MassHunter Personal Compound Database and Library Manager Software

Quick Start Guide

Agilent Technologies

This *Quick Start Guide* helps you launch PCDL Manager Software, become familiar with the user interface, view PCDLs, and perform typical workflows to create and edit a custom PCDL.

What is Agilent MassHunter PCDL Manager?

Agilent MassHunter Personal Compound Database and Library Manager Software (PCDL Manager) is stand-alone software used to manage the content of any personal compound database and library (PCDL). A PCDL contains a compound database, an ion mobility database, and a spectral library.

You can use PCDL Manager to add, remove and edit the compounds in your custom PCDL to meet the specific needs of your laboratory and your analyses. The compounds in your PCDL must contain, at a minimum, identification and mass. You can add retention times based on standards and/or based on your sample data acquisition method for compounds you routinely analyze. For a custom PCDL, you can also add your own spectra, in addition to the spectra provided in the master PCDL.

With MassHunter Qualitative Analysis B.07.00 and later, you can send GC/MS and MS/MS spectra to PCDL Manager. After you perform a Find by Formula search to identify compounds in your sample data, you can then send the GC/MS or MS/MS spectra to your custom PCDL; however, when you send spectra be sure to use comparable software versions, such as version B.08 for both Qualitative Analysis and PCDL Manager. You can also filter spectral noise and correct the fragment ions to their theoretical accurate mass. Qualitative Analysis can also be used to automate or manually perform searches of a PCDL to identify compounds and spectrum peaks in your data files.

What's new in B.08.00?

- PCDL Manager has been expanded to include ion mobility support.
- Updated user interface with fewer, task-oriented tabs: Compounds, Spectra, Ion Mobility, and Import.
- Improved search functionality is available in the Compounds, Spectra, and Ion Mobility tabs. The improved search functionality includes:

  - *Must also contain* and *Must not contain* filter boxes in the Compounds tab to allow more specificity in your compound searches
  - Limit results in the Compounds tab for compounds with spectra and/or collision cross section values
  - Ion species specific searching in the Spectra and Ion Mobility tabs
  - Searching of *MS Chemical Standard* and *CCS Chemical Standard* columns in the Spectra and Ion Mobility tabs
- PCDL Manager has been expanded to include additional chemical identifiers (BioCyc, Caymen Chemical, Chapman and Hall, ChEBI, InChi, InChi Key, Log P, NCBI, PubChem, Sigma Aldrich, SMILES, and UniProt) and new columns (CCS count, RT created, RT High (theoretical), RT Low (theoretical), and Synonyms).
- A new Import tab replaces the batch search mode and allows you to easily update or import retention times and collision cross section values.
- In-table editing of compound, spectra, and ion mobility information in your PCDL has replaced the Edit menu found in prior versions of PCDL Manager. When you view your compounds with editing enabled, a selected cell (compound and identifier column) is highlighted in a distinct green color indicating that the value can be directly edited.
- View compound information, spectra, and molecular structures all at the same time for each compound entry by launching the Spectra and Molecular Structure viewers.
- View multiple spectra at one time using the Spectra viewer.
- Create new spectra from published work by adding *m/z* versus relative abundance values.
- Create subset PCDLs directly from the Compounds tab by searching for multiple identifiers at one time in the *Compounds search criteria* and using the new *Must contain* and *Must not contain* filters.

- New traceability for each spectral or CCS entry with *MS Chemical Std* and *CCS Chemical Std* columns in the Spectra and Ion Mobility tabs (you can add the chemical supplier product number in these columns).
- Create and manage the external website links available in the Links menu to make finding the information you need to manage your PCDLs fast and intuitive.

Features of PCDL Manager

- Search for compounds using text, formula, accurate mass, and retention time - you can specify retention time as optional or required in your compound search. Using retention time increases your compound search specificity.
- Search and view GC/MS and MS/MS spectra in PCDLs.
- Create and edit custom PCDLs, including adding proprietary compounds, retention times, collision cross sections, and raw experimental or theoretically corrected MS/MS and GC/MS spectra.
- Import retention times and collision cross section values from CSV files.
- Send spectra to your customized PCDL directly from Qualitative Analysis to create your own library. Choose from options to filter spectral noise and/or to correct the fragment ions to their theoretical accurate mass.
- Load spectra from either a CEF file or using copy-and-paste mass spectra from Qualitative Analysis, and search for the spectra in the current PCDL.
- Create new spectra from published work by adding *m/z* versus relative abundance values.
- Perform private, on-site searches using your PCDLs to help keep your intellectual property safe.
- Link to websites for more information on compounds in your PCDL.

Terminology

Custom PCDL A PCDL that you can edit using PCDL Manager. A custom PCDL is designated *User* in the **Master or User** field as described in "View PCDL information" on page 25.

PCDL An accurate mass compound database that may also contain retention times, an MS/MS accurate mass spectral library, and an ion mobility database including collision cross section values.

Compound Name Many compounds are commonly known by their salts. The mass spectrometer, however, detects the anion or cation portion of the salt, rather than the neutral salt. 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.

Where to Find More Information

Use the online Help for in-depth information as you use PCDL Manager. Display online Help in one of two ways:

- Select **Contents**, **Index**, or **Search** from the **Help** menu.
- Press **F1** to get context specific information about an active window, tab, or dialog box.

Go to www.agilent.com for the most current information on Agilent products.

User Interface

Main window

The main PCDL Manager window consists of five parts: (1) Menu Bar, (2) Toolbar, (3) Action Tabs, (4) Action Pane, and (5) Compound Results Pane. The number of compounds that meet your search criteria is shown above the table in the *Compounds Results Pane*. The window areas are shown in Figure 1.

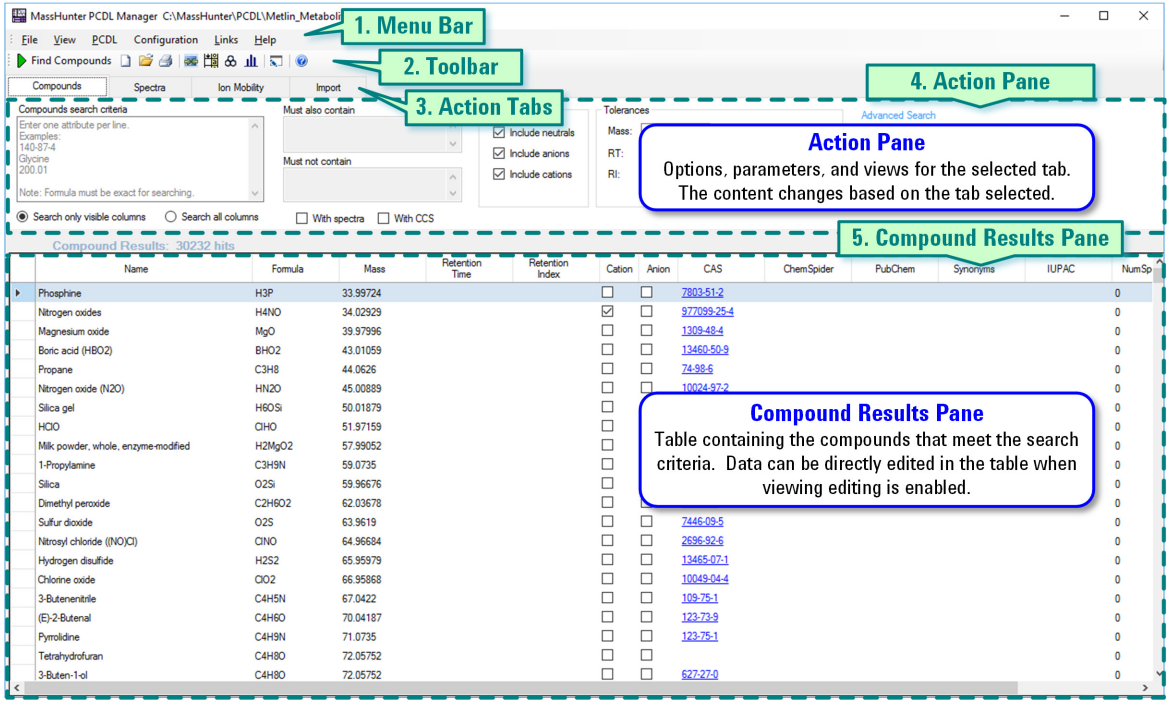

Figure 1 The main functional areas of PCDL Manager window

1. Menu Bar The menu bar provides actions that are used to create and manage your custom PCDL. More information regarding the menu bar is provided in the section "Menu bar" on page 8.

2. Toolbar The toolbar is located below the menu bar and contains buttons for commonly performed tasks. More information regarding the toolbar is provided in the section "Toolbar" on page 12.

3. Action Tabs Four tabs - **Compounds**, **Spectra**, **Ion Mobility**, and **Import** - provide options for you to search, view, and edit compound data and spectra in the open PCDL. More information regarding the tabs is provided in the section "Action Tabs" on page 13.

4. Action Pane The *Action Pane* is where you enter and select parameters, information, and options, and then view the compound, spectra, and ion mobility results. Content of the *Action Pane* changes based on the tab selected.

5. Compound Results Pane Lists the compounds and the compounds data that meet your search criteria. This pane changes based on the selected action tab and is replaced with a *Matched Compounds* table when you select the **Import tab**.

Menu bar

The menu options available in PCDL Manager are shown in Figure 2.

Figure 2 PCDL Manager menu bar

File: Open, backup, and create new PCDLs. You can also create subset PCDLs, convert older PCDLs, import compounds from a CSV file, and print and export your search results.

View: Manage the columns in the compound results table in the *Compounds Results* pane, view molecular structure details in a separate **Compound** window, and view spectra in a separate **Spectra Viewer** window.

PCDL: Search for compounds, spectra or conformers in your PCDL, toggle the **Allow Editing** mode, and review information about your PCDL.

Configuration: Manage the links (URLs) to online compound databases.

Links: Open your default Internet browser to the selected website. When the editing mode is enabled, you can add, edit, and remove links in this menu.

Help: Provides a link to online Help and information about PCDL Manager software.

File menu

New PCDL Create a custom PCDL that can be edited and personalized for your lab. You can create a new PCDL by making a clone of an existing PCDL, including the open PCDL, with a new name, or you can create a new empty PCDL. When you make a clone of a master PCDL, the clone can be edited. See "Create a new PCDL" on page 30.

Open PCDL Select and open an existing PCDL. The currently open PCDL is closed automatically when you open a new PCDL.

> ***Note:*** When you use **Open PCDL** on an older PCDL, PCDL Manager automatically notifies you that the PCDL is an older version and converts the PCDL to the current format. The original PCDL is archived in the folder **\MassHunter\PCDL\B.0X.00\Archive**, where **X** is the PCDL Manager version compatible with the original PCDL. If you click **Cancel** in the **Open PCDL** dialog box when you launch PCDL Manager, PCDL Manager has limited functionality until you open or create a new PCDL.

Backup PCDL Create a copy of the open PCDL. This is a convenient way to archive an existing PCDL and to save incremental progress while you are creating or editing a new PCDL.

Convert PCDL Opens the **Convert PCDL** dialog box. You must convert a PCDL which was developed with an older version of PCDL Manager to the current format. Once you convert a PCDL to version B.08, you cannot use the converted PCDL in a version of Qualitative Analysis that is prior to B.08.

> ***Note:*** When you use **Convert PCDL** on an older PCDL, PCDL Manager saves the original PCDL in the folder **\MassHunter**

PCDL\B.0X.00\Archive, where **X** is the PCDL Manager version compatible with the original PCDL.

Create Subset PCDL Create a new PCDL containing the only the selected compound rows in the open PCDL.

Import Compounds Add compounds from a CSV file to the open PCDL. If you start with an empty PCDL, then you are creating a new PCDL from the imported compounds. This menu option is only available when editing is enabled.

Print Results Print search results and structures to a printer configured on your personal computer.

Exit Close the PCDL Manager window. The open PCDL is automatically saved.

View menu

Autosize Columns Changes the width of each column in the tables so that the data displayed in the tables is optimized.

Hide Empty Columns Hides columns in tables that do not have any content. You can display hidden columns again when you right-click on a table column heading and then click **Add/Remove Columns** or **Restore Default Columns**.

Molecular Viewer Opens the **Compound** window where you can view, edit, and load the molecular structure data related to the selected compound.

Spectra Viewer Opens the **Spectra Viewer** window where you can view, create, add, edit, delete, and load acquired spectral data for the selected compound.

PCDL menu

Find Compounds Searches the PCDL for compounds that match the criteria specified in the *Action Pane*. This menu option is only available when **Compounds tab** is active. You can also press the **F5** key to find compounds.

Find Spectra Searches the PCDL for spectra that match the criteria specified in the *Action Pane* when the **Spectra tab** is active. This menu option is only available when the **Spectra tab** is active. You can also press the **F5** key to find spectra.

Find Conformers Searches the PCDL for compounds that match the criteria specified in the *Action Pane* when the *Ion Mobility* tab is active. This menu option is only available when the *Ion Mobility* tab is active. You can also press the **F5** key to find conformers.

Allow Editing Enable, or disable, editing operations for a custom PCDL. You can also press the **F2** key to enable and disable editing. When editing is enabled, a check mark ( ) appears next to this menu option and an **Add** button indication (Add) appears above the *Compounds Results* table in the **Compounds tab**.

Note: A master PCDL cannot be edited.

PCDL Information Opens the **PCDL Information** dialog box where you can view information about the current PCDL. When editing is enabled, you can edit the PCDL **Type** and **Description**.

Configuration

Modify URLs in Link Columns Manage the links (URLs) to online compound databases that are contained in the chemical identifier columns in the PCDL.

Links menu

Quick, customizable access to websites specific to your custom PCDL application area such as pesticides or metabolites web sites that contain additional chemical information on compounds or metabolites. When editing is enabled, you can edit, add new links, and delete links in the **Links** menu.

Help menu

Contents, Index, and Search Opens the online Help window for 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, build, and notes of the MassHunter PCDL Manager software.

Toolbar

The toolbar is located below the menu bar and contains four groups of buttons for commonly performed tasks.

Button	Equivalent Command
	Button changes based on the active *action tab*: **PCDL > Find Compounds**, or press **F5** **PCDL > Find Spectra**, or press **F5** **PCDL > Find Conformers**, or press **F5**
	**File > New PCDL**, or press **Ctrl+N**
	**File > Open PCDL**, or press **Ctrl+O**
	**File > Print Results**, or press **Ctrl+P**
	**View > Autosize Columns**
	**View > Hide Empty Columns**
	**View > Molecular Viewer**
	**View > Spectra Viewer**
	**PCDL > Allow Editing**, or press **F2** This command is not available when a master PCDL is open.
	**Help > Contents**, or press **F1**

Action Tabs

Four *Action Tabs* are available in PCDL Manager: **Compounds**, **Spectra**, **Ion Mobility**, and **Import**.

Working with the Action Tabs

Searching for compounds in a PCDL is performed by entering search criteria in one of the *Action tabs*: **Compounds**, **Spectra**, or **Ion Mobility**. Each of these *Action Tabs* provides you with search parameters optimized to search your PCDL based on either the compound data columns (**Compounds tab**), basic compound information with spectra specific parameters (**Spectra tab**), and basic compound information with ion mobility specific parameters (**Ion Mobility tab**). The search results in the **Spectra** and **Ion Mobility** tabs include an additional results table to help you view the spectra or ion mobility data for the compounds results from your search.

The search results obtained by performing a search in any one of the *Action Tabs* can be viewed in any of the other *Action Tabs* by simply changing tab. For example, if you search for a compound in the **Compounds tab** using formula, switching to the **Spectra tab** and **Ion Mobility tab** allows you to view the corresponding spectral and ion mobility information for each compound that matched your original search.

> ***Note:*** Each time you perform a search, the previous results are disregarded. When you change between *Action Tabs* without performing a new search on the PCDL, the compound results displayed do not match the search criteria present in the current action tab until you perform a search.

The **Import tab** is used to update your PCDL with new retention times or CCS values and related information.

Compounds tab

You can search for compounds in the PCDL using parameters in the *Action Pane* when the **Compounds tab** is selected. Search results are displayed in a *Compound Results* table in the *Compound Results Pane*. When editing is enabled, you can edit the compound data directly in the Compound Results table.

Figure 3 on page 14 shows a view of the **Compounds tab** using the *Search Action Pane*. Figure 4 on page 15 shows a view of the **Compounds tab** using the *Advanced Search Action Pane*.

For more information on using the **Compounds tab** see: "Editing a PCDL" on page 30 and "Find Compounds in your PCDL" on page 47.

Search tips

Use the following search tips to help find your compounds more efficiently:

- Enter one search element per line.
- When searching for a molecular formula, the formula must match an entry in the *Formula* column exactly. Partial molecular formulas are not matched during the search.
- Enter the first digits of the *CAS* number and include the hyphen. For example, to search for 551-92-8 enter *551-* in the search.
- When searching for Mass, RT, and RI values, include a decimal point in your value as shown in the following examples:
  - **Mass:** For mass 121, search for 121.12, 121.123, 121.1234
  - **RT:** For a retention time of 10 minutes, search for 10.0
  - **RI:** For a retention index of 10, search for 10.0 or 10.00

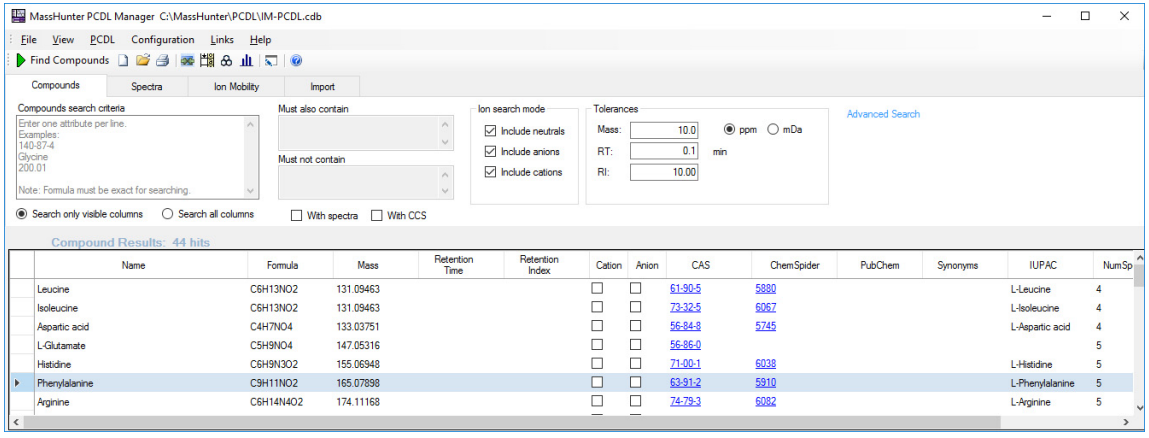

Figure 3 The **Compounds tab** for the *Search Action Pane* in PCDL Manager without any search criteria entered for **Find Compounds**

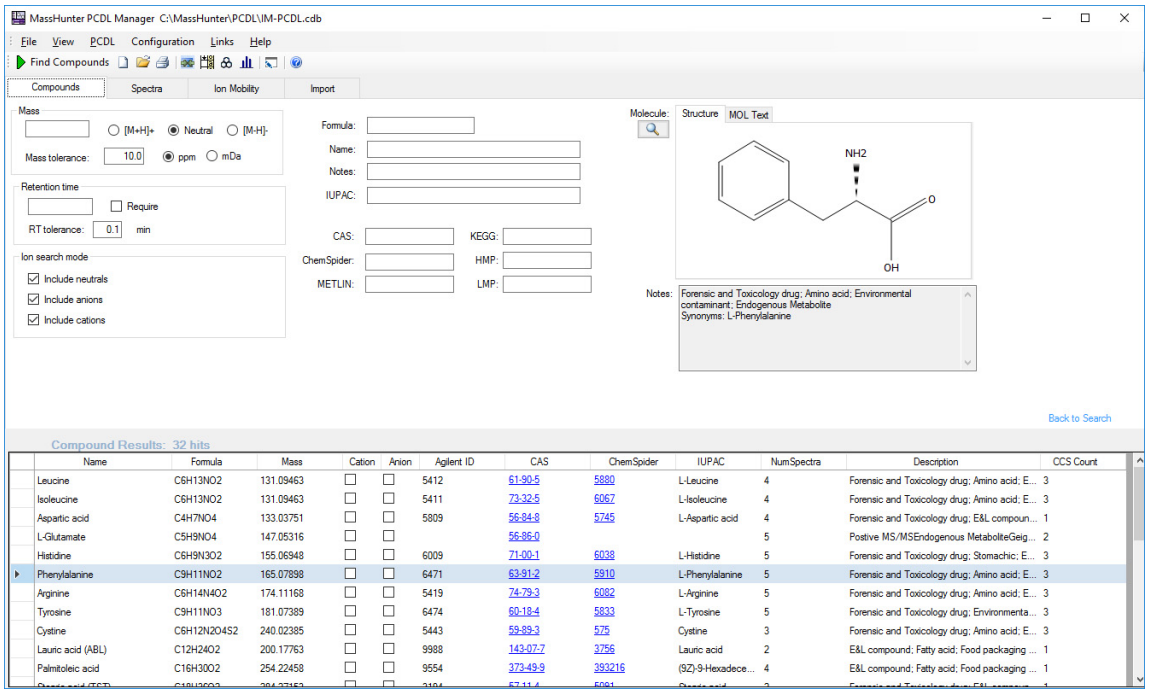

Figure 4 The **Compounds tab** for the *Advanced Search Action Pane* in PCDL Manager without any search criteria entered for **Find Compounds**

Viewing structures

When available in your PCDL, the molecular structure of the selected compound can be viewed in the *Advanced Search* view on the **Compounds tab** or in a separate **Molecular Viewer** dialog box. The **Molecular Viewer** dialog box is visible even when you change your views among the *Action Tabs* allowing you to view structural information at the same time as compound, spectral, and ion mobility information.

See "View molecular structures" on page 26 for more information about viewing molecular structures.

Spectra tab

You can search for spectra and their associated compounds in the PCDL using parameters in the *Action Pane* when **Spectra tab** is selected. Search results are displayed in two tables, *Spectra for Compound* and *Compound Results*, that are shown in the *Compound Results Pane* (*Figure 5*).

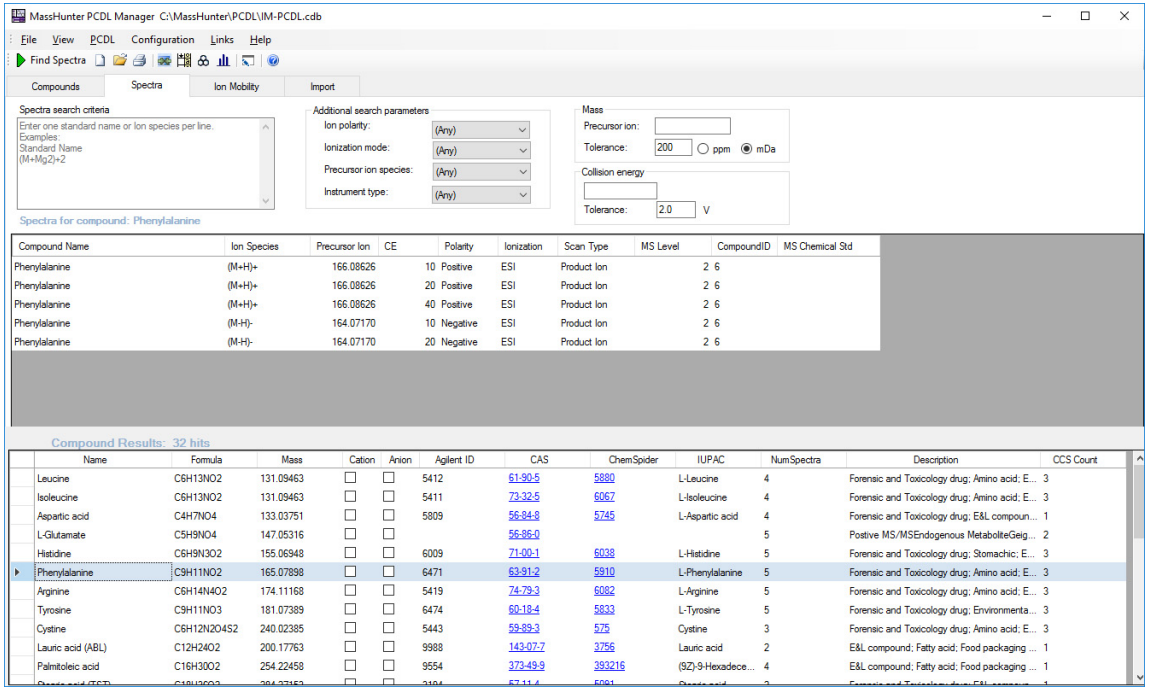

Figure 5 The **Spectra tab** in PCDL Manager without any search criteria entered for **Find Spectra**

Viewing spectra

When available in your PCDL, the spectra of the selected compound are viewed in the **Spectral Viewer** window that is visible even when you change your views among the *Action Tabs* (see Figure 6 on page 17). The spectra of the selected compound can be viewed in one of several ways:

- **From the Menu bar:** Click **View > Spectra Viewer** to launch the **Spectra Viewer** window.

- **From the Toolbar:** Click the **View Spectra** icon , located on the toolbar, to launch a the **Spectra Viewer** dialog box.

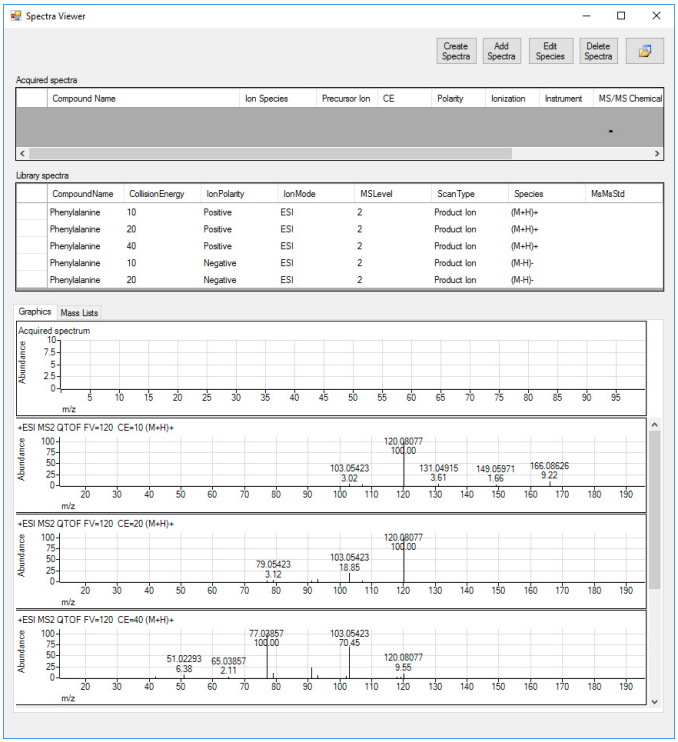

Figure 6 **Spectra Viewer** dialog box

Working with spectra

If editing is enabled, you can create, add, edit, and delete spectra in a custom PCDL from within the **Spectra Viewer** dialog box. You can edit the molecular or precursor ion information, including ion species, precursor ion *m/z* and the MS Chemical Standard information. You can also remove noise peaks from raw experimental spectra such as spectra which were loaded from a **CEF** file. Before you can work with the spectra for a compound, you must perform a search so that the compounds and associated spectra you want to manage are present in the *Compound Results* table.

Note: It is recommended to use the **Send Spectra to PCDL** feature in MassHunter Qualitative Analysis to import spectra to a PCDL when creating your own custom PCDL, rather than using copy and paste of spectra from MassHunter Data Analysis software or loading spectra from CEF files. This feature allows you to apply the following options: to filter spectral noise, set a pass/fail base peak height filter, and correct the fragment ions to their theoretical accurate mass.

Ion Mobility tab

You can search for compounds in the PCDL using parameters associated with ion mobility in the *Action Pane* when the **Ion Mobility tab** is selected. Search results are displayed in two tables, *Ion Mobility information for compound* and *Compound Results*, that are shown in the *Compound Results Pane* (*Figure 7*).

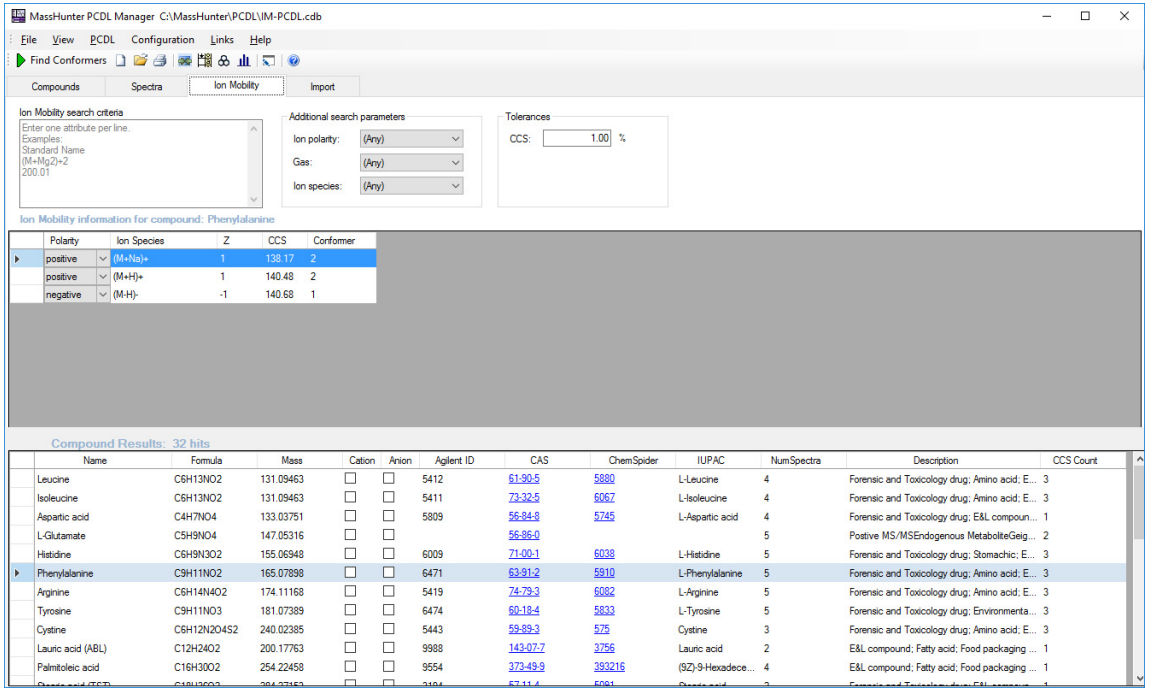

Figure 7 The **Ion Mobility tab** in PCDL Manager without any search criteria entered for **Find Conformers**

Import tab

You can import retention times (RTs) and collision cross section (CCS) values for the compounds in your PCDL. The imported values are obtained from a previously prepared CSV file (see "Import CSV File Format" on page 33).

The compounds in your open PCDL that match compounds in the import file are displayed in the *Matched Compounds* table (the left table in Figure 8 and Figure 9) that replaces the *Compound Results Pane*.

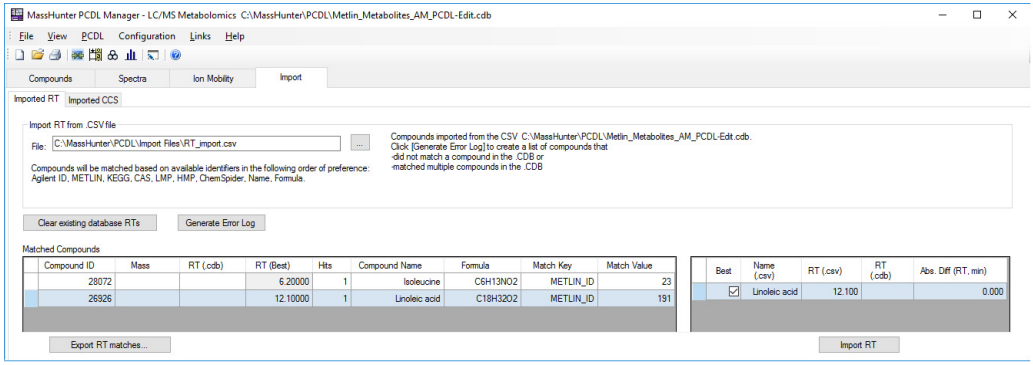

Figure 8 The **Import tab** in PCDL Manager, **Imported RT** tab

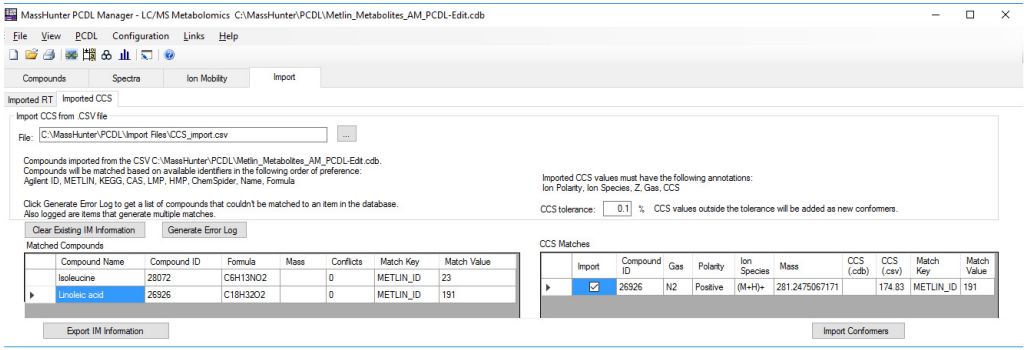

Figure 9 The **Import tab** in PCDL Manager, **Imported CCS** tab

When you select a compound in the *Matched Compounds* table, the table to the right shows the RT or CCS matches depending on whether the **Imported RT** tab (Figure 8) or the **Imported**

CCS tab (Figure 9 on page 19) is selected, respectively. If there is more than one match for an RT import, you select the match that is the best fit. If there is more than one match for the CCS import, you can select which matches you want to import as new conformers and which matches you want to ignore.

Getting Started

The following topics help you get started using PCDL Manager to open, convert, backup, and view PCDLs:

Install and run PCDL Manager

1. Install PCDL Manager. Follow the instructions in "PCDL Manager Installation" on page 77.
2. Double-click the **PCDL Manager B.08.00** icon  located on your desktop.

   Alternatively, you can click **Start > All Programs > Agilent > MassHunter Workstation > PCDL Manager B.08.00** (Windows 7), or click **Start > All apps > Agilent > PCDL Manager B.08.00** (Windows 10) to launch PCDL Manager.
3. Select the example PCDL **Sulfas_AM_PCDL.cdb** in the **Open PCDL** dialog box.

   To open a different PCDL, see "Open a PCDL" on page 22.

   Note: The PCDL that was last viewed is displayed as the default PCDL to open in the **Open PCDL** dialog box.
4. Click **Open**. You are now ready to become familiar with the operations available in PCDL Manager.

Open a PCDL

You open a PCDL when you (1) launch PCDL Manager and (2) when you want to change the active PCDL after PCDL Manager is running. PCDL files have a **.cdb** extension.

Note: Master PCDLs cannot be edited, but they can be used to create custom PCDLs that can be edited. See "Create a new PCDL" on page 30.

(1) Launch PCDL Manager When you initially start PCDL Manager you are prompted to select a PCDL to open.

1 Double-click the **PCDL Manager B.08.00** icon  located on your desktop.

Note: From *File Explorer* you can double-click on a **.cdb** file to launch PCDL Manager and open the chosen PCDL.

Alternatively, you can click **Start > All Programs > Agilent > MassHunter Workstation > PCDL Manager B.08.00** (Windows 7), or click **Start > All apps > Agilent > PCDL Manager B.08.00** (Windows 10) to launch PCDL Manager.

2 Select the PCDL to open in the **Open PCDL** dialog box.

Note: The PCDL that was last viewed is displayed as the default PCDL to open in the **Open PCDL** dialog box. You can choose to open the previously opened PCDL, or navigate to and select a different PCDL.

3 Click **Open**.

Note: If you click **Cancel** in the **Open PCDL** dialog box when you launch PCDL Manager, PCDL Manager has limited functionality until you open or create a new PCDL.

(2) Open a different PCDL After PCDL Manager is open, perform the following steps to open a different PCDL.

1 Click **File > Open PCDL**, click  on the toolbar, or press **Ctrl+O** to open the **Open PCDL** dialog box.

2 Select the PCDL file of interest.

3 Click **Open**.

Note: When you open an older PCDL, PCDL Manager automatically notifies you that it detected that the PCDL is an older version and converts the PCDL to the current format. The original PCDL is archived in the folder **MassHunter\PCDL\ B.0X.00\Archive**, where **X** is the PCDL Manager version compatible with the original PCDL.

Convert an older PCDL

PCDLs created from previous versions of PCDL Manager can be converted for use in PCDL Manager B.08.00 and later.

1 Click **File > Convert PCDL** to open the **Convert PCDL** dialog box (Figure 10).

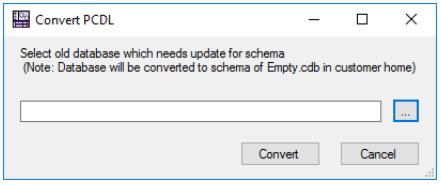

Figure 10 **Convert PCDL** dialog box

2 Click the select PCDL icon ... to open the **Open PCDL** dialog box.

Alternatively, you can type the full path and filename of a PCDL to convert directly into the **Convert PCDL** dialog box (Figure 11 on page 24) and skip the next step.

3 Select the PCDL that you want to convert and then click **Open** to return the path and filename to the **Convert PCDL** dialog box.

4 Click **Convert**. The PCDL is converted to the latest schema.

- If the PCDL is converted, the original PCDL is archived in the folder **MassHunter\PCDL\B.0X.00\Archive**, where **X** is the PCDL Manager version compatible with the original PCDL.

- If a copy of the PCDL is already saved in the **\MassHunter\PCDL\B.0X.00\Archive** folder, a dialog box informs you that the conversion was not performed because the PCDL was previously converted. To proceed with the conversion you need to either delete or change the file name of the PCDL in the **\MassHunter\PCDL\B.0X.00\Archive** folder and then repeat the steps to convert the PCDL.

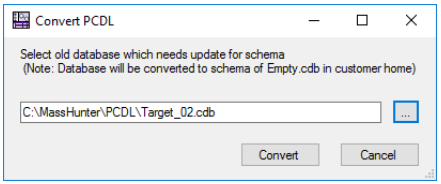

Figure 11 **Convert PCDL** dialog box with a PCDL specified

Backup a PCDL

When you edit a PCDL the changes are made to your PCDL immediately and in real-time. Since PCDL Manager does not have an *undo* function, you can create a backup of the current state of your PCDL at any time. You can save time restoring a previous version of your PCDL if you create a backup of your PCDL at various times.

1. Click **File > Backup PCDL** to launch the **Backup PCDL** dialog box.
2. Select a folder for the backup file, or accept the default folder **MassHunter\PCDL\Archive**.
3. Type a file name for the backup file, or accept the proposed file name - the proposed file name is the PCDL file name with the current date appended in the form **<name>.<yyyy.mm.dd>.cdb** where **name** is the name of the open 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 in the specified location.

View PCDL information

You can view general information about an open PCDL using the **PCDL Information** dialog box. If the open PCDL is not a master but a user PCDL, and if editing is enabled, you can edit some of the general information.

1 Click **PCDL > PCDL Information** to launch the **PCDL Information** dialog box.

2 View the following information about the open PCDL. If editing is enabled, you can edit the fields marked **editable field** while you are viewing the PCDL information.

- **File name**
- **# Compounds**
- **Master or User:** ***Master*** indicates the PCDL is not editable and ***User*** indicates the PCDL is editable (also referred to as a custom PCDL).
- **Type** (**editable field**): Select a type from the list.

  Note: The **Type** value is used to determine the default data columns that are shown in the *Compounds Results* table and the default **Links** available in the menu bar.
- **Edit allowed**: An indication of the current status of the PCDL. ***Yes*** indicates PCDL editing is enabled and ***No*** indicates that PCDL editing is disabled.
- **Last modified**: A time stamp indicating when the PCDL was last modified using PCDL Manager.
- **Version**: The PCDL Manager schema version of the PCDL.
- **Description** (**editable field**): Text that describes the PCDL.

3 Click **Apply** if you made changes to the PCDL **Type** or edited the **Description** (see Figure 12 on page 26).

4 Click **Close** to exit the **PCDL Information** dialog box.

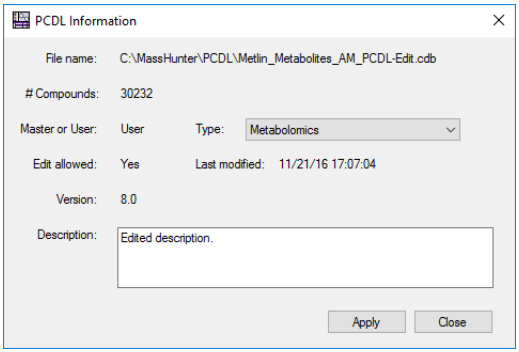

Figure 12 **PCDL Information** dialog box with editing enabled

View molecular structures

When available in your PCDL, the molecular structure of the selected compound can be viewed in the *Advanced Search* view on the **Compounds tab** or in a separate **Molecular Viewer** dialog box. The **Molecular Viewer** dialog box is visible even when you change your views among the *Action Tabs* allowing you to view structural information at the same time as compound, spectral, and ion mobility information.

Molecular structures can be viewed in one of several ways:

- **From the Menu bar:** Click **View > Molecular Viewer** to launch the **Molecular Viewer** dialog box.
- **From the Toolbar:** Click the **View Molecular Structure** icon , located on the toolbar, to launch the **Molecular Viewer** dialog box (Figure 13 on page 27).
- **From the Action Pane:** Click the view **Molecule** icon , located in the **Advanced Search** part of the *Action Pane*, to launch the **Molecular Viewer** dialog box (see Figure 13 on page 27).
- **In the Action Pane:** Click **Advanced Search** in the *Action Pane*. When available, the molecular structure is visible in the *Action Pane* (Figure 4 on page 15). The parameters and options available for searching the PCDL also change when you are in *Advanced Search*.

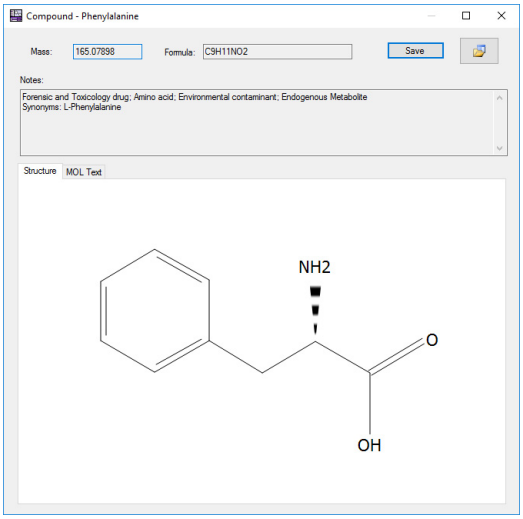

Figure 13 **Molecular Viewer** dialog box

Editing the molecular structure

When editing is enabled, you can edit the molecular structure information for a custom PCDL. Within the *MOL Text* tab you can edit and perform cut-and-paste operations to edit the molecular structure. See "Edit a molecular structure" on page 41 for information on editing the molecular structure. If you edit the information in the **Molecular Viewer** dialog box, click **Save** to update the PCDL with your changes.

Editing the notes

When editing is enabled, you can edit the notes information for a custom PCDL. If you edit the information in the **Molecular Viewer** dialog box, click **Save** to update the PCDL with your changes.

> ***Note:*** The content displayed in the **Notes** field in the **Molecular Viewer** dialog box is identical to the values in the compound *Description* column of the *Compound Results* table.

View mass spectra

When available in your PCDL, the mass spectra of the selected compound can be viewed in the **Spectra Viewer** dialog box. The **Spectra Viewer** dialog box is visible even when you change your

views among the *Action Tabs* allowing you to view spectral information at the same time as compound, structure, and ion mobility information.

Mass spectra can be viewed in one of several ways:

- **From the Menu bar:** Click **View > Spectra Viewer** to launch the **Spectra Viewer** dialog box.
- **From the Toolbar:** Click the **View Spectra** icon , located on the toolbar, to launch the **Spectra Viewer** dialog box (Figure 14).

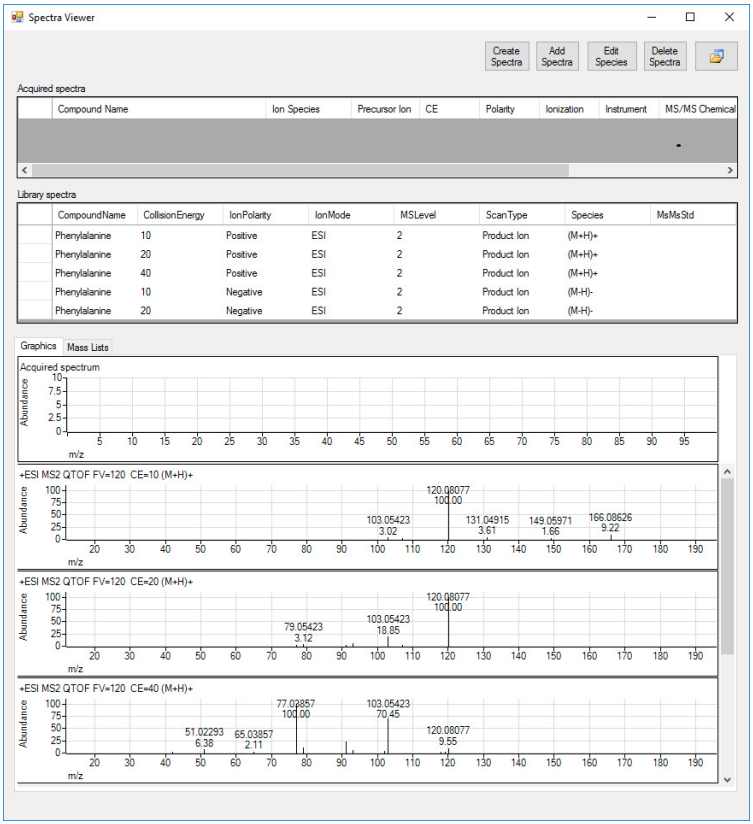

Figure 14 **Spectra Viewer** dialog box

View linked websites

The PCDL Manager interface allows you to create customized links to websites, such as pesticides, metabolomics, or forensics websites, that contain additional chemical information on compounds or metabolites.

1 Click **Links**.

2 Click a website link of interest as shown in Figure 15. The selected website opens in your default Internet browser.

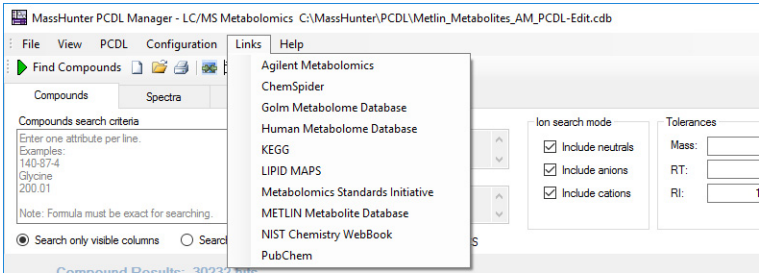

Figure 15 Linked websites for a PCDL **Type** *LC/MS Metabolomics* with editing disabled

Edit links

When editing is enabled, you can edit, add new links, and delete links in the **Links** menu as shown in Figure 16.

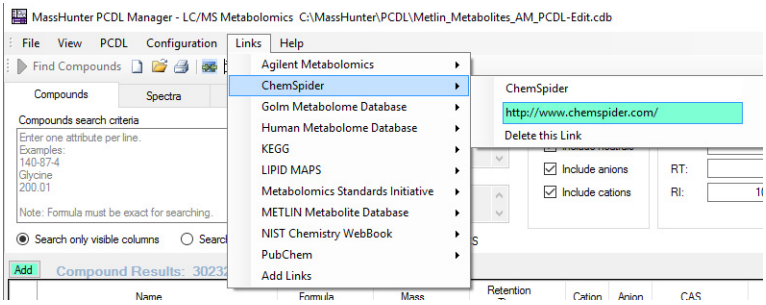

Figure 16 Linked websites with editing enabled

Editing a PCDL

The following topics help you get started using PCDL Manager to create and edit PCDLs:

- "Create a new PCDL" below
- "Import compounds into a PCDL" on page 32
- "Import CSV File Format" on page 33
- "Add compounds manually to a PCDL" on page 35
- "Append compounds to a PCDL" on page 36
- "Create a subset PCDL" on page 39
- "Edit a molecular structure" on page 41

Create a new PCDL

These steps describe how you can create a new PCDL.

Note: You can also create a new PCDL by creating a subset of an existing PCDL as described in "Create a subset PCDL" on page 39

1 Click **File > New PCDL**, click the **Create a New PCDL** icon on the toolbar, or press **Ctrl+N** to launch the **Create New PCDL** dialog box.

2 Select whether to create an *empty* PCDL or to create a PCDL by starting with a copy of the compounds in an already existing PCDL (see Figure 17 on page 31).

- Select **Create New PCDL** to create an empty PCDL that does not contain any initial compounds. Continue with step 4.
- Select **Clone Existing PCDL** to create a PCDL containing a copy of the compounds in an existing PCDL. Continue with step 3.

3 Select a PCDL to clone for the new PCDL from the **Select an existing PCDL** list.

The default path is **\MassHunter\PCDL**.

A small example PCDL (**Sulfas_AM_PCDL.cdb**) is supplied with PCDL Manager and can be used to create a custom PCDL; remember to remove the example compounds from your custom PCDL.

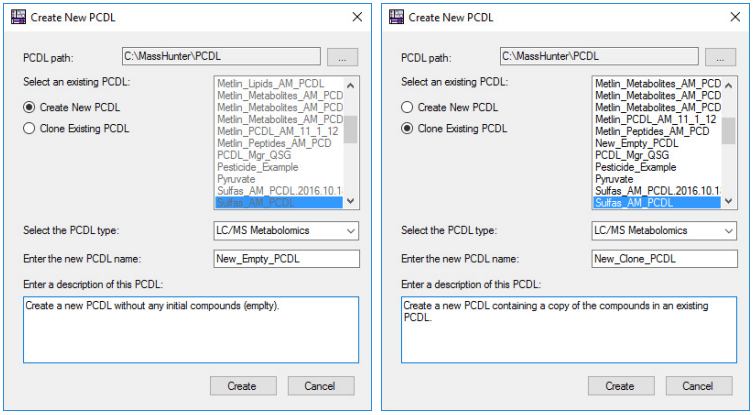

Figure 17 **Create New PCDL** dialog box parameters: **Create New PCDL** (left) and **Clone Existing PCDL** (right)

4 Select the type of new PCDL from the list available in **Select the PCDL type** (see Figure 18).

The PCDL type you select determines the default data columns shown in the *Compound Results* table and the default URLs available in the **Links** menu.

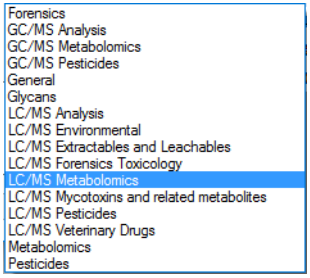

Figure 18 List of available **PCDL types**

5 Type a name in **Enter the new PCDL name**.

6 Type a description in **Enter a description of this PCDL**.

7 Click **Create** to generate the new PCDL and automatically open the new PCDL in PCDL Manager.

8 You can add compounds to the new, and now active, PCDL in any of the following ways:

- "Import compounds into a PCDL" starting below
- "Add compounds manually to a PCDL" on page 35

Import compounds into a PCDL

Use the following steps to import compounds into an open custom PCDL, or to create a custom PCDL from a compound list created by another application.

Note: When you start with an empty PCDL using **Create New PCDL** (see step 2 on page 30) you are creating a new custom PCDL from the compounds you import.

1 Prepare an import file.

An example **Compound_import.csv** file can be found in **\\MassHunter\PCDL\Import Files**; this file can be used as a template. The format required for the import file is described in "Import CSV File Format" on page 33 and in the online Help topic **Import File Format**. The import CSV file can be created manually using a spreadsheet or text editing program.

2 Open the custom PCDL of interest, or create a new PCDL as described in "Create a new PCDL" on page 30.

3 Click **PCDL > Allow Editing**, click  on the toolbar, or press **F2** to enable editing of the open PCDL.

4 Click **File > Import Compounds**.

5 Select the **.CSV** file you prepared in step 1 that contains the compounds of interest.

6 Click **Open**.

7 Click **PCDL > Allow Editing**, click  on the toolbar, or press **F2** to disable editing of the open PCDL.

8 Click **PCDL > Find Compounds,** click 

on the toolbar, or press **F5** to view the compounds in the PCDL. The compounds are listed in the *Compound Results* table.

9 Examine the log file, if created. Compounds that were *not* imported due to problems with the input file are saved in a file **<ImportFileName>-ImportLog.csv**, where **<ImportFileName>** is the name of the PCDL selected in step 5. Examine the log file to determine how to fix the problem and then import the corrected file.

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

10 (*Optional*) See "Editing a PCDL" on page 30 if you want to change information for the imported compounds.

Import CSV File Format

A file for importing compounds into a PCDL must have the values separated by commas (CSV file). The file can be created in any of the following ways:

- Export from another application such as Qualitative Analysis.
- Create manually using a spreadsheet program or text editor (saved in CSV format).

The first line(s) in the CSV file may be designated for your comments. Start such comment lines in your CSV file with a **#**. The first non-comment line of the CSV file contains the column header names with each column identifier name separated by a comma. The subsequent lines contain the values for each column separated by a comma, one compound per line.

Compound import

- For **File > Import Compounds**, you must have at minimum a name and either a formula or a mass to create a new compound in the PCDL. The mass is auto-calculated from the formula if there is no mass.

- Typical data column header names for compound import include: **Name**, **Formula**, **Mass**, **Anion**, **Cation**, **METLIN**, **KEGG**, **CAS**, **LMP**, **HMP**, **ChemSpider**, **RT**, **RI**, **Log P**, **RT Low(Theor.)**, **RT high(Theor.)**, **Synonyms**, **SMILES**, **InChI**, **InChI Key**, **Sigma-Aldrich**, **Cayman Chemical**, **Description**, **PubChem**, **ChEBI**, **BioCyc**, **Chapman Hall**, **NCBI**, **Uniprot**, **IUPAC**.
- Multiple synonyms can be entered into the **Synonyms** column when separated by a semicolon (;), for example, **L-Isoleucine; 2-Amino-3-methylvaleric acid**.
- All compounds are assumed to be represented in their neutral form, unless a value of **1** is entered in the *Cation* or *Anion* column.

Tips when importing compounds

- Review the import file format and column headers to make sure they conform to the expected format described in this section and in one of the example CSV files.
- If errors are found while importing a file, a log file consisting of the following name is created during import. The log file contains lines that were not correctly parsed and not imported: **<ImportFileName>-ImportLog.csv**, where **ImportFileName** is the original import file name. You can edit this file, make corrections, and then import the corrected file.
- The **Mass** is calculated from the formula, unless the difference between the mass calculated from the formula versus the mass indicated in the import file is > 0.0001 Da. Then the mass difference is greater than > 0.0001 Da, the compound is not imported into the PCDL but instead the **Mass** and **Formula** values are read from the input file added to the mass error log file: **<ImportFileName>-MassErrorsLog.csv**.

  The information in the log file can be used to determine the correct **Formula** or **Mass**. Typically errors occur when (1) the **Mass** value was the mass from the spectrum and not a neutral mass, or (2) the **Formula** contained an adduct (such as Cl^-).
- Special characters cause PCDL Manager to fail to import the compounds contained in a CSV file. This can sometimes arise when values are copied and pasted from Internet chemical database sources.

- If a compound name, or other data column containing an alphanumeric string, contains a comma, be sure to enclose the text containing a comma in double quotation marks as shown in the compound name **"1,3-bisphoglycerate"**.

  Many spreadsheet programs automatically enclose text with commas in quotes when saving a file in a **CSV** format. Open a saved **CSV** file in a text editor to view characters that may be hidden when viewed in a spreadsheet.

RT import

- For RT import, available in the **Import tab**, you must have at minimum one identifier (Agilent ID, Metlin ID, KEGG, CAS, Formula, Name, LMP, or HMP, ChemSpider) and a retention time.

CCS import

- For CCS import, available in the **Import tab**, you must have at minimum one identifier (Agilent ID, Metlin ID, KEGG, CAS, Formula, Name, LMP, or HMP, ChemSpider) and a CCS value, Ion Polarity, Ion Species, and Gas.

Example CSV files

Three example import file templates are provided in the **\MassHunter\PCDL\Import Files** folder. Use one of these three example files as a template when you manually create your own CSV file for import.

- **Compound_import.csv** - An example compound import file that can be used to import compounds using **File > Import Compounds** (**Import Compounds** dialog box).
- **CCS_import.csv** - An example collision cross section import file that can be used to import CCS values from the **Import tab**, **Imported CCS** tab.
- **RT_import.csv** - An example retention time import file that can be used to import RT values from the **Import tab**, **Imported RT** tab.

Add compounds manually to a PCDL

You can add compounds individually to any custom PCDL by enabling editing mode and entering the information directly in the **Compounds tab**.

1 Press the **F2** key, click  on the toolbar, or click **PCDL > Allow Editing** to enable editing, if editing is not already enabled.

When editing is enabled, a check mark ( ) appears next to the **PCDL > Allow Editing** menu option and an **Add** button and indication (Add) appears above the *Compounds Results* table in the **Compounds tab**.

2 Click **Add** to create a new compound row to the end of your PCDL (see Figure 19).

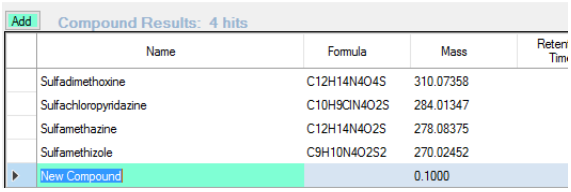

Figure 19 New compound added and ready for your data (shown added to the example PCDL Sulfas_AM_PCDL .cdb)

3 Click on the cells under the respective heading and type the information for the new compound.

When editing is enabled, a selected cell is highlighted in a distinct green color indicating that the value can be directly edited. You must tab through to the next cell that you wish to enter data, or press **Enter**, to save the value to the cell.

Append compounds to a PCDL

You use the following procedure to add the compounds selected in the *Compounds Results* table of your open PCDL to a saved PCDL. You can only append to a custom PCDL (a PCDL designated *User* in the **Master or User** field as described in "View PCDL information" on page 25).

1 View the compounds in the PCDL. Click **PCDL > Find Compounds**, click Find Compounds on the toolbar, or press **F5**, if necessary, to view the compounds in the PCDL. The compounds are listed in the *Compound Results* table.

2 Sort on any of the compound identifier columns or use the advanced searching functionality of the *Compound search criteria*, along with the *Must also contain* and *Must not contain* filters to find your compounds of interest (see "Find Compounds in your PCDL" on page 47).

3 Select the compounds you want to append to the saved PCDL.

To select a set of adjacent compound rows, click the first compound row, and then hold down the **Shift** key while you click on the last compound row.

To add additional compounds, adjacent or nonadjacent, to your selection, hold down the **Ctrl** key while you individually click additional compound rows.

You can use the scroll bar while holding down the **Ctrl** key to bring additional compounds into view within the *Compounds Results* table to add to your selection.

4 Right-click on any highlighted compound, and then click **Append to PCDL** as shown in Figure 20.

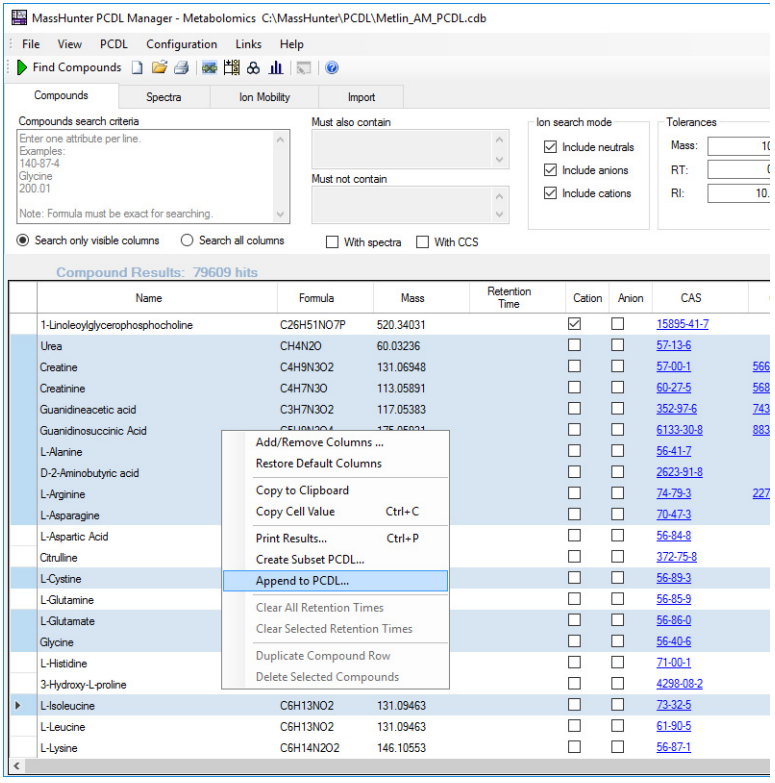

Figure 20 Append to PCDL

5 Click the select folder icon ... to open the **Browse for Folder** dialog box or skip to step 6 on page 38.

Alternatively, you can type the full PCDL path directly into the **Append to PCDL** dialog box (Figure 21).

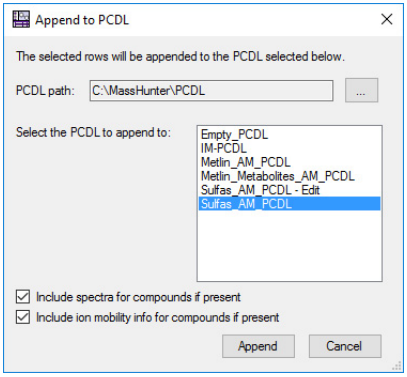

Figure 21 **Append to PCDL** dialog box

6 Select the PCDL that you want to append to from the list of PCDLs in **Select the PCDL to append to** (see Figure 21).

7 Mark **Include spectra for compounds if present** to include mass spectra for each compound when available.

8 Mark **Include ion mobility info for compounds if present** to include ion mobility data for each compound when available.

9 Click **Append** to add the compounds you highlighted to the selected PCDL (Figure 20 on page 37).

10 Click **Yes** in the **Compounds Appended** dialog box to open the PCDL that contains the appended compounds (see Figure 22 on page 39).

Click **No** to continue appending additional compounds to the same or another custom PCDL; repeat steps 1 through 7.

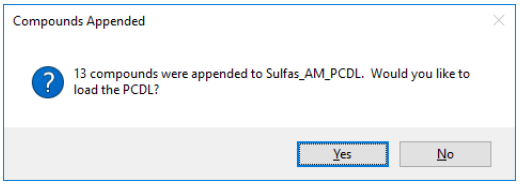

Figure 22 **Append to PCDL** dialog box

11 Review the custom PCDL that contains the appended compounds. In the default view of the *Compound Results* table, the appended compounds are found at the end of the table.

Create a subset PCDL

You use the following procedure to create a custom subset PCDL from the open PCDL. You can use a master PCDL or a custom PCDL as the starting template.

1 Click **File > Open PCDL**, click on the toolbar, or press **Ctrl+O** to open the **Open PCDL** dialog box.

2 Navigate to and click on the PCDL that contains the compounds you want to save as a subset PCDL.

3 Click **Open**.

4 View the compounds in the PCDL. Click **PCDL > Find Compounds**, click Find Compounds on the toolbar, or press **F5**, if necessary, to view the compounds in the PCDL. The compounds are listed in the *Compound Results* table.

5 Sort on any of the compound identifier columns or use the advanced searching functionality of the *Compound search criteria*, along with the *Must also contain* and *Must not contain* filters to find your compounds of interest (see "Find Compounds in your PCDL" on page 47).

6 Select the compounds you want to include in the subset PCDL.

To select a set of adjacent compound rows, click the first compound row, and then hold down the **Shift** key while you click on the last compound row.

To add additional compounds, adjacent or nonadjacent, to your selection, hold down the **Ctrl** key while you individually click additional compound rows.

You can use the scroll bar while holding down the **Ctrl** key to bring additional compounds into view within the *Compounds Results* table to be added to your selection.

7 Click **File > Create Subset PCDL** to open the **Create Subset PCDL** dialog box (see Figure 23).

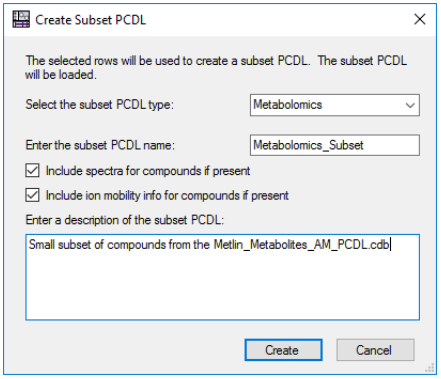

Figure 23 **Create Subset PCDL** dialog box

8 **Select the subset PCDL type** from the list of available types (see Figure 18 on page 31).

9 Type a name for the subset PCDL in **Enter the subset PCDL name**.

10 Mark **Include spectra for compounds if present** to include mass spectra for each compound when available.

11 Mark **Include ion mobility info for compounds if present** to include ion mobility data for each compound when available.

12 Type in a description for the subset PCDL in **Enter a description of the subset PCDL**.

13 Click **Create**.

The subset PCDL is created and a message is displayed that informs you of the subset PCDL file name and the number of compounds that were copied into the new subset PCDL.

14 Review the information presented in the **Subset PCDL Created** dialog box (see Figure 24).

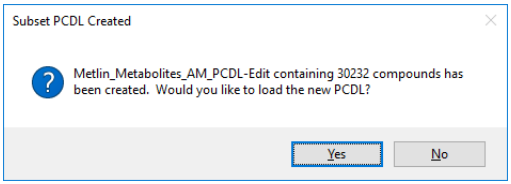

Figure 24 **Subset PCDL Created** dialog box

15 Click **Yes** to load the new subset PCDL into PCDL Manager.

Click **No** if you want to continue working with the current PCDL.

Edit a molecular structure

You use the following procedure to edit the molecular structure of a compound in your custom PCDL.

1 Select the compound of interest in the *Compound Results* table. Click any data cell in the same row of the compound of interest to select the compound.

2 Enable editing. Press the **F2** key, click on the toolbar, or click **PCDL > Allow Editing** to enable editing, if editing is not already enabled.

When editing is enabled, a check mark ( ) appears next to the **PCDL > Allow Editing** menu option and an **Add** button and indication (Add) appears above the *Compounds Results* table in the **Compounds tab**.

3 Open the **Molecular Viewer** dialog box (Figure 13 on page 27) in one of the following ways:

- **From the Menu bar:** Click **View > Molecular Viewer**.
- **From the Toolbar:** Click the **View Molecular Structure** icon located on the toolbar.
- **From the Action Pane:** Click the view **Molecule** icon , located in the **Advanced Search** part of the *Action Pane*.

4 Edit molecular structure information in either of the following ways:

- Click the **MOL Text** tab and paste MOL file text that you have copied from a molecular drawing tool (**Ctrl+V**, or right-click, and then click **Paste** from the shortcut menu), *or*
- Click load structures file icon  to open the **Open Structure File** dialog box to select a **MOL** file to load.

Both MOL and glycan structures are supported by PCDL Manager. If the structure attached to the currently selected compound is in the glycan format, then the glycan cartoon is displayed in the Structures tab. Right-click on a glycan drawing to change the display settings, such as **Show Linkage** and **Switch Direction**.

The **MOL Text** tab displays the text version of the molecular structure. If the current PCDL is a custom PCDL and 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 edit the structure of the selected compound. You can also click the **Load Structure from File**  button in the **Molecular Viewer** dialog box to load a structure from a Mol (**.mol**), an SDF (**.sdf**), a Keff Glycan (**.kcf**), a Linucs Glycan (**.linucs**), or a GlycoCT Condensed (**.glycoct_condensed**) file.

Note: If the new **MOL** file contains a structure with a different molecular formula from the value currently in the **Formula** box, a warning appears stating that the mass for the new molecular structure differs from the mass associated with the **Formula** box:

Click **Yes** to apply the new structure's formula and automatically update the **Formula** and **Mass** information boxes.

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

5 Click **Save** when you are satisfied with your changes to the molecular structure and notes.

Note: The content displayed in the **Notes** field in the **Molecular Viewer** dialog box is identical to the values in the compound *Description* column in the *Compound Results* table.

Edit mass spectra

You use one of the following procedures to edit mass spectra in your open PCDL. You can edit the molecular or precursor ion information, including ion species, precursor ion *m/z* and the MS Chemical Standard information. You can also remove noise peaks from raw experimental spectra such as spectra which were loaded from a **CEF** file.

> ***Note:*** The recommend procedure to add spectra to your PCDL is to use "Send Spectra to a PCDL from Qualitative Analysis" on page 66. The Qualitative Analysis workflow automatically adds the correct ion species and provides you with options to set the options to filter spectral noise, set a pass/fail base peak height filter, and correct the fragment ions to their theoretical accurate mass.

The following procedures allow you to edit spectra from within PCDL Manager.

Load a spectrum from a CEF file

This procedure loads spectra that have been exported to a **CEF** file from another program such as MassHunter Qualitative Analysis software.

1. Select the compound of interest in the *Compound Results* table. Click any data cell for the compound of interest to select the compound.
2. Enable editing. Press **F2**, click on the toolbar, or click **PCDL > Allow Editing** to enable editing, if editing is not already enabled.

   When editing is enabled, a check mark ( ) appears next to the **PCDL > Allow Editing** menu option and an **Add** button and indication (Add) appears above the *Compounds Results* table in the **Compounds tab**.
3. Open the **Spectra Viewer** dialog box (Figure 14 on page 28) in one of the following ways:
   - **From the Menu bar:** Click **View > Spectra Viewer**.
   - **From the Toolbar:** Click the **View Spectra** icon , located on the toolbar.

4 Click the load spectra icon to open the **Load Spectra** dialog box.

5 Navigate to and select the **CEF** file of interest.

6 Click **Open**. The available spectra in the **CEF** file are loaded.

If profile spectra or spectra which are not supported in PCDL Manager are contained in the file, a message is displayed saying that they have been skipped. Only centroided GC/MS and MS/MS spectra can be loaded for use in MassHunter PCDL Manager.

The spectra appear in the *Acquired spectra* table and can be compared to the library spectra in either a graphics or table format as shown in Figure 25.

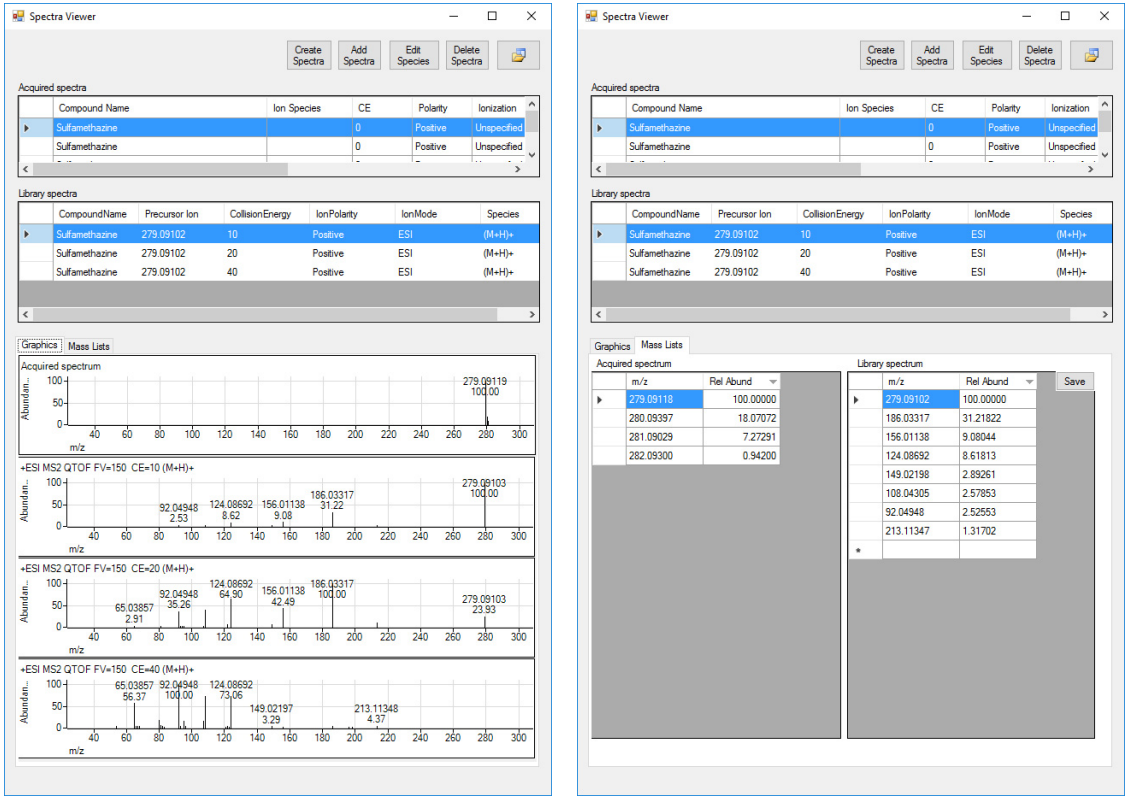

Figure 25 **Spectra Viewer** dialog box with acquired spectra imported from a CEF file: *Graphics* tab (left) and *Mass Lists* tab (right)

Add spectra to the compound

1 Click to select the spectrum of interest in the *Acquired Spectra* table. Use **Ctrl+click** or **Shift+click** select multiple spectra.

2 Click **Add Spectra**. The *Library spectra* table is refreshed to show the new list of spectra for the compound.

3 Click each spectrum and then click **Edit Species** to enter the revised or corrected information in the **Edit Species** dialog box (Figure 26).

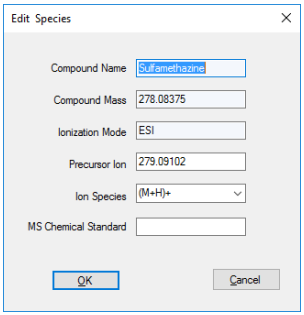

Figure 26 **Edit Species** dialog box

Delete spectra from the compound

1 Click to select the spectrum of interest in the *Library spectra* table. Use **Ctrl+click** or **Shift+click** select multiple spectra.

2 Click **Delete Spectra**. The *Library spectra* table is refreshed to show the revised list of spectra for the compound.

Move spectra between compounds

The following procedure moves spectra between compounds and can be performed within a single PCDL running on a single instance of PCDL Manager, or between two PCDLs running on two instances of PCDL Manager.

1 Click the compound to copy the spectra **from** in the *Compound Results* table, or the *Spectra for Compound* table.

   The spectra for the selected compound are listed in the *Spectra Results* table, and simultaneously listed and shown in the **Spectra Viewer** dialog box.

2 Click to select the spectra of interest in the *Library spectra* table in the **Spectra Viewer** dialog box, press **Ctrl+C** or right-click and then click **Copy Spectra** from the shortcut menu.

   Use **Ctrl-click** or **Shift-click** before copying if you want to select multiple spectra.

3 Press **Ctrl+V** in the *Acquired spectra* table, or right-click in the upper left cell of the table and then click **Paste Spectra** from the shortcut menu.

   The *Acquired spectra* table of interest can be from within the open PCDL or from a second instance of PCDL Manager that has different PCDL (**.cdb**) file open.

   The spectra are added to the *Acquired spectra* table.

4 Click to select the compound to copy the spectra **to** in the *Compound Results* table, or the *Spectra for Compound* table.

5 Click **Add Spectra** in the **Spectra Viewer** dialog box.

The *Library spectra* table is refreshed to show the revised list of spectra for the compound.

Find Compounds in your PCDL

Search for compounds in the PCDL using parameters you enter in the *Action Pane*. Search results are displayed in the *Compound Results* table in the *Compound Results Pane*. When editing is enabled, you can also edit the compound data directly in the *Compound Results* table.

Figure 3 on page 14 shows a view of the **Compounds tab** using the *Search Action Pane*. Figure 4 on page 15 shows a view of the **Compounds tab** using the *Advanced Search Action Pane*.

The following topics help you find compounds in your PCDL:

- "Prepare to find compounds" below
- "Enter search parameters" on page 48
- "Change how data is displayed in the results tables" on page 51
- "Print compound results" on page 52

Prepare to find compounds

1. Click **File > Open PCDL**, click  on the toolbar, or press **Ctrl+O** if the PCDL you want to search is not already open.
2. Click the **Compounds tab**.
3. Disable editing. Press **F2**, click  on the toolbar, or click **PCDL > Allow Editing** to disable editing, if editing is already enabled.

   When editing is enabled, a check mark () appears next to the **PCDL > Allow Editing** menu option and an **Add** button and indication () appears above the *Compounds Results* table in the **Compounds tab**.

Enter search parameters

1. Enter your search parameters in the *Action pane*. To return the contents of the entire PCDL, leave the search parameters

blank. See Figure 3 on page 14 for the **Search** *Action Pane*.

a **Compounds search criteria**

- Enter one search attribute per line; each line is combined as a logical **OR**. For example:
  140-87-4
  Glycine
  200.01
  C6H14N4O2
- When searching for a molecular formula, the formula must match an entry in the *Formula* column exactly. Partial molecular formulas are not matched during the search.
- Enter the first digits of the *CAS* number and include the hyphen. For example, to search for 551-92-8 enter **551-** in the search.
- When searching for *Mass*, *RT*, and *RI* values, include a decimal point in your value, for example:
  Mass: For mass 121, search for **121.12**, **121.123**, or **121.1234**
  RT: For a retention time of 10 minutes, search for **10.0**
  RI: For a retention index of 10, search for **10.0** or **10.00**

b *(Optional)* **Must also contain:** Enter criteria that must be found in each compound that matches an attribute in the **Compounds search criteria**. Enter one search attribute per line; each line is combined as a logical **OR**. If there are no entries in the **Compounds search criteria**, the **Must also contain** filter box is disabled.

c *(Optional)* **Must not contain**: Enter criteria that must not be found in any compound that matches an attribute in the **Compounds search criteria**. Enter one search attribute per line; each line is combined as a logical **OR**. If there are no entries in the **Compounds search criteria**, the **Must not contain** filter box is disabled.

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

- **Include neutrals** is typically marked. Clear the check box if you want to search anions and cations only.
- Mark **Include anions** if the data was acquired in *negative* ion mode and you want the search to include anions.

- Mark **Include cations** if the data was acquired in *positive* ion mode and you want the search to include cations.

  Note: All three modes are marked as default. Ensure to mark **Include anions** *or* **Include cations** if you also want to consider those chemicals that don't pick up or lose a proton to ionize.

e Enter applicable **Tolerances** for **Mass**, **RT**, and **RI**.

f Select whether the search includes only visible data columns (**Search only visible columns**) or all of the data columns, even if the column is not currently displayed in the *Compound Results* table (**Search all columns**).

Note: Searching all columns on a large PCDL may take a significant amount of time depending on the search parameters entered. METLIN is an example of a large PCDL.

g *(Optional)* Mark whether the search requires the compound to have spectra (**With spectra**) and/or a collision cross section value (**With CCS**).

2 *(Optional)* Click **Advanced Search** to enter more specific search criteria. Each of the criteria is combined as a logical **AND**. See Figure 4 on page 15 for the **Advanced Search** *Action Pane*.

a Select type of **Mass** (**[M+H]+**, **Neutral**, or **[M-H]-**)

- Select **[M+H]+** mass type if you are searching for an observed positive ion in the compound entries. The neutral mass value is automatically calculated, assuming the ion was a positive protonated ion. If **Include cations** is selected in Step 4d, the neutral mass of a cation is also calculated.
- Select **Neutral** mass type if the mass is the calculated neutral mass value, usually a value that was calculated by Molecular Feature Extraction (MFE). *Do not select this value for a mass observed in a spectrum.* Ions observed in a spectrum have a charge and need to be converted to neutral to work with the PCDL. For observed ions use either the **[M+H]+** or **[M-H]-** selection.

- Select **[M-H]-** mass type if you are searching for an observed negative ion in the compound entries. The neutral mass value is automatically calculated, assuming the ion was a negative deprotonated ion. If **Include anions** is selected in Step 4d, the neutral mass of an anion is also calculated.

3 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.
- 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.

4 If desired, enter search text for **Formula**, **Name**, **Notes**, **IUPAC**, and/or identifiers **CAS**, **ChemSpider**, **METLIN**, **KEGG**, **HMP**, and **LMP** to find compounds based on these chemical identifier fields. You can also enter text in the **Notes** field to search for a text string, such as “antidiabetic”. Your search text may include any special character typically used in a chemical name (hyphens, spaces, commas, single quote, or other specific characters).

5 Start the compound search in any of the following ways:

- Click Find Compounds on the toolbar,
- Click **PCDL > Find Compounds**, *or*
- Press the **F5** key.

6 View the search results in the *Compound Results* table. Data that match your search criteria are highlighted in a light yellow color, for example the column for a compound with an exact formula match appears as C6H14N4O2.

- Click on a compound in the *Compound Results* table to view its molecular structure information, when applicable, in the **Advanced Search** and the **Molecular Viewer** dialog box. See “View molecular structures” on page 26 for more information.

- Click on a compound in the *Compound Results* table to view its mass spectra, when applicable, in the **Spectra tab**, and the **Spectral Viewer** dialog box. See "View mass spectra" on page 27 for more information.
- Click on a compound in the *Compound Results* table to view its collision cross section, when applicable, in the **Ion Mobility tab**. See "Find Conformers in your PCDL" on page 58 for more information.
- See "Editing a PCDL" on page 30 for more information regarding editing your PCDL

Change how data is displayed in the results tables

The available changes described are applicable to any results table in PCDL Manager.

1. **Sort the table by the entries in a particular column:** Click the heading for the column of interest.
2. **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. **Resize a column to fit the information contained in the column:** Double-click on the right column divider in the heading of the column of interest.
4. **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. **Resize a column to fit the information:** Click **View > Autosize Columns**, or click  on the toolbar, to resize the widths of columns to the width of the widest content in any cell of the column.
6. **Change the columns of information displayed in the table:**
   a. Right-click the table and click **Add/Remove Columns** from the shortcut menu to open the **Add/Remove Columns** dialog box.
   b. Move the items of information that you want to display from the **Available columns** list to the **Show these**

columns list by clicking **Add ->** or by double-clicking on them.

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

d Click **OK** to save your changes. The results table is refreshed to reflect the selected columns of information.

e Click **View > Hide Empty Columns**, or click  on the toolbar, to automatically hide columns that do not have any content. The results table is refreshed to reflect the selected columns of information.

f Right-click anywhere in a table, and then click **Restore Default Columns** in the shortcut menu to automatically restore the default setting for the table view. The results table is refreshed to reflect the selected columns of information.

Print compound results

If you want to print only certain compounds, first highlight those rows in the *Compound Results* table:

To select a set of adjacent compound rows, click the first compound row, and then hold down the **Shift** key while you click on the last compound row.

To add additional compounds, adjacent or nonadjacent, to your selection, hold down the **Ctrl** key while you individually click additional compound rows.

You can use the scroll bar while holding down the **Ctrl** key to bring additional compounds into view within the *Compounds Results* table to be added to your selection.

1 Open the **Print Results** dialog box in one of several ways:

- **From the Menu bar:** Click **File > Print Results**.
- **From the Toolbar:** Click the **Print Results** icon  located on the toolbar.
- **From the *Compound Results* table:** Right-click and then click **Print Results**, or press **Ctrl+P**.

2 Select the desired **Report destination** options from the following:

- **Printer** - Choose from your PCs default system printers.
- **Print Preview** - Mark if you want to view the report in the **Print Preview** dialog box before sending the report to your selected **Printer**.
- **Fit to page** to size the report to fit the height and width of the page.
- **Orientation** (**Landscape** or **Portrait**). The default is Landscape; it allows more columns of information.

3 Select the desired **Report contents** options from the following:

- Select **All rows** or **Only highlighted rows** of the *Compounds Results* table
- Mark whether to **Print structures** and the size (**240 x 160**, **360 x 240**, or **540 x 360**)
- Mark whether print the report in a summary format, **Print in Summary Format**.

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

If you clear the **Print in Summary Format** check box, then up to the first 30 Agilent created compounds selected are printed with all of the columns displayed in the *Compound Results* table.

If you mark the **Print in Summary Format** check box, then all compounds selected, or all compounds, are printed with enough information to unambiguously identify the compound. The compounds are printed in the following summary format:

For compounds created by Agilent (compounds that have either an **Agilent** or **METLIN ID**), the following values are printed:

Compound Name

Formula

Mass

RT

RT Modified

Agilent ID

One of the following external chemical identifiers are printed using the following priority list:

CAS registry number - if this value is empty then go to

Chemspider ID - if this value is also empty then go to

IUPAC Name

METLIN ID

Date Modified

For user created compounds, the values listed above are printed, with the following exceptions:

The **Agilent ID** and **METLIN ID** values are not included since these identifiers are blank in user created compound entries.

5 Click  on the toolbar to print from the **Print Preview.**

Find Spectra in your PCDL

The following topics help you find spectra in your PCDL:

- "Prepare to find spectra" below
- "Enter search parameters" below
- "Clean up noisy spectra" on page 56

Prepare to find spectra

1 Click **File > Open PCDL**, or click on the toolbar, if the PCDL you want to search is not already open.

2 Click the **Spectra tab**.

3 Disable editing. Press **F2**, click on the toolbar, or click **PCDL > Allow Editing** to disable editing, if editing is already enabled.

When editing is enabled, a check mark ( ) appears next to the **PCDL > Allow Editing** menu option and an **Add** button and indication (Add) appears above the *Compounds Results* table in the **Compounds tab.**

Enter search parameters

1 Enter your search parameters in the *Action pane*. To return the contents of the entire PCDL with compounds which contain spectra leave the search parameters blank. See Figure 5 on page 16 for the **Spectra tab** *Action Pane*.

a Spectra search criteria

Enter one search attribute per line. Only the *Compound Name*, *Ion Species*, and *MS Chemical Std* columns are searched for text that you enter; each line is combined as a logical **OR**. For example:
Glycine
(M+H)+

b *(Optional)* Select values for the **Additional search parameters**: **Ion polarity**, **Ionization mode**, **Precursor**

ion species, and **Instrument type**. Each parameter line is combined as a logical **AND** to the **Spectra search criteria**.

c *(Optional)* Enter values for the **Mass** section: **Precursor ion** and **Tolerance**.

d *(Optional)* Enter values for the **Collision energy** section: collision energy and **Tolerance** in volts.

2 Start the spectra search in any of the following ways:

- Click Find Spectra on the toolbar,
- Click **PCDL > Find Spectra**, *or*
- Press the **F5** key.

3 Open the **Spectra Viewer** dialog box (Figure 14 on page 28) in one of the following ways:

- **From the Menu bar:** Click **View > Spectra Viewer**.
- **From the Toolbar:** Click the **View Spectra** icon , located on the toolbar.

4 View the search results in the *Spectra for compound* tables in the **Spectra tab** and the corresponding spectra in the **Spectra Viewer** dialog box. Data that match your search criteria are highlighted in a light yellow color in the *Spectral results pane* (upper table) which is labeled **Spectra for compound: <highlighted compound name>**.

5 Click on a compound in the *Compound results pane* (lower table in the **Spectra tab**) to refresh the spectra list for the highlighted compound in the *Spectral results pane* (upper table).

6 See "View mass spectra" on page 27 and "Edit mass spectra" on page 43 for more information.

Clean up noisy spectra

Use this procedure to remove small noise peaks from spectra in a user (custom) PCDL. Using the **Send Spectra to PCDL** feature in MassHunter Qualitative Analysis Workflows eliminates the need for this step. Qualitative Analysis Workflows automatically

sets the correct ion species and provides options for filtering spectral noise, setting a pass/fail base peak height filter, and correcting the fragment ions to their theoretical accurate mass.

1. Click **PCDL > Allow Editing**, click  on the toolbar, or press **F2** to enable editing of the open PCDL.
2. Open the **Spectra Viewer** dialog box in one of several ways:
   - **From the Menu bar:** Click **View > Spectra Viewer**.
   - **From the Toolbar:** Click the **View Spectra** icon  .
3. Select the spectrum of interest from the *Library spectra* table.
4. Click the **Mass Lists** tab. 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.
5. Click on a row in the **Library masses** list to select a mass to delete. Use **Ctrl-click** or **Shift-click** to select multiple rows.
6. Press **Delete** on the keyboard.
7. Click **Save** to update the selected library compound with modified (cleaned) spectra.

Find Conformers in your PCDL

The following topics help you find conformers in your PCDL. A conformer is an isomer of a molecule that differs from another isomer by the rotation of a single bond in the molecule. Conformers can be resolved with the addition of ion mobility data.

Prepare to find conformers

1. Click **File > Open PCDL**, click  on the toolbar, or press **Ctrl+O**, if the PCDL you want to search is not already open.
2. Click the **Ion Mobility tab**.
3. Disable editing. Press **F2**, click  on the toolbar, or click **PCDL > Allow Editing** to disable editing, if editing is already enabled.

   When editing is enabled, a check mark () appears next to the **PCDL > Allow Editing** menu option and an **Add** button and indication () appears above the *Compounds Results* table in the **Compounds tab.**

Enter search parameters

1. Enter your search parameters in the *Action pane*. To return the contents of the entire PCDL with compounds which contain collision cross section values leave the search parameters blank. See Figure 7 on page 18 for the **Ion Mobility tab** *Action Pane*.

   a. **Ion Mobility search criteria**

      Enter one search attribute per line. Only the *Ion Species*, *CCS column*, *Description*, *CCS Chemical Std*, and *Notes* columns are searched for text or numbers that you enter here. Each line is combined as a logical **OR**.

   b. *(Optional)* Select values for the **Additional search parameters**: **Ion polarity**, **Gas**, and **Ion species**. Each

parameter line is combined as a logical **AND** to the **Ion Mobility search criteria**.

c *(Optional)* Enter values for the **Tolerance** section: **CCS** value.

2 Start the conformer search in any of the following ways:

- Click Find Conformers on the toolbar,
- Click **PCDL > Find Conformers**, *or*
- Press the **F5** key.

3 Click on a compound in the lower table to refresh the ion mobility list for the highlighted compound in the upper table.

4 View the search results in the *Ion Mobility information for compound* tables. Data that match your search criteria are highlighted in a light yellow color in the *Ion Mobility Results* table (upper table).

Import RT and CCS Values

Importing works on the current dataset shown in the **Compounds tab**. For example, if you searched and found a subset of the compounds in the PCDL, then when you try to import values, the import is restricted to the compounds in the *Compound Results* table. To match the entire PCDL, first find compounds in the **Compounds tab** with all of the search criteria cleared.

The following topics help you import RT and CCS values into your PCDL:

Prepare to import

1. Click **File > Open PCDL**, click  on the toolbar, or press **Ctrl+O**, if the PCDL you want to search is not already open.
2. Find the compounds you want to be part of the import ("Find Compounds in your PCDL" on page 47). From the **Compounds tab**, find your compounds in any of the following ways:
   - Click  on the toolbar,
   - Click **PCDL > Find Compounds**, *or*
   - Press the **F5** key.
3. Review the compounds shown in the *Compound Results* table on the **Compounds tab**.
4. Click the **Import tab**.
5. Disable editing. Press **F2**, click  on the toolbar, or click **PCDL > Allow Editing** to disable editing, if editing is already enabled.

When editing is enabled, a check mark ( ) appears next to the **PCDL > Allow Editing** menu option and an **Add** button and indication (Add) appears above the *Compounds Results* table in the **Compounds tab.**

6 Click either the **Imported RT** tab or the **Imported CCS** tab and proceed to the section that covers the data you are importing, RT or CCS values.

RT CSV files

You can manually create an RT import file by copying and editing the provided example retention time import file. The template is located in the **\MassHunter\PCDL\Import Files** folder:

RT_import.csv - An example retention time import file that can be used to prepare the **CSV** file according to the correct format to import RT values from the **Import tab**, **Imported RT** tab.

You can also import retention times from compound results files exported directly from MassHunter Qualitative Analysis Workflows. Perform the following steps within MassHunter Qualitative Analysis Workflows:

1 Identify the compounds of interest in your PCDL using MassHunter Qualitative Analysis Workflows. For example, use Find by Formula or Library/DB Search to identify your compounds.

2 Export the compound results. Right-click in the *Compound List* table and then click **Export** as shown in Figure 27 on page 62. Use the default settings in the **Export** dialog box to export a CSV file which you can use for RT import.

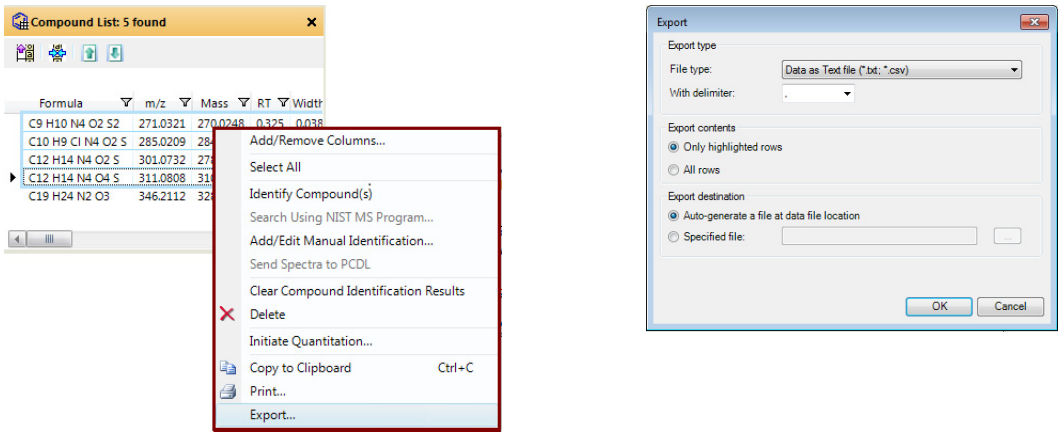

Figure 27 Shortcut menu from the *Compound List* table (left) and **Export** dialog box (right) in MassHunter Qualitative Analysis Workflows

Import RT User Interface

Browse button ... Opens the **Open Import List** dialog box.

Clear existing database RTs Clears any retention times from the compounds in the PCDL.

Generate Error Log Generates a log file that is saved in the **\MassHunter\PCDL\Import Files** folder.

Matched Compounds list The first list (left) contains the compounds from the PCDL that were matched to your imported file.

The second list (right) shows you the difference between the retention time in the PCDL and the retention time in the imported file. This list contains all of the matches from the PCDL with the current compound in the first list. Mark the *Best* match when there is more than one match to the compound.

You can also clear all *Best* matches and choose not to import a RT for certain *Matched Compounds*. This feature is useful when you have used a compound results file from MassHunter Qualitative Analysis as the input file, and you do not wish to update the RTs for all of compounds contained in this file.

Note: The following two buttons are at the bottom of the **Import tab**; you may need to adjust your main window size to view these buttons.

Export RT matches Creates an export file that contains a list of the matched compounds.

Import RT Updates the retention times in the *Compound Results* table for all of the compounds in the first (left) *Matched Compounds* list.

CCS CSV files

You can manually create a CCS import file by copying and editing the provided example collision cross section import file. The template is located in the **\MassHunter\PCDL\Import Files** folder:

CCS_import.csv - An example collision cross section import file that can be used to import CCS values from the **Import tab**, **Imported CCS** tab.

Import CCS User Interface

Browse button ... Opens the **Open Import List** dialog box.

CCS tolerance The tolerance value to use when adding the CCS information to the PCDL.

The CCS tolerance is a tool used to prevent duplicate conformers being added to a compound. Duplicate CCS values may not have exactly the same CCS values as the current conformers, but are essentially duplicates of current conformers within the instrument resolution.

If the CCS values are without the tolerance percentage given from the current value in the PCDL, then the CCS values are added as additional conformers. If the CCS values are within the tolerance percentage, then the blue highlighted *Import* check box in the *CCS Matches* list is cleared by default, generating a conflict in the *Matched Compounds* list. If you want to also import these values as additional conformers, then mark the appropriate *Import* check boxes in the *CCS Matches* list.

Click **Generate Error Log** to generate a log file containing a record of the unmatched compounds which were not imported and compounds which registered as multiple matches which were imported as individual conformers. You can use this information to curate your CCS entries.

Clear Existing IM Information Clears any ion mobility information from the compounds in the PCDL.

Generate Error Log Generates a log file that is saved in the **\MassHunter\PCDL\Import Files** folder.

This file contains unmatched compounds which were not imported and compounds which registered as multiple matches which were imported as individual conformers

Matched Compounds table The left table in the **Imported CCS** tab in the **Import tab** (Figure 28 on page 65). The *Matched Compounds* table contains the compounds from the PCDL that were matched when you selected the import file.

CCS Matches table The right table in the **Imported CCS** tab in the **Import tab** (Figure 28 on page 65). The *CCS Matches* table shows you the difference between the CCS values in the PCDL if available and the CCS values in the import file. If the difference is below the CCS tolerance, then a conflict is shown in the *Matched Compounds* list, and the blue highlighted *Import* check box is cleared so that additional conformers which are duplicates are not created upon import. You can choose to mark the *Import* check box and import it as an additional conformer. Multiple matches are noted in the error log.

If the difference between the CCS values are more than the CCS tolerance, then the CCS values are added as additional conformers.

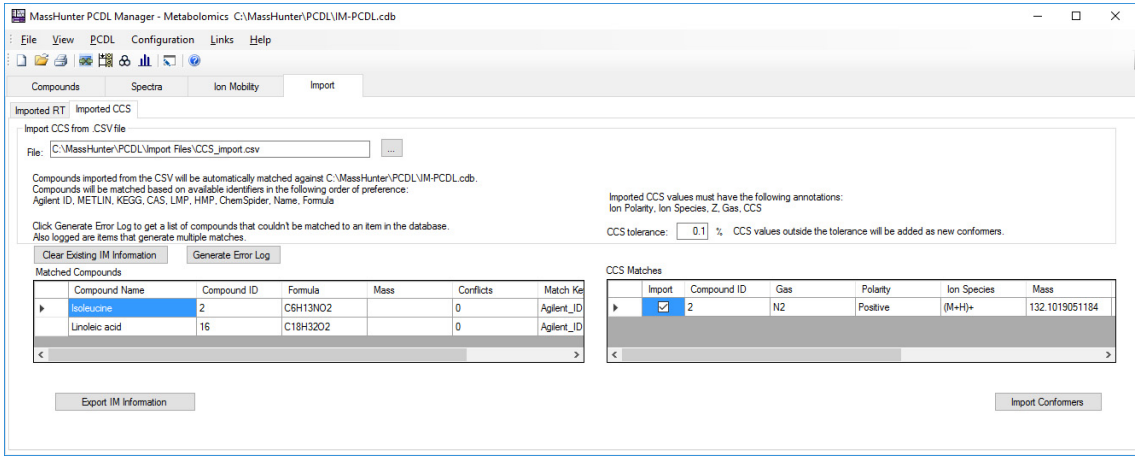

Figure 28 The **Import tab** in PCDL Manager, **Imported CCS** tab

Note: The following two buttons are at the bottom of the **Import tab**; you may need to adjust your main window size to view these buttons.

Export IM Information Creates an export file that contains a list of the matched compounds.

Import Conformers Adds the information in the *Compound Results* table for all of the compounds in the *Matched Compounds* list which have the *Import* check box marked in the *CCS Matches* table. CCS data is not updated or overwritten within the **Import tab**.

Send Spectra to a PCDL from Qualitative Analysis

You can use the following procedures to send spectra of identified compounds from MassHunter Qualitative Analysis to PCDL Manager. The following procedures are performed in the Qualitative Analysis software.

- "Send spectra from Qualitative Analysis Workflows"
- "Send spectra from Qualitative Analysis Navigator" on page 68
- "Options to send theoretically mass corrected spectra to a PCDL" on page 69

Note: Use the *Find by Formula* algorithm to identify compounds for sending spectra to a PCDL. Fragment annotations, needed for sending theoretically corrected spectra, are not currently supported by Database search.

For MS/MS spectra creation: In order to obtain the best scoring, it is highly recommend that you only select the lowest monoisotopic *m/z* ion as the precursor ion in MS/MS library acquisition, the use of higher isotope precursor *m/z* ions is not currently supported in PCDL Manager related workflows. In order to ensure that higher isotope *m/z* ions do not interfere with the lowest monoisotopic precursor ion fragmentation pattern the quadrupole resolution during acquisition must be set to narrow in order to ensure the best possible match to the MS/MS fragmentation library when you have complex mixtures.

Send spectra from Qualitative Analysis Workflows

1. Launch MassHunter Qualitative Analysis Workflows.
2. Open an MS/MS or GC/MS data file.
3. Create the spectrum that you want to send to a PCDL. See "Extract spectra in Qualitative Analysis Workflows" on page 71.

Note: When you use a large PCDL, such as METLIN, as the **Formula source** for identification, multiple hits for each compound are expected and require manual sorting to identify the correct compound.

4 Select all of the compounds that you want to send to PCDL in the *Compound List* window.

5 Open the **Send Spectra to PCDL** dialog box by performing one of the following actions:

Right-click the selected compounds in the *Compound List* window, and then click **Send Spectra to PCDL**, or right-click the selected spectra in the *Compound Fragment Spectrum Results* window, and then click **Send Spectra to PCDL**.

6 Select the **Library path**. The spectra are added to the selected PCDL

7 *(Optional)* Mark **Minimum base peak height** if you want to enter the minimum base peak counts that are needed to add the spectrum to the library. A default value of 1000 counts is recommended. You can change this value as necessary to achieve your desired results. This option allows you to set a pass/fail criteria based on base peak height to ensure good ion statistics in the spectral library.

8 Click one of the **Annotation filter** options. You can click either **Formula annotated peaks (excludes unknowns) if present else all peaks** or **All peaks**. When **Formula annotated peaks (excludes unknowns) if present else all peaks** is selected, the program checks that the *m/z* fragment ions observed are consistent with the assigned precursor ion species (for MS/MS spectra) or molecular ion species (GC/MS spectra) and assigns the fragment ion species as an annotation above each fragment ion peak.

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

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

Note: If profile or spectra which are not supported in PCDL Manager are contained in the file, a message is displayed stating that spectra have been skipped. Only identified, centroided MS/MS and GC/MS spectra are loaded for use in PCDL Manager.

11 The spectra can be viewed in the **Spectra Viewer** dialog box in PCDL Manager.

Send spectra from Qualitative Analysis Navigator

1 Launch MassHunter Qualitative Analysis Navigator.

2 Open a GC/MS data file. You should only send GC/MS spectra from the Qualitative Analysis Navigator.

3 Create the spectrum that you want to send to a PCDL. See "Extract spectra in Qualitative Analysis Navigator" on page 75.

4 Select all of the spectra that you want to send to PCDL in the *MS Spectrum Results* window.

5 Right-click the selected spectra in the *MS Spectrum Results* window, and then click **Send Spectra to PCDL** to open the **Send Spectra to PCDL** dialog box.

6 Select the **Library path**. The spectra are added to the selected PCDL

7 *(Optional)* Mark **Minimum base peak height** if you want to enter the minimum base peak counts that are needed to add the spectrum to the library. A default value of 1000 counts is recommended. You can change this value as necessary to achieve your desired results. This option allows you to set a pass/fail criteria based on base peak height to ensure good ion statistics in the spectral library.

8 Click one of the **Annotation filter** options. You can click either **Formula annotated peaks (excludes unknowns) if present else all peaks** or **All peaks**. When **Formula annotated peaks (excludes unknowns) if present else all peaks** is selected, the program checks that the *m/z* fragment ions observed are consistent with the assigned precursor ion species (for MS/MS spectra) or molecular ion species (GC/MS spectra) and assigns the fragment ion species as an annotation above each fragment ion peak.

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

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

Note: If profile or spectra which are not supported in PCDL Manager are contained in the file, a message is displayed stating that spectra have been skipped. Only identified, centroided MS/MS and GC/MS spectra are loaded for use in PCDL Manager.

11 The spectra can be viewed from the **Spectra tab**.

Options to send theoretically mass corrected spectra to a PCDL

The following options should be selected to send theoretically mass corrected spectra to a PCDL:

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

Before sending the spectra to the PCDL, manually inspect each spectrum and ensure that all peaks have been annotated. Annotated peaks are green and have the formula annotated above each peak. You may need to expand the x-axis to view the annotation.

Any un-annotated peaks indicate the following:

1 An impurity ion in the chemical standard which cannot be present according to the assigned precursor ion species (for MS/MS spectra) or molecular ion species (GC/MS spectra) empirical formula.

2 A background ion in the GC/MS spectra.

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

4 An unsupported workflow has been used for fragment annotation.

- Only Find by formula fragment annotation is supported for the **Send Spectra to PCDL** function for MS/MS spectra.
- Manual identification and annotation is recommended for GC/MS spectra.

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

Extract Spectra for a PCDL in Qualitative Analysis

This topic describes how to extract spectra using MassHunter Qualitative Analysis so you can send the spectra to a PCDL.

Extract spectra in Qualitative Analysis Workflows

1. Launch MassHunter Qualitative Analysis Workflows.
2. In the method editor, review the *Target/Suspect Screening* > *Find by Fragments* section to extract GC/MS spectra or the *Target/Suspect Screening* > *Find by Formula* section to extract MS/MS spectra and identify compounds.
   a. Click the *Target/Suspect Screening* > *Find by Fragments* tab (for GC/MS) or the *Target/Suspect Screening* > *Find by Formula* tab (for MS/MS) in the Method Editor window.
   b. Click the *Target Source* tab and select a PCDL that contains the compounds of interest.

   Note: When you use a large PCDL, such as METLIN, as the **Formula source** for identification, multiple hits for each compound are expected and require manual sorting to identify the correct compound.
3. Setup **Generate Formulas** parameters:

   ### Assign correct possible ion species

   a. In the Method Editor window, click the *Compound Identification* > *Generate Formulas* section.
   b. Click the *Allowed Species* tab.
   c. Mark all desired ion species under **Charge carrier to be assumed if not known**.
   d. Verify the appropriate elements and limits are set under **Elements and Limits**.

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

Add fragment annotation

a For GC/MS spectra click the *Find by Fragments* > *Fragment Annotation* tab. For MS/MS spectra click the *Find by Formula* > *Fragment Annotation* tab.

Note: If the *Find by Fragments* > *Fragment Annotation* tab is not visible, click **Configuration > Show Advanced Settings** and then click the *Find by Fragments* > *Fragment Annotation* tab.

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

Note: When **Annotate fragment spectrum peaks with formulas** is marked in the *Target Screening* workflow in Qualitative Analysis Workflows, observed *m/z* fragment ions are compared to the assigned precursor, or molecular ion species, for consistency. The fragmented ion species is assigned as an annotation above each fragment ion peak.

Note: When using **Find by Formula** for MS/MS spectra, it is highly recommended to mark **Annotate fragment spectrum peaks with formulas**. This allows you to send theoretically corrected mass spectra to your PCDL.

When using **Find by Fragments** with **Annotate fragment spectrum peaks with formulas** marked, GC/MS ions which have been automatically annotated as an allowed fragment ion, based on the molecular ion formula, must be rigorously inspected to ensure background ions, such as column bleed, which also correspond to an allowed fragment ion formula are not sent to the PCDL.

Set spectral noise filters for GC/MS spectra

a Click the *Find by Fragments* > *Fragment Annotation* tab.

b Mark **Absolute height** and type `50` for the **counts**.

c Clear the **Relative height** check box.

Set spectral noise filters for MS/MS spectra

a Click the *Find by Formula* > *Fragment Annotation* tab.

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

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

Note for spectral noise filters for both GC/MS and MS/MS

Note: The spectral noise filters can be adjusted to achieve desired results.

Note for spectral noise filters for both GC/MS and MS/MS

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

4 Click **Find > Find by Fragments** (for GC/MS spectra) or **Find > Find by Formula** (for MS/MS spectra) to run the algorithm.

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

6 *(Optional)* Click a compound in the *Compound List* window. Right-click the compound and then click **Add/Edit Manual Identification**. You can enter a **Formula**, **Charge**, **Ion Species**, **CAS ID**, **KEGG ID**, **UniProt ID**, **LMP ID**, and **HMP ID** in the dialog box. You can also add **Notes** and load a structure.

7 *(Optional)* Click a compound in the *Compound List* window. Right-click the *Compound Fragment Spectrum Results* window (for MS/MS spectra) or the *Compound MS Spectrum Results* window (for GC/MS spectra), and then click **Adjust Peak Threshold**. You can change the threshold to label a peak.

Annotated peaks are green and have the formula annotated above each peak. You may need to expand the x-axis to view the annotation. In the case when the spectrum itself is green, right-click either the *Compound MS Spectrum Results* window or the *Compound Fragment Spectrum Results* window, and then click **Choose Defined Color** and choose a different color.

Any un-annotated peaks indicate the following:

a An impurity ion in the chemical standard which cannot be present according to the assigned precursor ion species

(for MS/MS spectra) or molecular ion species (for GC/MS spectra) empirical formula.

b A background ion in GC/MS spectra.

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

d An unsupported workflow has been used for fragment annotation.

- Only Find by Formula fragment annotation is supported for the **Send Spectra to PCDL** function for MS/MS spectra.
- Manual identification and annotation is recommended for GC/MS spectra.

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

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

Extract spectra in Qualitative Analysis Navigator

1. Launch MassHunter Qualitative Analysis Navigator.
2. Extract an EIC of your compound of interest.
   a. Click **Chromatograms > Extract Chromatograms**.
   b. Set **Type** to **EIC**.
   c. Mark the **Integrate when extracted** check box.
   d. Set the **m/z value(s)** to your compound of interest.
   e. Click the *Advanced* tab.
   f. Select **Symmetric (m/z)** and type `+/- 0.5` for GC/MS spectra.
   g. Click **OK**.
3. *(Optional)* Extract a background spectrum. Select a range before and after the peak in the *Chromatogram Results* window. Right-click the window and then click **Extract Spectrum to Background**.
4. *(Optional)* Modify the method to subtract the background spectrum when you manually extract a spectrum. In the *Method Editor* window, click **Spectra > Extract (MS)**. On the *Manual Extraction* tab, select **Current background spectrum**.
5. Extract a spectrum from the EIC in the *Chromatogram Results* window. Select a region in the EIC near the peak. Right-click and then click **Extract MS Spectrum**. You can instead double-click the selected region.
6. Right-click the spectrum and then click **Find Spectrum Peaks**.
7. Right-click the spectrum and then click **Add/Edit Manual Identification**. You can add or edit the **Compound name**, **Formula**, **Charge**, **Ion Species**, **CAS ID**, **Notes, Structure**, and other identifiers in the **Add/Edit Manual Identification** dialog box.
8. *(Optional)* Right-click the spectrum and then click **Edit Peak Annotations**. You can change the **Species**, **Formula**, and **Ion Type** for peaks in the spectrum.

Note: If **Edit Peak Annotations** is not available, click **Configuration > Show Advanced Settings**, and then right-click the spectrum and then click **Edit Peak Annotations**.

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

PCDL Manager Installation

Install PCDL Manager B.08.00

PCDL Manager is installed from a Setup Wizard, which you run from the main installation program. You can install this version of PCDL Manager concurrent with a prior version.

- Double-click **PCDLSetup.exe**, or right-click **PCDLSetup.exe**, and then click **Run as administrator**.

PCDL Manager is installed along with the following example PCDL:

Sulfas_AM_PCDL.cdb - a small example custom PCDL containing four compounds with spectra that can be used to become familiar with PCDL Manager and to create your own custom PCDL.

Uninstall a prior copy of PCDL Manager

Since this version of PCDL Manager provides tools for you to convert PCDLs created using prior versions of PCDL manager, maintaining a prior version of PCDL Manager is optional. You can remove an older version of PCDL Manager using **Programs and Features** found on your PC.

1. Click **Start > Control Panel** on a PC running Windows 7, or click **Start > All apps > Windows System > Control Panel** on a PC running Windows 10.
2. Click **Programs and Features**.
3. Click **Agilent MassHunter PCDL Manager Software**.
4. Click **Uninstall/Change** to uninstall PCDL Manager.

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In this Book

The *Agilent G3336 MassHunter Personal Compound Database and Library Manager Software - Quick Start Guide* describes how to install and use the PCDL Manager Software. The familiarization exercises included in this guide help you get started with using the software.

This *Quick Start Guide* applies to MassHunter PCDL Manager B.08.00 and later, until superseded.

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