 3 To return the contents of the entire PCDL, leave the search fields blank and skip to Step 6. Otherwise, set the desired mass search criteria:
  - a **Mass and Mass tolerance in ppm or mDa**
  - b **Type of mass ([M+H]<sup>+</sup>, Neutral, or [M-H]<sup>-</sup>)**
    - Select **[M+H]<sup>+</sup>** 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]<sup>+</sup>** or **[M-H]<sup>-</sup>** selection.
    - Select **[M-H]<sup>-</sup>** 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 Select the **Ion search mode**, keeping in mind the following guidelines:
    - **Include neutrals** is typically selected. Clear it if you want to search anions and cations only.

- Select **Include anions** or **Include cations** if you also want to consider those chemicals that don't pick up or lose a proton to ionize. Searching *both* modes may return false matches.
  - Choose **Include anions** if the data was acquired in *negative* ion mode.
  - Choose **Include cations** if the data was acquired in *positive* ion mode.
- 4 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,
    - Select **Find Compounds** from 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 21 and [“To change how data is displayed in results tables”](#) on page 21.

## To view compound search results

- 1 Do a search on the Single Search tab as described in [“To find compounds”](#) on page 19.
- 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 21.
- 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 on the **Edit Compounds** tab, as described in [“To edit compounds in a custom PCDL”](#) on page 32.
- 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 36.

### See Also

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

- [“To print compound results”](#) on page 23.
- [“To create a subset PCDL from selected compounds”](#) on page 24.
- [“To append compounds to a PCDL”](#) on page 25.


## To change how data is displayed in results tables


- 1 To sort the table by the entries in a column, click the heading for the column of interest.
- 2 To change the order of the columns of information in the table, drag a column heading to a different position. Repeat this until the desired order is achieved.
- 3 To resize a column to fit the information contained in it, double-click on the right column divider in the heading of the column of interest.
- 4 To resize a column to a specific width, drag the separator between the column headings to the right or left until the column is the desired width.

- 5 To change which columns of information are displayed in the table:
  - a Right-click in the table and select **Add/Remove Columns** from the shortcut menu to open the Add/Remove Columns dialog box.
  - b Move the items of information that you want to display from the **Available columns** list to the **Show these columns** list 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**.

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

## To print compound results

- 1 If you want to print only certain compounds, highlight those rows in the Compound Results table using **Ctrl+click** or **Shift+click**.
- 2 Open the Print Results dialog box in *any* of the following ways:
  - Select **Print Results** from the File menu.
  - Click  on the toolbar.
  - Right-click in the results table and select **Print Results** from the shortcut menu.
- 3 Select desired report options from the following:
  - **Printer** (destination)
  - **Print Preview** if you want to view the report on the screen first.
  - **Fit to page** to size the report to fit the width of the page.
  - **Orientation (Landscape or Portrait)**. The default is Landscape, as it allows more columns of information.
- 4 Select the desired report content options from the following:
  - **All rows** or **Only highlighted rows** of the results table
  - **Include search parameters**
  - **Include unmatched masses**
  - **Print structures** and the size (240 x 160, 360 x 240, or 540 x 360)
- 5 Click **OK** to generate the report.

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

### NOTE

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

---

## 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 19
  - “To find compounds from a mass list” on page 26
- 2 To select the compounds of interest, highlight those rows in the table.
- 3 To open the Create Subset PCDL dialog box, right-click in the table, 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 25.



## 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 19
  - “To find compounds from a mass list” on page 26
- 2 To select the compounds of interest, highlight those rows in the table.
- 3 To open the Append to PCDL dialog box, right-click in the table, 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” (below)
- “To view batch search results” on page 28
- “To view batch summary results” on page 29
- “To export batch summary results” on page 30

### 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 on the **Batch Search** tab.
- 3 Enter a mass list in *one* of the following ways:
  - Click the **File** button to the left of the mass list table to open a mass list file output by MassHunter Qualitative Analysis (.csv or .txt file), Mass Profiler (.xls file), or GeneSpring MS (.txt file).
  - Copy and paste a compound list from MassHunter Qualitative Analysis.
  - Type 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 Select **Ion search mode** options as follows:
  - **Include neutrals** is typically selected.
  - Select **Include anions** and/or **Include cations** if you also want to consider those few chemicals that don't pick up or lose a proton to ionize.
- 6 Select one of the following options for **Retention times**:

| Option | Meaning   | Application  |
|--------|---|--|
| Ignore | Don't consider retention time even if it is present in the list | When searching the sample master PCDL or any custom PCDL <i>without</i> retention time data. |

|                 |  |   |
|-----------------|--|---|
| <b>Optional</b> | 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 <i>some</i> compounds.                         |
| <b>Required</b> | 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.
  - Select **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 on a row in the Mass List table to display the compounds found for that mass in the Compound Results table in the lower part of the window. For more information on viewing batch search results, see [“To view batch search results”](#) on page 28.
- 10 Select and view the best compound hit for each mass as described in [“To view batch summary results”](#) on page 29.

## 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 26.
- 2 When the search is complete, the number of hits for each mass appears in the **Hits** column of the mass list, and the list is automatically sorted to show the masses with the most hits at the top of the list. To sort the list by a different criterion, click the heading for the column of interest (**Mass** or **RT**). Masses with conflicting hits are shown in red text in the Mass List table.
- 3 Click on a row in the Mass List table to display the compounds found for that mass in the Search Results table in the lower part of the window.

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

- 4 (Optional) Change how the batch search results are displayed as described in [“To change how data is displayed in results tables”](#) on page 21.
- 5 See [“To view batch summary results”](#) on page 29 for information on selecting and viewing the best compound hit for each mass.
- 6 Click on a compound in the Compound Results table to view its structure information in the Structures area on the right side of the window, if the structure is available in the PCDL.
- 7 Click on 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 32.
- 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 36.


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

- [“To print compound results”](#) on page 23.
- [“To create a subset PCDL from selected compounds”](#) on page 24.
- [“To append compounds to a PCDL”](#) on page 25.

## 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 26.
- 2 Click on a row in the Mass List table to display the compounds found for that mass in the Batch Search Results table in the lower part of the window. Masses with conflicting hits are shown in red text in the Mass List table.
- 3 Review the entries marked in the **Best** column for each mass and if necessary, edit the Batch Search Results table to select the best compound hit by marking the desired row (compound). You can also *clear* the box for the selected hit to ignore all the results for that compound.
- 4 Click the **Batch Summary** tab to view only the best hits from the Batch Search Results table. Compounds with conflicting mass hits are shown in red text in the results table.
- 5 (*Optional*) Change how the batch summary results are displayed as described in [“To change how data is displayed in results tables”](#) on page 21.
- 6 Click on a compound in the results table to view its structure information in the Structures area on the right side of the window, if the structure is available in the PCDL.
- 7 Click on 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 32.
- 8 To export batch summary results, see [“To export batch summary results”](#) on page 30.
- 9 To print batch summary results, see [“To print compound results”](#) on page 23.
- 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 31.

## To export batch summary results

- 1 Do a batch search as described in “[To find compounds from a mass list](#)” on page 26.
- 2 Select and view the best compound hit for each mass as described in “[To view batch summary results](#)” on page 29, 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 21.
- 4 Open the Export Results dialog box in *any* of the following ways:
  - Select **Export Results** from the File menu.
  - Click  on the toolbar.
  - Right-click in the results table and select **Export Results** from the shortcut menu in the Batch Summary results table.
- 5 Click **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 is used:
  - If the mass list was opened from a file, the export file name is:  
**<massListFileName>-<TimeStampInSecs>.txt**
  - If you entered the mass list manually, the export file name is:  
**MassList-<TimeStampInSecs>.txt**
  - The default location for the export file is **MassHunter\PCDL\Results**.
  - The default output file format is **.TXT** (tab-separated values), but you can select **.CSV** (comma-separated values) instead.
- 6 Select one or more of the following types of information to include in the report: **Search parameters**, **Results**, and **Unmatched masses** (available only if the **Results** checkbox is marked).
- 7 Mark the **Open results file after exporting** option to open the batch summary results file automatically in the associated application.
- 8 Click **OK** to output the results.
- 9 The results will open in the associated application such as Excel if you selected the **Open results file** option in Step 7. Otherwise open the exported results file in your application of choice at a later time.

### NOTE

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

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

## Editing a custom PCDL

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

- [“To update retention time data”](#) on page 31
- [“To edit compounds in a custom PCDL”](#) on page 32

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

### NOTE

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

- 
- 4 Select *one* of the following options for **Retention times**:
    - **Ignore** - Use this option to search a 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 26.
  - 6 Initiate the search in *any* of the following ways:
    - Click **Find Compounds** on the toolbar.
    - Select **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 on a row in the Mass List table to display the compounds found for that mass in the Search Results table in the lower part of the window. For more information on viewing batch search results, see [“To view batch search results”](#) on page 28.
- 9 Select and view the best compound hit for each mass as described in [“To view batch summary results”](#) on page 29 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 19.
  - [“To find compounds from a mass list”](#) on page 26.
- 4 When the search is complete, click the **Edit Compounds** tab.
- 5 To update information for a particular compound:
  - a Select the compound of interest by clicking on it in the Search Results table. Information for the selected compound is displayed in the **Edit Compounds** tab.
  - b Update information on the left side of the Edit Compounds tab, such as Name, Mass, RT, Formula, CAS or ChemSpider ID, and Ion type.
  - c Update structure information if desired in either of the following ways:
    - Click on the MOL Text tab and paste in MOL file text that you have copied from a molecular drawing tool (**Ctrl+V**), or



- Click  in the Structures area to open a **.MOL** file.
  - 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.

**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 on it in the Search Results table. Use **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” - below](#)
- [“To copy spectra from MassHunter Qualitative Analysis” - below](#)
- [“To paste spectra into MassHunter PCDL Manager” on page 35](#)
- [“To search spectra in a PCDL” on page 35](#)
- [“To browse spectra in the PCDL” on page 36](#)
- [“To view spectra for a compound” on page 36](#)
- [“To add, move, or remove spectra in a custom PCDL” on page 37](#)
- [“To clean up noisy spectra” on page 38](#)

## 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 35](#)
- [“To add, move, or remove spectra in a custom PCDL” on page 37](#)
- [“To clean up noisy spectra” on page 38](#)

## To copy spectra from MassHunter Qualitative Analysis

- 1 Open the data file of interest in MassHunter Qualitative Analysis software.
- 2 Run **Find by Targeted MS/MS** or **Find by Auto MS/MS**, depending on how the data was acquired.
- 3 Expand the compounds of interest in Data Navigator to see the spectral results.
- 4 Select the product ion spectra of interest.

- 5 If the data was acquired in Profile mode, right-click and select **Convert Profile to Centroid and Replace** from the shortcut menu.
- 6 Right-click the MS Spectrum Results window and select **Copy to Clipboard**.  
All spectra displayed in the MS Spectrum Results window are copied, not just the highlighted ones.

## To paste spectra into MassHunter PCDL Manager


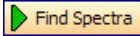
- 1 Copy spectra from MassHunter Qualitative Analysis as described in [“To copy spectra from MassHunter Qualitative Analysis”](#) on page 34.
- 2 Click to display the **Spectral Search** or **Edit Spectra** tab.
- 3 Right-click in the **Acquired spectra** table and select **Paste Spectra**.  
If profile spectra or non-MS/MS spectra were copied from MassHunter Qualitative Analysis, a message is displayed saying that they have been skipped. Only centroided MS/MS spectra are pasted into MassHunter PCDL Manager. The spectra are listed in the Acquired spectra table.

### NOTE

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

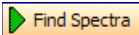
---

## 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 on a row of the results table to view the mass spectrum plot for the selected compound in the Spectral Plot window to the right of the table.
- 7 Click the **Mass Lists** tab in the Spectral Plot window to view a list of masses and 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 21.
- 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 19.
  - [“To find compounds from a mass list”](#) on page 26.
- 2 When the compound search is complete, click the **Browse Spectra** tab.

The compound search results are displayed in the Compound Results table in the lower part of the tab.
- 3 Click on a compound of interest in the Compound Results table. The 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 on a row of the Spectral Results table to view the mass spectrum plot for the selected spectrum in the Spectral Plot window to the right of the table.
- 5 Click the **Mass Lists** tab in the Spectral Plot window to view a list of masses and relative abundance values for the selected spectrum.
- 6 Repeat Steps 3 - 5 for other compounds of interest.

## To add, move, or remove spectra in a custom 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.

- 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 19.
  - [“To find compounds from a mass list”](#) on page 26.
- 3 When the compound search is complete, click the **Edit Spectra** tab.  
The compound search results are displayed in the Compound Results table in the lower part of the tab.
- 4 Click on a compound you want to view or modify in the Compound Results table. The spectra associated with the selected compound are displayed in the Library spectra table in the middle of the tab.
- 5 Load spectra into the Acquired spectra table at the top of the tab in either of the following ways:
  - From a **.CEF** file as described in [“To import spectra from a .CEF file”](#) on page 34, *or*
  - From Qualitative Analysis, as described in [“To copy spectra from MassHunter Qualitative Analysis”](#) and [“To paste spectra into MassHunter PCDL Manager”](#) on page 35.
- 6 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.
- 7 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.

- 8 To move spectra between compounds:
  - a Click to select the compound to copy spectra from in the **Compound Results** table in the lower part of the tab.

The spectra for that compound are displayed in the Library spectra table in the middle of the tab.
  - b Click to select the spectra of interest in the **Library spectra** table, then right-click in the table and select **Copy Spectra** from the shortcut menu. Use **Ctrl-click** or **Shift-click** before copying if you want to select multiple spectra.
  - c Right-click in the **Acquired spectra** table in the upper part of the tab and select **Paste Spectra** from the shortcut menu.

The spectra are added to the Acquired spectra table.
  - d Click to select the compound to copy the spectra to in the Compound Results table in the lower part of the tab.
  - e Click **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.

- 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:


- “Exercise 1. Search for compounds” on page 39
- “Exercise 2. View spectra for compounds” on page 42
- “Exercise 3. Batch search from a mass list” on page 44
- “Exercise 4. Search a spectral library” on page 47
- “Exercise 5. Browse spectra in the PCDL” on page 49


Custom PCDL operations:

- “Exercise 6. Create a custom PCDL” on page 51
- “Exercise 7. Edit compounds” on page 52
- “Exercise 8. Add retention times to a PCDL” on page 54



### 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.   | <p><b>a</b> Select <b>Open PCDL</b> from the File menu, <i>or</i> click the  button on the toolbar.</p> <p><b>b</b> Select the <b>Sulfas_AM_PCDL.cdb</b> file, and click the <b>Open</b> button.</p> | Skip this step if the Sulfas PCDL is already open.  |
| 2 Click on the <b>Single Search</b> tab.                               |  |   |
| 3 Leave the search fields blank.                                       | Be sure that the <b>Require</b> checkbox for Retention time is <i>cleared</i> , since the example Sulfas PCDL does <i>not</i> contain retention time information.  | This will return all compounds in the PCDL. See “ <a href="#">To find compounds</a> ” on page 19 for a discussion of search parameters to narrow your search. |
| 4 Begin searching.   | Click the <b>Find Compounds</b> button on the toolbar.   | Alternate methods: <ul style="list-style-type: none"> <li>• Select <b>Find Compounds</b> from the PCDL menu.</li> <li>• Press the <b>F5</b> key.</li> </ul>   |
| 5 Review the search results in the table in the lower half of the tab. | See <a href="#">Figure 1</a> on page 41.   | The results are sorted from low mass to high mass.  |

| Steps  | Detailed Instructions   | Comments  |
|--|---|---|
| 6 View structure information for a selected compound.              | Click on a compound in the Compound Results table. Its structure is displayed in the Structures area on the right side of the window.   | <ul style="list-style-type: none"> <li>Clicking the  button displays a larger image of the structure.</li> <li>Clicking the <b>MOL Text</b> tab displays the text version of the structure.</li> </ul>   |
| 7 Sort the table by name.  | Click the heading of the <b>Compound Name</b> 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.                                | <ol style="list-style-type: none"> <li>Drag a column heading to a different position.</li> <li>Repeat until the desired order is achieved.</li> </ol>   |   |
| 9 Resize a column.   | <ul style="list-style-type: none"> <li>Double-click on the right column divider in the heading of the column of interest to resize the column to fit the information contained in it.</li> </ul>  | <p>Alternate Method:</p> <ul style="list-style-type: none"> <li>Drag the separator between column headings to the right or left until the column of interest is the desired width.</li> </ul>   |
| 10 Change which columns of information are displayed in the table. | <ol style="list-style-type: none"> <li>Right-click in the table and select <b>Add/Remove Columns</b> from the shortcut menu.</li> <li>Move the items of information that you want to display from the <b>Available columns</b> list into the <b>Show these columns</b> list using the <b>Add-&gt;</b> button.</li> <li>Move the items of information that <i>you don't want to display</i> out of the <b>Show these columns</b> list into the <b>Available columns</b> list using the <b>&lt;-Remove</b> button.</li> <li>Click <b>OK</b>.</li> </ol> | <p>Alternate Methods:</p> <ul style="list-style-type: none"> <li>You can also open the Add/Remove Columns dialog box by selecting <b>Add/Remove Compound Columns</b> from the View menu.</li> <li>You can move individual items between the two lists by double-clicking them.</li> </ul> <p>Note that the original column layout can be restored at anytime by selecting <b>Restore Default Compound Columns</b> from the View menu.</p> |
| 11 Create a subset PCDL from selected compounds.                   | <ol style="list-style-type: none"> <li>To select the compounds of interest, highlight those rows in the table.</li> <li>Right-click in the table, then click <b>Create Subset PCDL</b>.</li> <li>Enter the information on the Create Subset PCDL dialog box.</li> <li>Click <b>Create</b>.</li> </ol>   | <ul style="list-style-type: none"> <li>For more information, see <a href="#">“To create a subset PCDL from selected compounds”</a> on page 24.</li> <li>You can also append selected results to an existing PCDL as described in <a href="#">“To append compounds to a PCDL”</a> on page 25.</li> </ul>   |



| Steps             | Detailed Instructions   | Comments   |
|-------------------|---|--|
| 12 Print results. | <p><b>a</b> Click the  button on the toolbar to open the Print Results dialog box.</p> <p><b>b</b> Select print options. For a discussion of print options, see “<a href="#">To print compound results</a>” on page 23.</p> <p><b>c</b> Click <b>OK</b>. If you selected the Print Preview option, review the report in the Print Preview window, then click the  button to print it.</p> | To print only selected results, highlight those rows in the Compound Results table using <b>Ctrl+click</b> or <b>Shift+click</b> , then select <b>Only highlighted rows</b> as one of the print options in Step c. |

Find Compounds       


Single Search    Batch Search    Batch Summary    Edit Compounds    Spectral Search    Browse Spectra    Edit Spectra

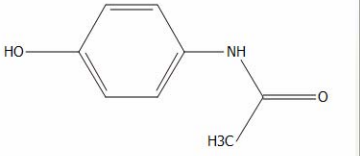
Mass:  [M+H]<sup>+</sup> ☒ Neutral ☐ [M-H]<sup>-</sup>  
 Mass tolerance:  10.0 ppm ☐ mDa

Retention time:  ☐ Require  
 RT tolerance:  0.1 min

Ion search mode:  
☒ Include neutrals  
☐ Include anions  
☐ Include cations

Formula:   
 Name:   
 Notes:   
 IUPAC:   
 CAS:   
 ChemSpider:

Molecule:  Structure MOL Text



Notes: 4-Acetamidophenol

Single Search Results: 10 hits

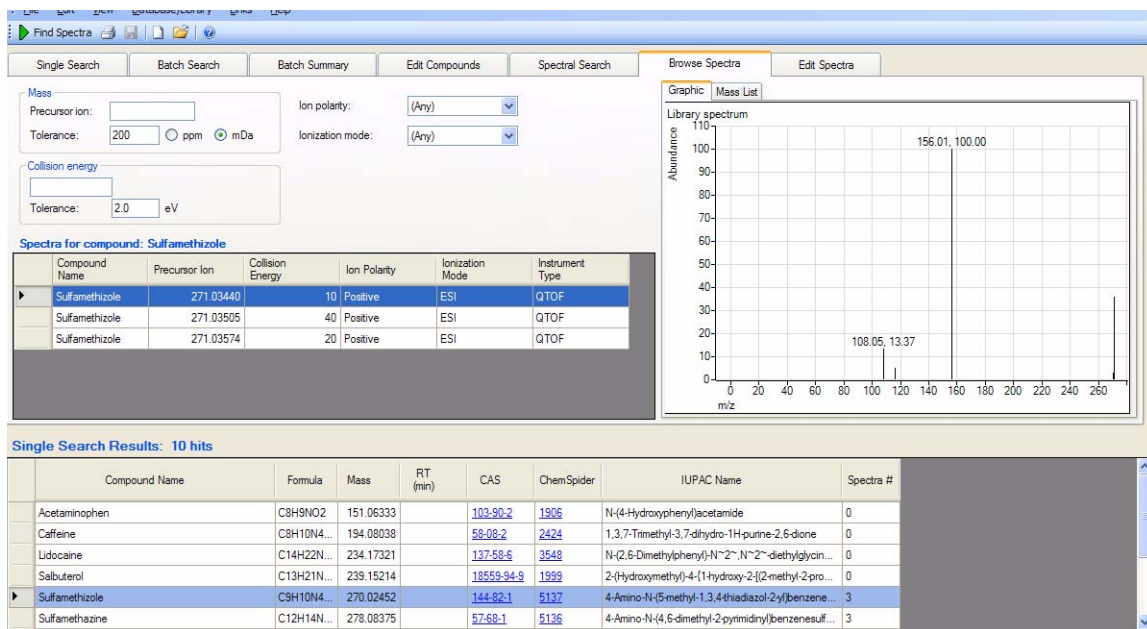
|   | Compound Name         | Formula  | Mass      | RT (min) | CAS                        | ChemSpider           | IUPAC Name  | Spectra # |
|---|-----------------------|----------|-----------|----------|----------------------------|----------------------|---|-----------|
| ▶ | Acetaminophen         | C8H9NO2  | 151.06333 |          | <a href="#">103-90-2</a>   | <a href="#">1906</a> | N-(4-Hydroxyphenyl)acetamide                          | 0         |
|   | Caffeine              | C8H10N4  | 194.08038 |          | <a href="#">58-08-2</a>    | <a href="#">2424</a> | 1,3,7-Trimethyl-3,7-dihydro-1H-purine-2,6-dione       | 0         |
|   | Lidocaine             | C14H22N2 | 234.17321 |          | <a href="#">137-58-6</a>   | <a href="#">3548</a> | N-(2,6-Dimethylphenyl)-N'-2'-N"-2"-diethylglycin...   | 0         |
|   | Salbutamol            | C13H21N  | 239.15214 |          | <a href="#">18559-94-9</a> | <a href="#">1999</a> | 2-(Hydroxymethyl)-4-[(1-Hydroxy-2-[(2-methyl-2-pro... | 0         |
|   | Sulfamethizole        | C9H10N4  | 270.02452 |          | <a href="#">144-82-1</a>   | <a href="#">5137</a> | 4-Amino-N-(5-methyl-1,3,4-thiadiazol-2-yl)benzene...  | 3         |
|   | Sulfamethazine        | C12H14N4 | 278.08375 |          | <a href="#">57-68-1</a>    | <a href="#">5136</a> | 4-Amino-N-(4,6-dimethyl-2-pyrimidinyl)benzenesulf...  | 3         |
|   | Sulfachloropyridazine | C10H9Cl  | 284.01347 |          | <a href="#">80-32-0</a>    | <a href="#">6382</a> | 4-Amino-N-(6-chloro-3-pyridazinyl)benzenesulfona...   | 3         |
|   | Sulfadimethoxine      | C12H14N4 | 310.07358 |          | <a href="#">122-11-2</a>   | <a href="#">5132</a> | 4-Amino-N-(2,6-dimethoxy-4-pyrimidinyl)benzenes...    | 3         |
|   | Progesterone          | C21H30O2 | 314.22458 |          | <a href="#">57-83-0</a>    | <a href="#">5773</a> | Pregn-4-ene-3,20-dione                                | 0         |
|   | Reserpine             | C33H40N  | 608.27338 |          | <a href="#">50-55-5</a>    | <a href="#">5566</a> | Methyl (3beta,16beta,17alpha,18beta,20alpha)-1...     | 0         |

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 <b>Browse Spectra</b> tab.  | This procedure can also be performed from the <b>Edit Spectra</b> tab.  |
| 2 Select Sulfamethizole from the Single Search Results table. | Click on the <b>Sulfamethizole</b> 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 <b>Compound Name, Precursor Ion, Collision Energy, Ion Polarity, Ionization Mode, and Instrument type</b> 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 <b>Graphic</b> tab in the spectral plot window.<br>See <a href="#">Figure 2</a> on page 43.  | The spectral plot window is on the right side of the tab.   |
| 5 View the mass list for Sulfamethizole.                      | Click the <b>Mass List</b> tab in the spectral plot window.  |   |
| 6 View information for another Sulfamethizole spectrum.       | <b>a</b> Click on a different row of the spectral information table.<br><b>b</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 <b>Sulfamethazine</b> 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 Spectral Information for Single Search results

### 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.  | <ol style="list-style-type: none"> <li>Select <b>Open PCDL</b> from the File menu, or click the  button on the toolbar.</li> <li>Select the <b>Sulfas_AM_PCDL.cdb</b> file, and click the <b>Open</b> button.</li> </ol>  | Skip this step if the Sulfas PCDL is already open, as it is after Exercise 2.   |
| 2 Click on the <b>Batch Search</b> tab.   |  |   |
| 3 Open a mass list.   | <ol style="list-style-type: none"> <li>Click the <b>File</b> button to the left of the mass list table.</li> <li>Select the <b>sulfa_compounds.txt</b> mass list file in the <b>MassHunter\PCDL\Mass List Files</b> folder.</li> <li>Click the <b>Open</b> button.</li> </ol>  | <ul style="list-style-type: none"> <li>Mass lists can also be copy-and-pasted into PCDL Manager from MassHunter Qualitative Analysis.</li> <li>See online help in MassHunter Qualitative Analysis for instructions on how to output a mass list.</li> </ul> |
| 4 Set the batch search parameters.  | <ol style="list-style-type: none"> <li>In this case the following default search parameters can be used for the search:               <ul style="list-style-type: none"> <li><b>Neutral Masses</b> option marked.</li> <li><b>Mass tolerance</b> 10 ppm.</li> <li><b>Optional for Retention times</b> marked.</li> <li>Only the <b>Include neutrals</b> option marked for <b>Ion search mode</b>.</li> </ul> </li> </ol> | The example PCDL does <i>not</i> include retention times.   |
| 5 Begin searching.  | Click the <b>Find Compounds</b> button on the toolbar.   | Alternate methods: <ul style="list-style-type: none"> <li>Select <b>Find Compounds</b> from the PCDL menu.</li> <li>Press the <b>F5</b> key.</li> </ul>   |
| 6 Review search results.  | <ul style="list-style-type: none"> <li>When the search is complete, the number of hits for each mass appears in the <b>Hits</b> column of the mass list.</li> <li>The list is automatically sorted to show the masses with the most hits at the top of the list. See <a href="#">Figure 3</a> on page 46.</li> </ul>   | <ul style="list-style-type: none"> <li>To sort the mass list by a different criterion, click the heading for the column of interest.</li> <li>Masses with conflicting hits are shown in red text in the Mass List table.</li> </ul>                         |
| 7 (Optional) Create a subset PCDL from selected compounds or append selected compounds to an existing PCDL. | <ul style="list-style-type: none"> <li>See <a href="#">“To create a subset PCDL from selected compounds”</a> on page 24.</li> </ul>  | <ul style="list-style-type: none"> <li>See <a href="#">“To append compounds to a PCDL”</a> on page 25.</li> </ul>   |

| Steps   | Detailed Instructions   | Comments  |
|---|---|---|
| 8 View hits for selected masses.              | Click on a row in the Mass List table to display the compounds found for that mass in the Batch Search Results table in the lower part of the window.   | For ease of reviewing results, use the <b>F4</b> key to scroll down the Mass List and the <b>Shift+F4</b> keys to scroll back up. The information in the results table will be updated as you scroll through the mass list.<br>The batch search results table can be resorted as described in <a href="#">“To change how data is displayed in results tables”</a> on page 21.   |
| 9 Select the best compound hit for each mass. | Mark the <b>Best</b> 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 <b>Batch Summary tab</b> . The Best hit for each mass is shown in the Batch Summary table in the lower part of the window. See <a href="#">Figure 4</a> on page 46.   | Compounds with conflicting mass hits are shown in red text in the results table.<br>The batch summary results table can be resorted as described in <a href="#">“To change how data is displayed in results tables”</a> on page 21.   |
| 11 Export batch summary results.              | <ol style="list-style-type: none"> <li>Click the  button on the toolbar to open the Export Results dialog box.</li> <li>Select the following options: <b>Search parameters</b>, <b>Results</b>, and <b>Unmatched masses</b>.</li> <li>Mark the <b>Open results file after exporting</b> option.</li> <li>Click <b>OK</b> to output the results.<br/>The results will open in the associated application such as Excel.<br/>The following export file is created in the <b>MassHunter\PCDL\Results</b> folder:<br/><b>sulfa_compounds-&lt;timestamp&gt;.txt</b></li> </ol> | <p>You can also open the Export Results dialog box in either of the following ways:</p> <ul style="list-style-type: none"> <li>Select <b>Export Results</b> from the File menu.</li> <li>Right-click in the Batch Summary results table and select <b>Export Results</b> from the shortcut menu.</li> </ul> <p>You can select a different file name, location or type as described in <a href="#">“To export batch summary results”</a> on page 30.</p> |

## Familiarization Exercises

Find Compounds

Single Search Batch Search Batch Summary Edit Compounds Spectral Search

Masses:

File ...

Clear

| Mass     | RT    | Hits |
|----------|-------|------|
| 278.0839 | 0.786 | 1    |
| 310.0738 | 1.218 | 1    |
| 270.0246 | 0.321 | 1    |
| 284.0132 | 0.509 | 1    |
| 403.2352 | 1.591 | 0    |
| 308.217  | 1.559 | 0    |
| 442.2216 | 1.756 | 0    |
| 430.2839 | 1.665 | 0    |
| 329.1998 | 1.745 | 0    |
| 417.2268 | 1.674 | 0    |
| 400.1886 | 1.749 | 0    |

Masses

☐ [M+H]<sup>+</sup> ☒ Neutral ☐ [M-H]<sup>-</sup>

Mass tolerance: 10.0 ☒ ppm ☐ mDa

Retention times

☐ Ignore ☒ Optional ☐ Required

RT tolerance: 0.1 min

Ion search mode

☒ Include neutrals ☐ Include anions ☐ Include cations

**Figure 3** Results of Batch Search - Mass List

Find Compounds

Single Search Batch Search Batch Summary Edit Compounds Spectral Search Browse Spectra Edit Spectra

Report comments:

Mass list search parameters

Mass list file: C:\MassHunter\Data\PCDL\Mass List Files\aulfa\_compounds.bt

Masses: +/- 10.0 ppm Neutral Search: Neutrals

Retention time parameters

RTs: +/- 0.1 min (Optional)

Apply Retention Times

Best mass match results

Total hits: 4 / 19 (21.1%)

Conflicting hits: 0 / 4 (0%)

Single matches: 4 / 19 (21.1%)

Molecule:

Structure MOL Text

Oc1cc(C(=O)Nc2ccc(O)cc2)nc(C)c1

Notes:



Batch Summary Results: 4 hits (4 total hits, 4 single matches, 19 submitted)

| Compound Name         | Formula    | Mass      | Mass Submitted | Delta Mass (ppm) | RT (min) | RT Submitted | Delta RT | CAS      | ChemSpider | IUPAC Name   | Spectra # |
|-----------------------|------------|-----------|----------------|------------------|----------|--------------|----------|----------|------------|--|-----------|
| Sulfamethazine        | C12H14N... | 278.08375 | 278.08390      | -0.54            | 0.786    | 0.786        |          | 57-68-1  | 5136       | 4-Amino-N-(4,6-dimethyl-2-pyrimidinyl)benzenesulf... | 3         |
| Sulfadimethoxine      | C12H14N... | 310.07358 | 310.07380      | -0.71            | 1.218    | 1.218        |          | 122-11-2 | 5132       | 4-Amino-N-(2,6-dimethoxy-4-pyrimidinyl)benzenes...   | 3         |
| Sulfamethizole        | C9H10N4... | 270.02452 | 270.02460      | -0.30            | 0.321    | 0.321        |          | 144-82-1 | 5137       | 4-Amino-N-(5-methyl-1,3,4-thiadiazol-2-yl)benzene... | 3         |
| Sulfachloropyridazine | C10H9Cl... | 284.01347 | 284.01320      | 0.95             | 0.509    | 0.509        |          | 80-32-0  | 6382       | 4-Amino-N-(6-chloro-3-pyridazinyl)benzenesulfona...  | 3         |

**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.         | <ol style="list-style-type: none"> <li>Select <b>Open PCDL</b> from the File menu, <i>or</i> click the  button on the toolbar.</li> <li>Select the <b>Sulfas_AM_PCDL.cdb</b> file, and click the <b>Open</b> button.</li> </ol>   | Skip this step if the Sulfas PCDL is already open, as it will be after Exercise 3.  |
| 2 Import spectra.                | <ol style="list-style-type: none"> <li>Click the  button on the <b>Spectral Search</b> tab.</li> <li>Select the <b>Sulfas.CEF</b> file in the <b>Example Data</b> folder on the PCDL installation disk.</li> <li>Click the <b>Open</b> button.</li> <li>When the message "Any profile or non-MS/MS spectra were skipped" appears, click <b>OK</b>.</li> </ol> | <ul style="list-style-type: none"> <li>See online help in MassHunter Qualitative Analysis for instructions on how to output spectra to a <b>.CEF</b> file.</li> <li>This message appears when the import file contains Profile spectra or non-MS/MS spectra, as is the case in the example <b>.CEF</b> file. Only centroided MS/MS spectra are imported for use in PCDL Manager.</li> </ul> |
|                                  | The imported spectra appear in the Acquired spectra table in the upper part of the tab.  | Often the <b>Compound Name</b> 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 <b>Sulfamethazine</b> row in the Acquired spectra table that has <b>Collision Energy</b> value of <b>0</b> .  |   |
| 4 Set search parameters.         | <i>Clear</i> the check mark for the <b>Collision energy Filter</b> .   | Use default values for the other search parameters.   |
| 5 Start searching.               | Click the <b>Find Spectra</b> button on the toolbar.   | You can also start the search in <i>either</i> of the following ways: <ul style="list-style-type: none"> <li>Select <b>Find Spectra</b> from the PCDL menu.</li> <li>Press the <b>F5</b> key.</li> </ul>  |

| Steps                                 | Detailed Instructions  | Comments  |
|---------------------------------------|--|---|
| 6 View search results.                | The search results are displayed in the Library spectra table in the lower part of the tab.<br>In this case, two library spectra are returned by the search.<br>See <a href="#">Figure 5</a> on page 48. | If desired, the spectral results display can be changed as described in <a href="#">“To change how data is displayed in results tables”</a> on page 21. |
| 7 Select a different results spectra. | Click on a different row of the Library spectra table.   | Notice that the lower spectrum in the <b>Graphics</b> tab of the Spectral Plot Window to the right of the table is updated.                             |
| 8 View the mass list.                 | Click the <b>Mass Lists</b> tab in the Spectral Plot window.   |   |

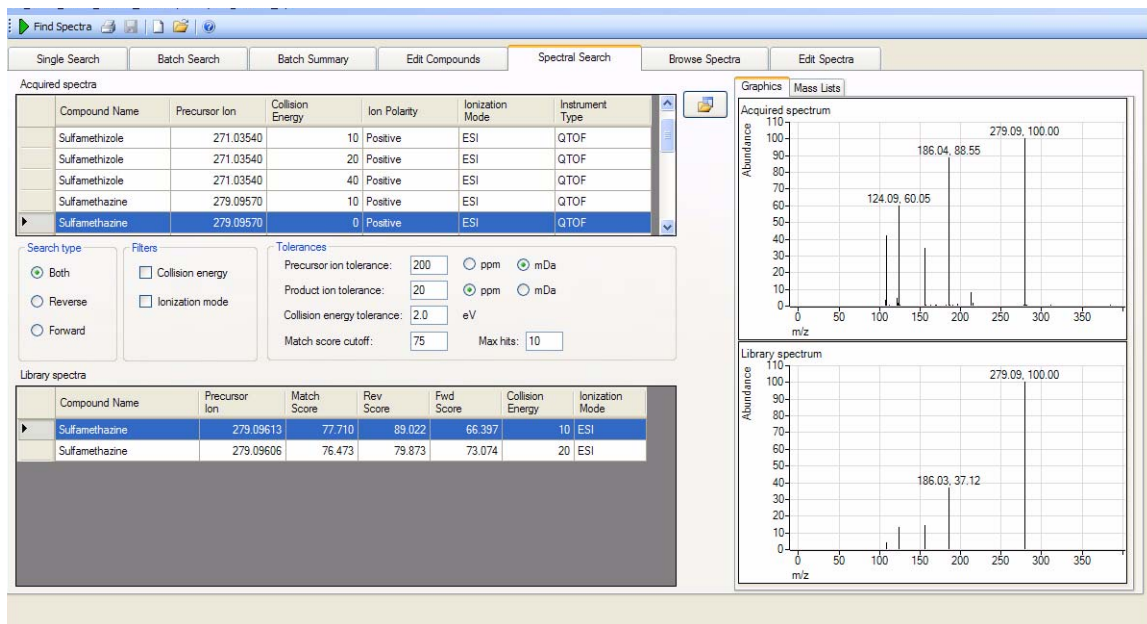



Figure 5 Spectral Search Results



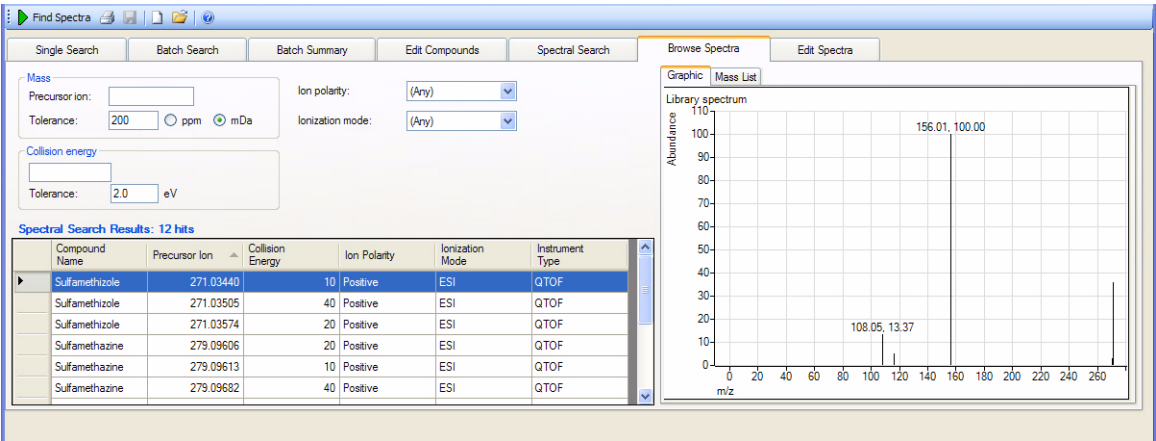
## Exercise 5. Browse spectra in the PCDL

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.                              | <ol style="list-style-type: none"> <li>Select <b>Open PCDL</b> from the File menu, or click the  button on the toolbar.</li> <li>Select the <b>Sulfas_AM_PCDL.cdb</b> file, and click the <b>Open</b> button.</li> </ol>  | 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 <b>Browse Spectra</b> tab.  |  |
| 3 View all compounds in the PCDL.                     | <ol style="list-style-type: none"> <li>Use the default search parameters:               <ul style="list-style-type: none"> <li><b>Precursor Ion Mass</b> and <b>Collision energy</b> blank</li> <li><b>Ion polarity</b> (Any)</li> <li><b>Ionization mode</b> (Any)</li> </ul> </li> <li>Click the <b>Find Spectra</b> button on the toolbar to start the search.</li> </ol> |  |
| 4 View spectral information.                          | View <b>Compound Name</b> , <b>Precursor Ion</b> , <b>Collision Energy</b> , <b>Ion Polarity</b> , <b>Ionization Mode</b> , and <b>Instrument type</b> in the Spectral Search Results table in the middle of the tab. See <a href="#">Figure 6</a> on page 50.   |  |
| 5 View the mass spectrum plot for one of the spectra. | <ol style="list-style-type: none"> <li>Click on a row of the results table to select a spectrum.</li> <li>Click the <b>Graphic</b> tab in the spectral plot window to the right of the table.</li> </ol>   |  |
| 3 View the mass list for the selected spectra.        | Click the <b>Mass List</b> tab in the spectral plot window.  |  |
| 4 Filter spectra by Precursor ion mass.               | <ol style="list-style-type: none"> <li>Set the Precursor ion mass to <b>279.09</b>.</li> <li>Click the <b>Find Spectra</b> button on the toolbar to start the search.</li> </ol>   | Note that only the three Sulfamethazine spectra are returned.                      |

# Familiarization Exercises


| Steps   | Detailed Instructions   | Comments   |
|---|---|--|
| 5 Reset the default search parameters.        | <b>a</b> Right click in the upper part of the Browse Spectra tab and select <b>Reset Search Fields</b> from the shortcut menu.        |  |
| 6 Filter spectra by Collision energy voltage. | <b>a</b> Set the Collision energy to <b>40</b> .<br><b>b</b> Click the <b>Find Spectra</b> 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. | Select <b>New PCDL</b> 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: <ul style="list-style-type: none"> <li>• <a href="#">“To create a subset PCDL from an input file”</a> on page 15</li> <li>• <a href="#">“To create a subset PCDL from selected compounds”</a> on page 24</li> </ul> |
| 2 Create the new PCDL.          | <ol style="list-style-type: none"> <li>Select <b>Sulfas_AM_PCDL</b> as the starting PCDL.</li> <li>Select <b>General</b> as the PCDL type.</li> <li>Type in a name for the new PCDL, such as <b>Sulfas_AM_Custom</b>.</li> <li>Enter a description for the new PCDL.</li> <li>Click the <b>Create</b> button to create the new PCDL.</li> </ol> | <ul style="list-style-type: none"> <li>• The new PCDL becomes the current working PCDL and is automatically enabled for editing.</li> <li>• The new custom PCDL will contain all compounds and spectra from the starting PCDL.</li> </ul>  |
| 3 Edit the PCDL.                | See <a href="#">“Exercise 7. Edit compounds”</a> .  |  |

## Exercise 7. Edit compounds


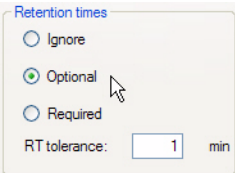
In this exercise, you will edit the custom PCDL that you created in Exercise 6.

| Steps  | Detailed Instructions   | Comments   |
|--|---|--|
| 1 Open the custom PCDL you created in Exercise 6, if it is not already open. | <b>a</b> Select <b>Open PCDL</b> from the File menu, or click the  button on the toolbar.<br><b>b</b> Select the <b>Sulfas_AM_Custom.cdb</b> file, and click the <b>Open</b> 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.  | <b>a</b> Open the <b>PCDL</b> menu.<br><b>b</b> Mark <b>Allow Editing</b> if it is not currently marked.  | A new PCDL is automatically enabled for editing when it is created.  |
| 3 Do a search.   | <b>a</b> Click the <b>Single Search</b> tab.<br><b>b</b> Click the <b>Find Compounds</b> 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 <b>Edit Compounds</b> tab.                                       |   |  |
| 5 Update information for a particular compound.                              | <b>a</b> Select the compound of interest by clicking on it in the Compound Results table.<br><b>b</b> Update information on the left side of the Edit Compounds tab, such as Mass, RT, Formula, Name, CAS ID, and Ion type.<br><b>c</b> Click the <b>Update Selected</b> button to apply the changes to the PCDL.   | <p>Information for the selected compound is displayed in the Edit Compounds tab.</p> <p>The updated information will be changed in the PCDL and reflected in the results table.</p>                    |
| 6 Update structure information for a particular compound.                    | <b>a</b> Select the compound of interest by clicking on it in the Compound Results table.<br><b>b</b> Click the  button in the Structures area to open a <b>.MOL</b> file.<br><b>c</b> Click the <b>Update Selected</b> 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 <b>MOL Text</b> tab and pasting in MOL file text that you copied from a molecular drawing tool ( <b>Ctrl+V</b> ). |

| Steps   | Detailed Instructions  | Comments  |
|---|--|---|
| 7 Add a new compound to the PCDL.                             | <p><b>a</b> Click the <b>Add New</b> button.<br/>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.</p> <p><b>b</b> Enter or change information for the new compound as described in Step 5 above.</p> <p><b>c</b> Click the <b>Update Selected</b> button.<br/>The information you entered for the new compound is updated in the PCDL and the information is reflected in the results table.</p> | <p><b>Alternate method:</b></p> <p><b>a</b> Enter information for a new compound on the left side of the Edit Compounds tab, such as Mass, RT, Formula, Name, and Ion type.</p> <p><b>b</b> Click the <b>Save As New</b> button.<br/>A new compound is created in the PCDL using the specified values. The new compound is displayed at the end of the results table.</p> |
| 8 Remove a compound from the PCDL.                            | <p><b>a</b> Select the compound of interest by clicking on it in the Compound Results table.</p> <p><b>b</b> Click the <b>Delete Selected</b> button.</p>  | 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. | <b>a</b> Select <b>Open PCDL</b> from the File menu, or click the  toolbar button.<br><b>b</b> Select the <b>Sulfas_AM_Custom.cdb</b> file, and click the <b>Open</b> button.  | None of the compounds in this example PCDL have retention times.                         |
| 2 Enable editing for this PCDL.   | <b>a</b> Open the <b>PCDL</b> menu.<br><b>b</b> Mark <b>Allow Editing</b> if it is not currently marked.  | A new PCDL is automatically enabled for editing when it is created.                      |
| 3 Click the <b>Batch Search</b> tab.  |   |  |
| 4 Open a mass list file that contains retention time information for the masses.                      | <b>a</b> Click the <b>File</b> button to the left of the mass list table.<br><b>b</b> Select <b>sulfa_compounds.txt</b> in the <b>MassHunter\PCDL\Mass List Files</b> folder.<br><b>c</b> Click the <b>Open</b> button.   | Each mass in the mass list must have an associated retention time value.                 |
| 5 Set the search parameters.  | <b>a</b> Set the <b>Mass tolerance</b> to 100 ppm.<br><b>b</b> Mark <b>Retention times Optional</b> .<br><b>c</b> Set the <b>RT tolerance</b> to 1 minute as shown below:   |  |
|   |    |  |
| 6 Start the search.   | Click the <b>Find Compounds</b> toolbar button. The number of hits for each mass appears in the <b>Hits</b> column of the mass list. In this example, hits were found for four masses, which appear at the top of the mass list. See <a href="#">Figure 7</a> . | To sort the list by a different criterion, click the heading for the column of interest. |
| 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.                          |

| Steps | Detailed Instructions  | Comments  |
|-------|--|---|
| 8     | Click the <b>Batch Summary</b> tab.                            | See <a href="#">Figure 8</a> .  |
| 9     | Update retention times in the PCDL from the current mass list. | Click the <b>Apply Retention Times</b> 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 <a href="#">Figure 9</a> .       |

Find Compounds

Single Search | **Batch Search** | Batch Summary | Edit Compounds | Spectral Search | Browse Spectra

Masses:

File ...

Clear

| Mass     | RT    | Hits |
|----------|-------|------|
| 278.0839 | 0.786 | 1    |
| 310.0738 | 1.218 | 1    |
| 270.0246 | 0.321 | 1    |
| 284.0132 | 0.509 | 1    |
| 403.2352 | 1.591 | 0    |
| 308.217  | 1.559 | 0    |
| 442.2216 | 1.756 | 0    |
| 430.2839 | 1.665 | 0    |
| 329.1998 | 1.745 | 0    |
| 417.2268 | 1.674 | 0    |
| 400.1886 | 1.748 | 0    |

Masses

☐ [M+H]<sup>+</sup> ☒ Neutral ☐ [M-H]<sup>-</sup>

Mass tolerance: 100 ☒ ppm ☐ mDa

Retention times

☐ Ignore ☒ Optional ☐ Required

RT tolerance: 1 min

Ion search mode

☒ Include neutrals ☐ Include anions ☐ Include cations

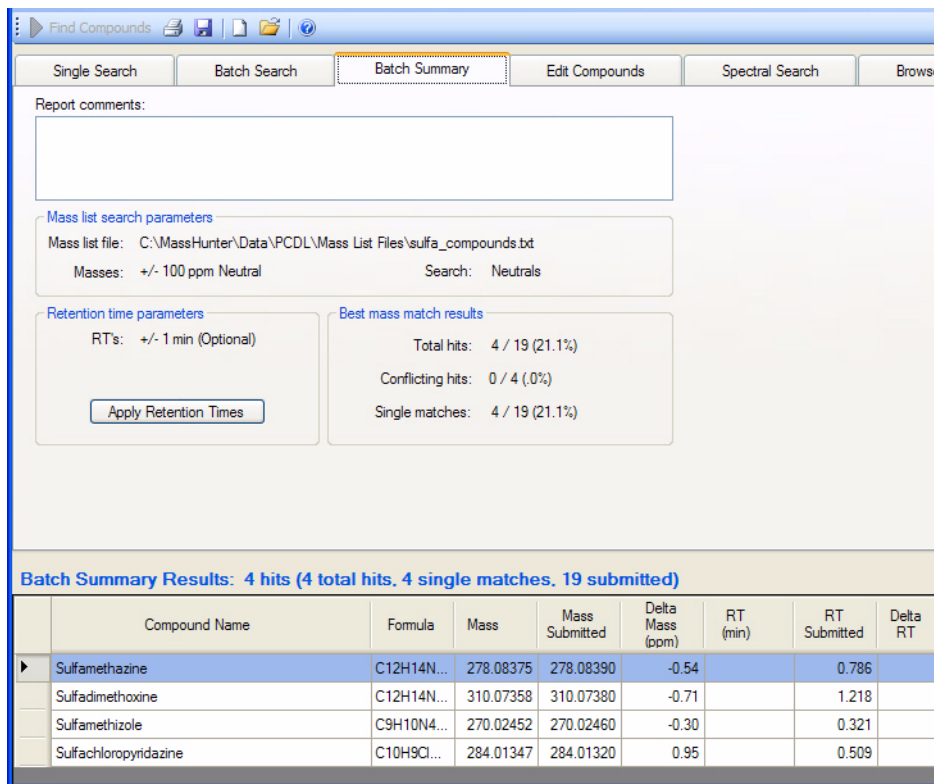
Molecule:

Notes:

**Batch Search Results: 1 hit for Mass: 278.0839 RT: 0.786**

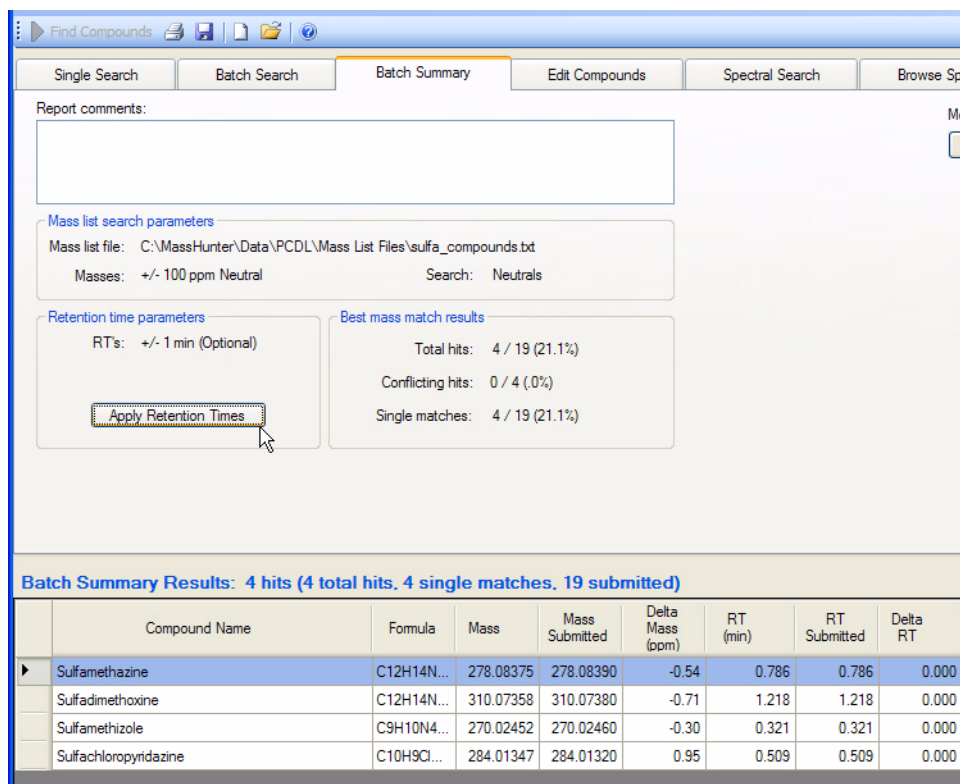
| Best                                | Compound Name  | Formula   | Mass      | Delta Mass (ppm) | RT (min) | Delta RT | CAS     | ChemSpider |
|-------------------------------------|----------------|---|-----------|------------------|----------|----------|---------|------------|
| <input checked="" type="checkbox"/> | Sulfamethazine | C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub> | 278.08375 | -0.54            |          |          | 57-68-1 | 5136       |

**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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