Agilent G6855AA MassHunter Personal Forensic Toxicology Database

Quick Start Guide

This guide describes how to install and use MassHunter Personal Forensic Toxicology Database.

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Where to find more information

Use the online help for in-depth information not given in this *Quick Start Guide*. Display online help in either of the following ways:

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

Agilent Technologies

What is Personal Forensic Toxicology Database software?

MassHunter Personal Forensic Toxicology Database provides tools to access a forensic database for compound searches based on LC/MS data.

Personal Forensic Toxicology Database software allows you to:

- Do automated searches on multiple compounds, which saves time.
- Do private, on-site searches, which keeps intellectual property safe.
- Customize the database by adding proprietary compounds.
- Customize the database by adding retention times to compounds in the database.
- Search a database using mass only, mass and optional retention time, or mass and retention time required. The use of retention time increases the compound identification specificity.
- Search on text.
- Search on empirical formula.
- Search on retention time.
- Do automated or manual searches from Agilent MassHunter Workstation Software–Qualitative Analysis program. See page 11.
- Link to websites for more information on many compounds.

Personal Forensic Toxicology Database software supports mass lists output from Agilent MassHunter Mass Profiler, GeneSpring MS, and Qualitative Analysis software.

Compound names in the database

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

Installation

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

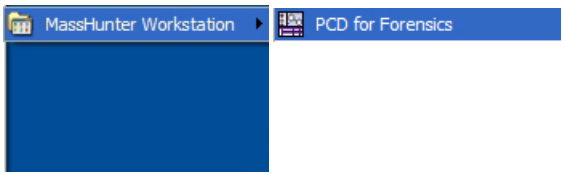
1. Insert the CD-ROM labeled Agilent G6855AA into the CDROM drive.
2. Click the Windows **Start** button and select **Run**.
3. Type **x:\setup**, where **x** is the letter of the CDROM drive, and click **OK**.
4. Follow the instructions on the screen to install the software.

To uninstall the software

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

Startup

Select **Programs > Agilent > MassHunter Workstation > PCD for Forensics** from the Windows Start menu, as shown below, to start the MassHunter Personal Forensic Toxicology Database software.



Main Window

The MassHunter Personal Forensic Toxicology Database main window has the following areas and controls.

- "Toolbar"(below)
- "Menus" (below)
- "Tabs" on page 7
- "Search Results Table" on page 8
- "Structures" on page 9

Toolbar

The following items are available on the MassHunter Personal Forensic Toxicology Database toolbar:

Button	Equivalent Menu Item
	Database > Find Compounds
	File > Print Results
	File > Export Results
	File > New Database
	File > Open Database
	Help > Contents

Menus

The following menus are available in MassHunter Personal Forensic Toxicology Database software:

- "File menu" on page 5
- "Edit menu" on page 5
- "View menu" on page 6
- "Database menu" on page 6
- "Links menu" on page 6
- "Help menu" on page 7

File menu

New Database Allows you to create a subset of the master Forensic database or to create a custom database that can be edited and personalized for your lab. This is done by creating a copy of an existing database with a new name.

Open Database Allows you to open a different database.

Backup Database Allows you to copy the database for archive purposes.

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

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

Print Results Allows you to print search results and structures.

Exit Closes the Personal Forensic Toxicology Database software window.

Edit menu

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

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

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

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

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

View menu

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

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

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

Database menu

Find Compounds Searches the database for compounds that match criteria specified on the Single Search tab or Batch Search tab. Compounds that match the search criteria are displayed in the Search Results table at the bottom of the window.

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

Database Information Allows you to view information about the current database and edit the description for custom databases with editing enabled.

Links menu

Allows you to access the following websites for information on compounds:

- PubChem (National Center for Biotechnology Information)
- Chem Industry
- TOXNET
- ChemBioFinder
- NIST Chemistry WebBook (National Institute of Standards and Technology)
- IPCS INTOX Databank (International Program on Chemical Safety)
- SOFT (Society of Forensic Toxicologists)

- TIAFT (The International Association of Forensic Toxicologists)
- AAFS (American Academy of Forensic Sciences)
- Related Forensics Websites

Help menu

Contents, Index, and Search Opens the online help window for Personal Forensic Toxicology Database software, with the appropriate tab displayed.

View EULA Displays the license agreement for Personal Forensic Toxicology Database software in a Notepad window.

About Displays the version and build number of the Personal Forensic Toxicology Database software.

Tabs

Single Search tab

Allows you to search for compounds in the database. The search is started by clicking the **Find Compounds** button on the toolbar, selecting **Find Compounds** from the Database menu, or pressing the **F5** key. Search results are displayed in the Results table in the lower part of the window. See "To find compounds" on page 13.

Batch Search tab

Allows you to search for compounds in the database by specifying a mass list and optional retention times. The search is started by clicking the **Find Compounds** button on the toolbar, selecting **Find Compounds** from the Database menu, or pressing the **F5** key. Search results are displayed in the Results table in the lower part of the window. See "To find compounds from a mass list" on page 17.

Batch Summary tab

Shows a summary view of all Best fit hits from a Batch Search. Results can be exported for use with other applications. You can also add comments and update retention times for custom databases with editing enabled. See "To view batch summary results" on page 20.

Edit Compounds tab

For custom databases that allow editing, you can use this tab to edit information for compounds and to add new compounds. Before editing existing compounds, do a Single or Batch search, so that the compounds to be modified are present in the Search Results table. See "To edit a custom database" on page 25.

Search Results Table

This area in the lower part of the Personal Forensic Toxicology Database software window allows you to view search results. It also allows you to select compounds for editing on the Edit Compounds tab (*custom databases with editing enabled only*).

Viewing search results

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

- To change which columns of information are displayed in the table, right-click in the table and select **Add/Remove Columns** from the shortcut menu.
- To sort the table by the entries in a column, click the heading for the column of interest.
- To change the order of the columns of information in the table, drag a column heading to a different position. Repeat this until the desired order is achieved.
- To resize a column to fit the information contained in it, double-click on the right column divider in the heading of the column of interest.
- To resize a column to a specific width, drag the separator between the column headings to the right or left until the column is the desired width.

Editing compound information in the database

You can edit information in the database for the compounds shown in the Search Results table as follows, if you are using a custom database with editing enabled.

- Select the row (compound) of interest in the table. Make changes to the values in the edit fields that appear in the Edit Compounds tab. When you click the **Update Selected** button, the database is updated and the changes are reflected in the results table.

- Add a compound to a custom database in either of the following ways:
  - **Add New** - Click the **Add New** button to create a new compound in the database with a mass of 0 named “New Compound”. The new compound is displayed at the end of the Results table. Enter information such as Mass, RT, Formula, Name, and Structure for the new compound in the Edit Compounds tab. The information for the new compound is updated in the database and reflected in the results table when you click the **Update Selected** button.
  - **Save As New** - Click the **Save As New** button to create a new compound in the database using the current values of the edit fields on the Edit Compounds tab. The new compound is displayed at the end of the Results table.
- To remove a compound from the database, select the row (compound) of interest in the table, then click the **Delete Selected** button. Use **Ctrl+click** or **Shift+click** to select multiple lines for deletion.

Structures

Structure tab

This area on the right side of the Personal Forensic Toxicology Database software window displays structure information for the compound currently selected in the Results table, if it is available in the database. Clicking the  button opens the Structure Details dialog box and displays a larger image of the structure.

MOL Text tab

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

Getting Started

The following topics will help you get started with Agilent MassHunter Personal Forensic Toxicology Database. This guide and the online help explain these activities.

- "Searching a Forensic Tox database in Qualitative Analysis" on page 11
- "Searching a database in Personal Forensic Toxicology Database software" on page 13
- "Doing a batch search" on page 17
- "Database operations" on page 23
- "Custom database operations" on page 25

Searching a Forensic Tox database in Qualitative Analysis

Use the following procedures to search a Forensic Tox database with MassHunter Workstation Software–Qualitative Analysis program. These steps apply to version B.02.00 of Qualitative Analysis and may be slightly different in later revisions.

To use a Forensic Tox database to identify compounds in Qualitative Analysis

Use this procedure to identify compounds with a Forensic Tox database: **1** Open the data file of interest in Qualitative Analysis.

2 Find compounds as described in Qualitative Analysis online help.

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

4 Set the database search criteria in the **Identify Compounds > Search Database** section of Method Editor:

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

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

- Select File Type **.mtl** to see a list of databases.
- Select the Forensic Tox database of interest.

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

To use a Forensic Tox database to identify spectrum peaks in Qualitative Analysis

Use this procedure to identify spectrum peaks with a Forensic Tox database:

1 Open the data file of interest in Qualitative Analysis.

2 Extract a mass spectrum or extract a peak spectrum as described in Qualitative Analysis online help.

3 If not already set, set the database search criteria in the **Identify Compounds > Search Database** section of Method Editor as described in Step 4 above.

4 Initiate the search by right-clicking on the spectrum and selecting **Search Database for Spectrum Peaks** from the shortcut menu (or in other ways described in Qualitative Analysis online help).

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

5 Review the results in the DB Search Results window.

Searching a database in Personal Forensic Toxicology Database software

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

- "To find compounds" (below)
- "To view search results" on page 15
- "To change how data is displayed in the Results table" on page 15
- "To print search results" on page 16

To find compounds

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

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

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

3 To return the contents of the entire database, leave the search fields blank and skip to Step 7. Otherwise, set the desired mass search criteria:

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

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

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

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

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

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

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

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

c **Ion search mode**:

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

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

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

6 Initiate the search in any of the following ways:

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

7 View search results in the Search Results table at the bottom of the window. For more information, see “To view search results” on page 15 and “To change how data is displayed in the Results table” on page 15.

To view search results

1. Do a search on the Single Search tab as described in "To find compounds" on page 13.
2. View search results in the Search Results table at the bottom of the window. You can change how search results are displayed as described in "To change how data is displayed in the Results table" on page 15.
3. Click on a compound in the Results table to view its structure information in the Structures area on the right side of the window, if the structure is available in the database.
4. Click on the **Edit Compounds** tab to edit information for custom databases that allow editing, as described in "To edit a custom database" on page 25.
5. To print results, see "To print search results" on page 16.

To change how data is displayed in the Results table

This topic relates to search results displayed on the Single Search, Batch Search, Batch Summary, and Edit Compounds tabs.

1. To sort the table by the entries in a column, click the heading for the column of interest.
2. To change the order of the columns of information in the table, drag a column heading to a different position. Repeat this until the desired order is achieved.
3. To resize a column to fit the information contained in it, double-click on the right column divider in the heading of the column of interest.
4. To resize a column to a specific width, drag the separator between the column headings to the right or left until the column is the desired width.
5. To change which columns of information are displayed in the table:
   a. Right-click in the table and select **Add/Remove Columns** from the shortcut menu to open the Add/Remove Columns dialog box.
   b. Move the items of information that you want to display into the **Show these columns** list.
   c. Click **OK**.

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

To print search results

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

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

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

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

Doing a batch search

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

- "To find compounds from a mass list" (below)
- "To view batch search results" on page 19
- "To view batch summary results" on page 20
- "To export batch summary results" on page 21

To find compounds from a mass list

1. If the database you want to search is not already open, open it in *either* of the following ways:
   - Select **Open Database** from the File menu.
   - Click the  button on the toolbar.
2. Click on the **Batch Search** tab.
3. Enter a mass list in *one* of the following ways:
   - Click the **File** button to the left of the mass list table to open a mass list file output by MassHunter Qualitative Analysis (**.csv** or **.txt** file), Mass Profiler (**.xls** file), or GeneSpring MS (**.txt** file).
   - Copy and paste a compound list from MassHunter Qualitative Analysis.
   - Type in masses and retention times directly into the table.
4. Select or enter the **Type of mass** (normally **Neutral** for Batch Search) and **Mass tolerance**, in **ppm** or **mDa**.
5. Select **Ion search mode** options as follows:
   - **Include neutrals** is normally always selected.
   - Select **Include anions** and/or **Include cations** if you also want to consider those few chemicals that don't pick up or lose a proton to ionize.
6. Select one of the following options for **Retention times**:

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

Optional	Use retention time information to rank a compound higher if its retention time matches with the observed retention time.	Any. Select this option if you plan to update retention times in a custom database from the mass list as described in "To update retention time data" on page 27.
Required	Consider only compounds that match the specified retention time range.	When searching a database that contains retention time information for compounds.

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

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

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

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

9 Click on a row in the Mass List table to display the compounds found for that mass in the Search Results table in the lower part of the window. For more information on viewing batch search results, see "To view batch search results" on page 19.

10 Select and view the best compound hit for each mass as described in "To view batch summary results" on page 20.

To view batch search results

1. Do a search on the Batch Search tab as described in "To find compounds from a mass list" on page 17.
2. When the search is complete, the number of hits for each mass appears in the **Hits** column of the mass list, and the list is automatically sorted to show the masses with the most hits at the top of the list. To sort the list by a different criterion, click the heading for the column of interest (**Mass** or **RT**). Masses with conflicting hits are shown in red text in the Mass List table.
3. Click on a row in the Mass List table to display the compounds found for that mass in the Search Results table in the lower part of the window.

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

4. (*Optional*) Change how the batch search results are displayed as described in "To change how data is displayed in the Results table" on page 15.
5. See "To view batch summary results" on page 20 for information on selecting and viewing the best compound hit for each mass.
6. Click on a compound in the Results table to view its structure information in the Structures area on the right side of the window, if the structure is available in the database.
7. Click on the **Edit Compounds** tab to edit information for custom databases that allow editing, as described in "To edit a custom database" on page 25.
8. To print batch results, see "To print search results" on page 16.

To view batch summary results

1. Do a search on the Batch Search tab as described in "To find compounds from a mass list" on page 17.
2. Click on a row in the Mass List table to display the compounds found for that mass in the Search Results table in the lower part of the window. Masses with conflicting hits are shown in red text in the Mass List table.
3. Review the entries marked in the **Best** column for each mass and if necessary, edit the Batch Search Results table to select the best compound hit by marking the desired row (compound). You can also *clear* the box for the selected hit to ignore all the results for that compound.
4. Click the **Batch Summary** tab to view only the best hits from the Batch Search Results table. Compounds with conflicting mass hits are shown in red text in the results table.
5. (*Optional*) Change how the batch summary results are displayed as described in "To change how data is displayed in the Results table" on page 15.
6. Click on a compound in the Results table to view its structure information in the Structures area on the right side of the window, if the structure is available in the database.
7. Click on the **Edit Compounds** tab to edit information for custom databases that allow editing, as described in "To edit a custom database" on page 25.
8. To export batch summary results, see "To export batch summary results" on page 21.
9. To print batch summary results, see "To print search results" on page 16.
10. (*Optional*) For a custom database with editing enabled, you can update retention times in the database for the compounds shown in the Batch Summary Results table. See "To update retention time data" on page 27.

To export batch summary results

1. Do a batch search as described in "To find compounds from a mass list" on page 17.
2. Select and view the best compound hit for each mass as described in "To view batch summary results" on page 20, or clear the box for the selected hit to ignore all the results for that compound.
3. (*Optional*) Change the display of data in the Batch Summary tab as described in "To change how data is displayed in the Results table" on page 15.
4. Open the Export Results dialog box in *any* of the following ways:
   - Select **Export Results** from the File menu.
   - Click the  button on the toolbar.
   - Right-click in the results table and select **Export Results** from the shortcut menu in the Batch Summary results table.
5. Click the **Select** button if you wish to specify a different file name, location, or file type for the export file. Otherwise the following default file name, location, and format is used:
   - If the mass list was opened from a file, the export file name is: **<massListFileName>-<timestampInSecs>.txt**
   - If you entered the mass list manually, the export file name is: **MassList-<timestampInSecs>.txt**
   - The default location for the export file is **MassHunter\Forensics\Results**.
   - The default output file format is **.TXT** (tab-separated values), but you can select **.CSV** (comma-separated values) instead.
6. Select one or more of the following types of information to include in the report: **Search parameters**, **Results**, and **Unmatched masses** (available only if the **Results** checkbox is marked).
7. Mark the **Open results file after exporting** option to open the batch summary results file automatically in the associated application.
8. Click **OK** to output the results.
9. The results will open in the associated application such as Excel if you selected the **Open results file** option in Step 7. Otherwise open the exported results file in your application of choice at a later time.

NOTE

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

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

Database operations

The following operations apply to both Master and custom databases and are described in the following pages:

- "To open a database" (below)
- "To back up a database" (below)
- "To view database information" on page 24

To open a database

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

- Select **Open Database** from the File menu.
- Click the  button on the toolbar.

2 Select the database of interest (**.mtl** file extension) and click the **Open** button.

The following database files are supplied with the software:

- **Forensics.mtl** - the master Forensic database. This database *cannot* be edited, but can be copied to create a custom database that can be edited. See "To create a custom database" on page 25.
- **Empty.mtl** - an empty master database, which can be used to create a custom database for importing compounds. To create a database and import compounds, see "To create a custom database" on page 25 and "To import compounds" on page 28.

To back up a database

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

2 Select a folder for the backup file or accept the default folder, which is:

MassHunter\databases\Archive

3 Type in a file name for the backup file or accept the default file name, which is in the form:

<dbname>.<yyyy.mm.dd>.mtl

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

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

To view database information

1. Select **Database Information** from the Database menu.
2. View the following information about the database:
   - Database file name
   - The number of compounds (entries) in the database
   - Type (**Master** or **User**)
   - Edit allowed (**Yes** or **No**)
   - Last modified timestamp
   - Version number
   - Description - the description can be edited if the current database is a custom database with editing enabled.
3. Click the **Close** button to close the Database Information dialog box.

Custom database operations

The following operations apply only to custom databases and are described in the following pages:

- "To create a custom database" (below)
- "To edit a custom database" (below). This includes adding and removing compounds.
- "To update retention time data" on page 27
- "To import compounds" on page 28

To create a custom database

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

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

a Select a starting database for the new database. Use **Empty.mtl** if you want to create an empty database for importing compounds.

b Type in a name for the new database.

c Enter a description for the new database.

d Click the **Create** button to create the new database.

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

To edit a custom database

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

1 Open the custom database of interest.

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

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

- "To find compounds" on page 13.
- "To find compounds from a mass list" on page 17.

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

5 To update information for a particular compound:

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

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

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

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

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

6 To add a new compound to the database:

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

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

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

Alternate method to add a new compound

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

7 To remove a compound from the database:

a Select the compound of interest by clicking on it in the Search Results table.

b Click the **Delete Selected** button.

To update retention time data

1. Open the custom database of interest. Be sure that editing is enabled by marking **Allow Editing** on the Database menu.
2. Click on the **Batch Search** tab.
3. Enter a mass list in *one* of the following ways:
   - Click the **File** button to the left of the mass list table to open a mass list file output by MassHunter Workstation Qualitative Analysis (**.csv** or **.txt** file), Mass Profiler (**.xls** file), or GeneSpring MS (**.txt** file).
   - Copy and paste a compound list from Qualitative Analysis.
   - Type in masses and retention times directly into the table.

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

4. Select *one* of the following options for **Retention times**:
   - **Optional** - Use this option to search a database that either has no retention time information or has retention times missing for some compounds that you now want to update.
   - **Required** - Use this option if you only want to identify and update those compounds that already have retention time information in the database. Specify an **RT tolerance** value in minutes as well.
5. Set other search criteria if desired as described in "To find compounds from a mass list" on page 17.
6. Initiate the search in *any* of the following ways:
   - Click the **Find Compounds** button on the toolbar.
   - Select **Find Compounds** from the Database menu.
   - Press the **F5** key.
7. When the search is complete, the number of hits for each mass appears in the **Hits** column of the mass list, and the list is automatically sorted to show the masses with the most hits at the top of the list. To sort the list by a different criterion, click the heading for the column of interest (**Mass** or **RT**).

   Masses with conflicting hits are shown in red text in the Mass List table.
8. Click on a row in the Mass List table to display the compounds found for that mass in the Search Results table in the lower part of the window. For more information on viewing batch search results, see "To view batch search results" on page 19.

9 Select and view the best compound hit for each mass as described in "To view batch summary results" on page 20 or clear the box for the selected hit to ignore that compound.

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

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

To import compounds

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

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

- Exported from Personal Compound Database software as described in "To export batch summary results" on page 21.
- Exported from another application such as Agilent Mass Profiler or GeneSpring MS software.
- Manually in Excel.

2 Open the custom database of interest or create a new database.

NOTE You can create a new database for importing compounds from **Empty.mtl** as described in "To create a custom database" on page 25.

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

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

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

6 To view the new compounds in the database, do a search on the Single Search tab with no criteria or criteria that you know will find the compounds of interest. The compounds will be listed in the Search Results table in the lower part of the window.

NOTE The mass is calculated from the formula, unless the difference is > 0.0001 Da. In that case, the Mass and Formula values will be as read from the input file, and those compounds will be added to the file: **<ImportFileName>-MassErrorsLog.csv**, where **<ImportFileName>** is the name of the import file selected in Step 5. The information in the log file can be used to determine the correct Formula or Mass. Typically errors will occur when 1) the mass value was the mass from the spectrum and not a neutral mass, or 2) the formula contained the adduct (such as Cl).

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

8 (*Optional*) See "To edit a custom database" on page 25 if you want to change information for the imported compounds.

Familiarization Exercises

These exercises will help you learn to use the MassHunter Personal Forensic Toxicology Database:

- "Exercise 1. Search for compounds in a database" on page 30
- "Exercise 2. Batch search from a mass list" on page 33
- "Exercise 3. Create a custom database" on page 37
- "Exercise 4. Edit a custom database" on page 38
- "Exercise 5. Add retention times to a database" on page 40

Exercise 1. Search for compounds in a database

In this exercise, you will search the master Forensic database and review the search results.

Steps	Detailed Instructions	Comments
1 Open the master Forensic database.	**a** Select **Open Database** from the File menu, *or* click the  button on the toolbar. **b** Select the **Forensics.mtl** file, and click the **Open** button.	Skip this step if the master Forensic database is already open.
2 Click on the **Single Search** tab.		
3 Leave the search fields blank.	Be sure that the **Require** checkbox for Retention time is *cleared*, since the master Forensic database does *not* contain retention time information.	This will return the contents of the entire database. See "To find compounds" on page 13 for a discussion of search parameters to narrow your search.
4 Click the **Find Compounds** button on the toolbar to begin searching.		You can also start the search in either of the following ways: • Select **Find Compounds** from the Database menu. • Press the **F5** key.
5 Review the search results in the table in the lower half of the window.		The results are sorted from low mass to high mass.

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

Steps	Detailed Instructions	Comments
11 Print results.	**a** To print only selected results, highlight those rows in the Results table using **Ctrl+click** or **Shift+click**, then select **Only highlighted rows** as one of the print options in Step 11c below. **b** Click the  button on the toolbar to open the Print Results dialog box. **c** Select print options. For a discussion of print options, see "To print search results" on page 16. **d** Click **OK**. If you selected the Print Preview option, review the report in the Print Preview window, then click the  button to print it.	You can also open the Print Results dialog box in either of the following ways: • Select **Print Results** from the File menu • Right-click in the results table and select **Print Results** from the shortcut menu.

Exercise 2. Batch search from a mass list

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

Steps	Detailed Instructions	Comments
1 Open the master Forensic database.	**a** Select **Open Database** from the File menu, *or* click the  button on the toolbar. **b** Select the **Forensics.mtl** file, and click the **Open** button.	Skip this step if the master Forensic database is already open, as it will be after Exercise 1.
2 Click on the **Batch Search** tab.		
3 Open a mass list.	**a** Click the **File** button to the left of the mass list table. **b** Select the **tox_compounds.txt** mass list file in the **MassHunter\PCD\Mass List Files** folder. **c** Click the **Open** button.	Mass lists can also be copy-and-pasted into Personal Forensic Toxicology Database software from Qualitative Analysis. See online help in MassHunter Qualitative Analysis for instructions on how to output a mass list.
4 Set the search parameters.	**a** Select the **Neutral Masses** option. **b** Set **Mass tolerance** to 10 ppm. **c** Mark **Ignore** for **Retention times**. **d** Mark only the **Include neutrals** option for **Ion search mode**.	The master Forensic database does *not* include retention times.
5 Click the **Find Compounds** button on the toolbar to begin searching.		You can also start the search in *either* of the following ways: • Select **Find Compounds** from the Database menu. • Press the **F5** key.
6 Review search results.	When the search is complete, the number of hits for each mass appears in the **Hits** column of the mass list, and the list is automatically sorted to show the masses with the most hits at the top of the list (e.g. mass 300.0662 in this example has 10 hits). Masses with conflicting hits are shown in red text in the Mass List table. See Figure 1 on page 35.	To sort the mass list by a different criterion, click the heading for the column of interest (**Mass** or **RT**).

Steps	Detailed Instructions	Comments
7 View hits for selected masses.	Click on a row in the Mass List table to display the compounds found for that mass in the Batch Search Results table in the lower part of the window.	For ease of reviewing results, use the **F4** key to scroll down the Mass List and the **Shift**+**F4** keys to scroll back up. The information in the Results table will be updated as you scroll through the mass list. The batch search results table can be resorted as described in "To change how data is displayed in the Results table" on page 15.
8 Review the entries marked in the Best column for each mass and edit the Batch Search Results table to select the best compound hit for a particular mass.	Mark the **Best** column for the row (compound) you believe is the best compound hit for each mass. In many cases, this will be the one already selected by the software.	You can also clear the box for the selected hit to ignore that mass.
9 View the best hit results.	Click the **Batch Summary tab**. The Best hit for each mass is shown in the Batch Summary table in the lower part of the window. See Figure 2 on page 36.	Compounds with conflicting mass hits are shown in red text in the results table. The batch summary results table can be resorted as described in "To change how data is displayed in the Results table" on page 15.
10 Export batch summary results.	**a** Click the  button on the toolbar to open the Export Results dialog box. **b** Select the options to include **Search parameters**, **Results**, and **Unmatched masses**. **c** Mark the **Open results file after exporting** option. **d** Click **OK** to output the results. The results will open in the associated application such as Excel. The following export file is created in the **MassHunter\PCD\Results** folder: **tox_compounds-<timestamp>.txt**	You can also open the Export Results dialog box in either of the following ways: • Select **Export Results** from the File menu. • Right-click in the Batch Summary results table and select **Export Results** from the shortcut menu. You can select a different file name, location or type as described in "To export batch summary results" on page 21.

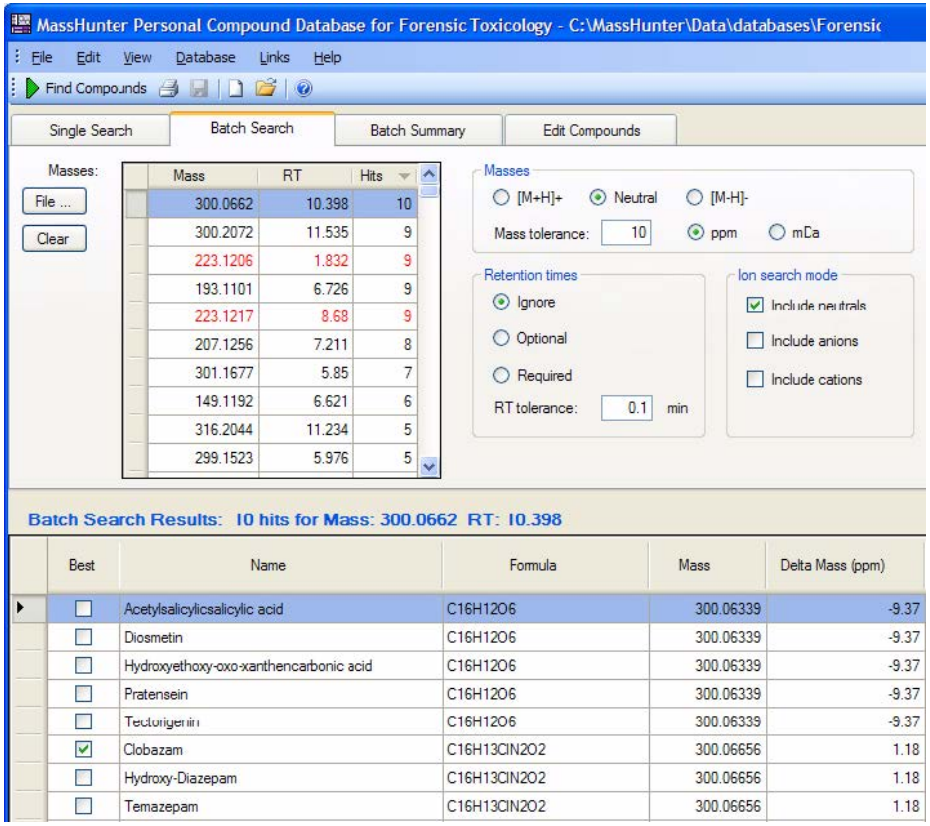


Figure 1 Results of Batch Search

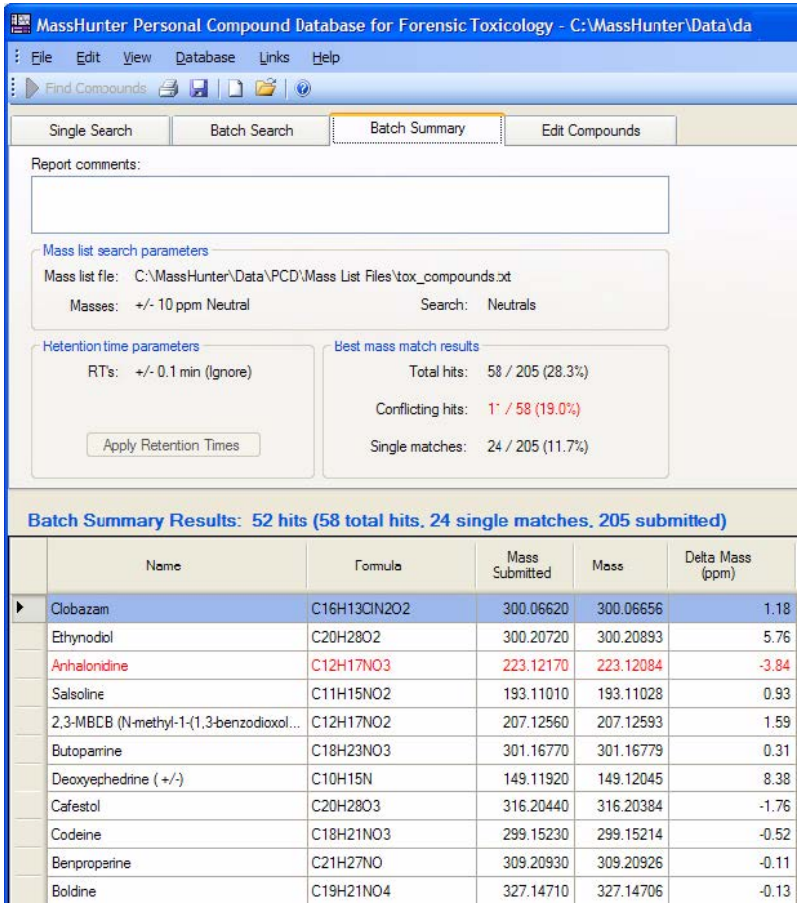


Figure 2 Batch Summary Results

Exercise 3. Create a custom database

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

Steps	Detailed Instructions	Comments
1 Open the New Database dialog box.	Select **New Database** from the File menu, or click the  button on the toolbar.	
2 Create the new database.	**a** Select **Forensics** as the starting database for the new database. **b** Type in a name for the new database, e.g. **Forensics_Subset**. **c** Enter a description for the new database, such as "My database". **d** Click the **Create** button to create the new database.	The new database becomes the current working database and is automatically enabled for editing.
3 Edit the database.	See "Exercise 4. Edit a custom database".	

Exercise 4. Edit a custom database

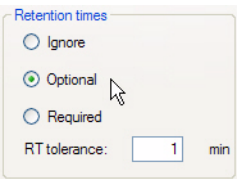
In this exercise, you will edit the custom database that you created in Exercise 3.

Steps	Detailed Instructions	Comments
1 Open the custom database you created in Exercise 3, if it is not already open.	**a** Select **Open Database** from the File menu, *or* click the  button on the toolbar. **b** Select the **Forensics_Subset.mtl** file, and click the **Open** button.	Skip this step if the custom database is already open, as it will be if you just completed Exercise 3.
2 Verify that editing is allowed for this database.	Open the **Database** menu and verify that there is a check mark next to **Allow Editing**.	
3 Do a search.	**a** Click the **Single Search** tab. **b** Click the **Find Compounds** button on the toolbar to start the search. The search results appear in the table in the lower half of the window.	See "Exercise 1. Search for compounds in a database" on page 30 for more information on the available search criteria. This search returns all neutral mass compounds in the database.
4 Click the **Edit Compounds** tab.		
5 Update information for a particular compound.	**a** Select the compound of interest by clicking on it in the Search Results table. **b** Update information on the left side of the Edit Compounds tab, such as Mass, RT, Formula, Name, CAS ID, and Ion type. **c** Click the **Update Selected** button to apply the changes to the database.	Information for the selected compound is displayed in the Edit Compounds tab. The updated information will be changed in the database and reflected in the Results table.
6 Update structure information for a particular compound.	**a** Select the compound of interest by clicking on it in the Search Results table. **b** Click the  button in the Molecule area to open a **.MOL** file. **c** Click the **Update Selected** button. The information you entered will be changed in the database.	You can also update structure information for a selected compound by clicking on the **MOL Text** tab and pasting in MOL file text that you copied from a molecular drawing tool (**Ctrl**+**V**).

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

Exercise 5. Add retention times to a database

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

Steps	Detailed Instructions	Comments
1 Open the custom database you created in Exercise 3 and edited in Exercise 4, if it is not already open.	**a** Select **Open Database** from the File menu, *or* click the  toolbar button. **b** Select the **Forensics_Subset.mtl** file, and click the **Open** button.	None of the compounds in this example database have retention times.
2 Verify that editing is allowed for this database.	Open the **Database** menu and verify that there is a check mark next to **Allow Editing**.	
3 Click the **Batch Search** tab.		
4 Open a mass list file that contains retention time information for the masses.	**a** Click the **File** button to the left of the mass list table. **b** Select **tox_compounds.txt** in the **MassHunter\PCD\Mass List Files** folder. **c** Click the **Open** button.	Each mass in the mass list must have an associated retention time value.
5 Set the search parameters.	**a** Set the **Mass tolerance** to 100 ppm. **b** Mark **Retention times Optional**. **c** Set the **RT tolerance** to 1 minute as shown below: 	
6 Start the search.	Click the **Find Compounds** toolbar button.	The results are shown in Figure 3.
7 Resolve conflicting hits.	**a** Click on a row in red in the Mass List table. **b** Mark the **Best** column for the desired row (compound) or clear the box for the selected hit to ignore the mass. **c** Repeat for all rows in red to resolve all conflicting results.	All conflicting results must be resolved before retention time data can be updated.

Steps	Detailed Instructions	Comments
8 Click the **Batch Summary** tab.	See Figure 4.	
9 Update retention times in the database from the current mass list.	Click the **Apply Retention Times** button. Note that this button is unavailable until all conflicting hits are resolved as described in Step 7.	Retention time information is updated in the database for each of the compounds listed in the Batch Summary table. See Figure 5.

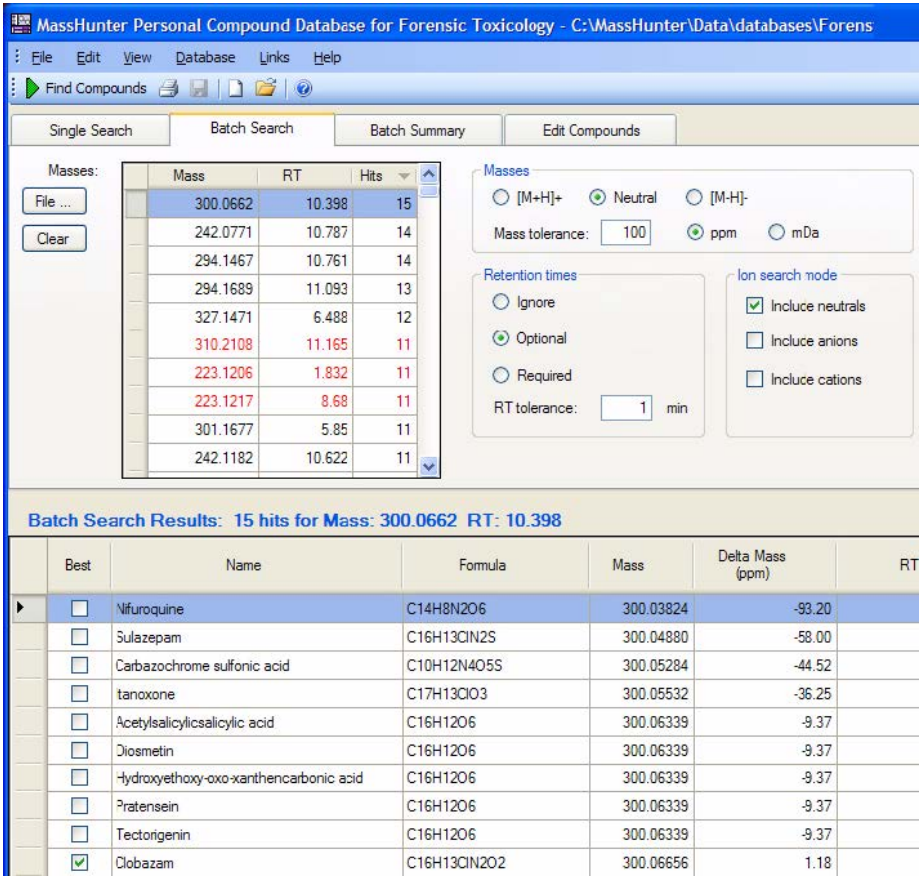
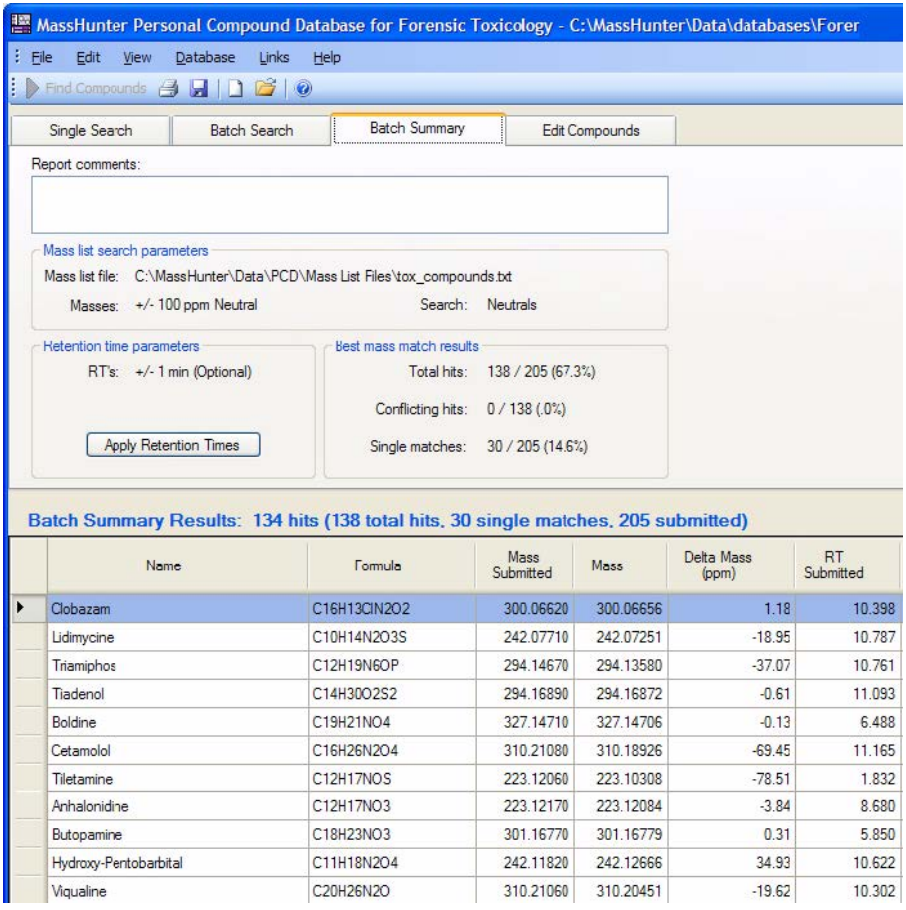
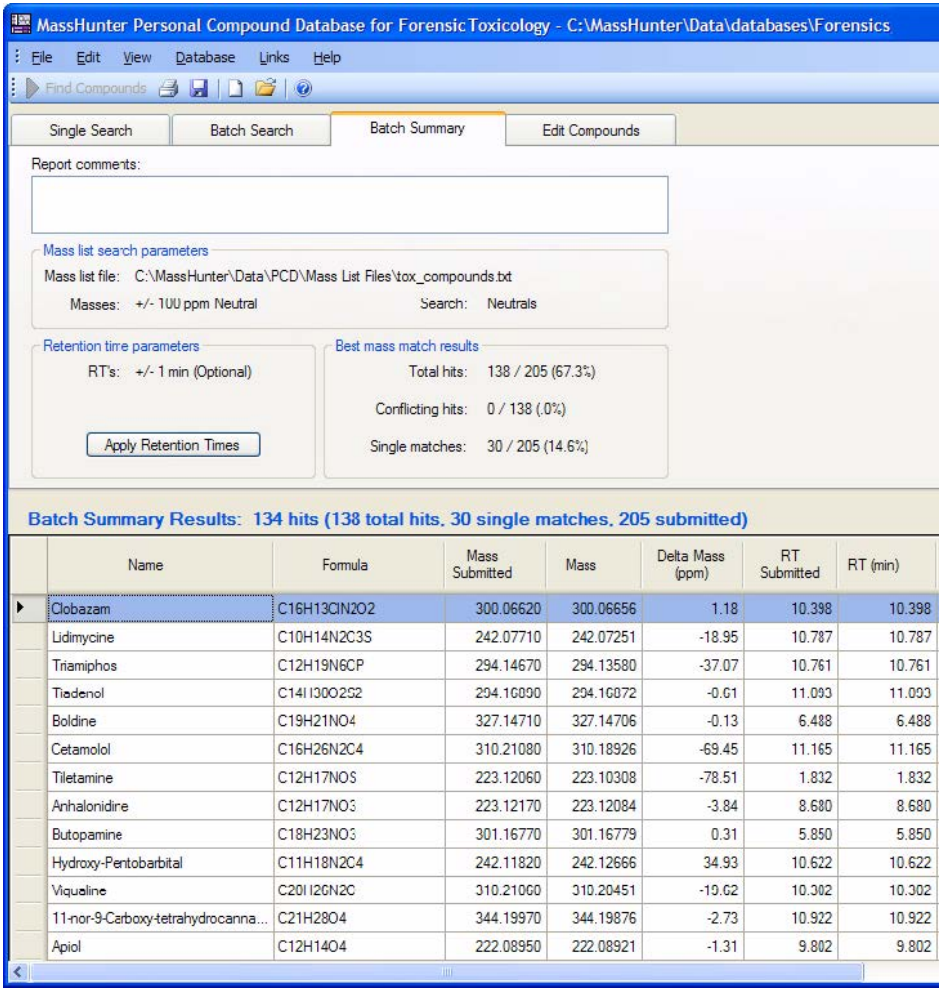


Figure 3 Batch Search Results with Retention Time Optional



Name	Formula	Mass Submitted	Mass	Delta Mass (ppm)	RT Submitted
Clobazam	C16H13ClN2O2	300.06620	300.06656	1.18	10.398
Lidimycine	C10H14N2O3S	242.07710	242.07251	-18.95	10.787
Triamiphos	C12H19N6OP	294.14670	294.13580	-37.07	10.761
Tiadenol	C14H30O2S2	294.16890	294.16872	-0.61	11.093
Boldine	C19H21NO4	327.14710	327.14706	-0.13	6.488
Cetamolol	C16H26N2O4	310.21080	310.18926	-69.45	11.165
Tiletamine	C12H17NOS	223.12060	223.10308	-78.51	1.832
Anhalonidine	C12H17NO3	223.12170	223.12084	-3.84	8.680
Butopamine	C18H23NO3	301.16770	301.16779	0.31	5.850
Hydroxy-Pentobarbital	C11H18N2O4	242.11820	242.12666	34.93	10.622
Viqualine	C20H26N2O	310.21060	310.20451	-19.62	10.302

Figure 4 Batch Summary Results with Retention Time Optional (before updating)



Name	Formula	Mass Submitted	Mass	Delta Mass (ppm)	RT Submitted	RT (min)
Clobazam	C16H13ClN2O2	300.06620	300.06656	1.18	10.398	10.398
Lidimycine	C10H14N2C3S	242.07710	242.07251	-18.95	10.787	10.787
Triamiphos	C12H19N6CP	294.14670	294.13580	-37.07	10.761	10.761
Tiadenol	C14H30O2S2	294.16090	294.16072	-0.61	11.093	11.093
Boldine	C19H21NO4	327.14710	327.14706	-0.13	6.488	6.488
Cetamolol	C16H26N2C4	310.21080	310.18926	-69.45	11.165	11.165
Tiletamine	C12H17NOS	223.12060	223.10308	-78.51	1.832	1.832
Anhalonidine	C12H17NO3	223.12170	223.12084	-3.84	8.680	8.680
Butopamine	C18H23NO3	301.16770	301.16779	0.31	5.850	5.850
Hydroxy-Pentobarbital	C11H18N2C4	242.11820	242.12666	34.93	10.622	10.622
Viqualine	C20H20N2C	310.21060	310.20451	-19.62	10.302	10.302
11-nor-9-Carboxy-tetrahydrocanna...	C21H28O4	344.19970	344.19876	-2.73	10.922	10.922
Apiol	C12H14O4	222.08950	222.08921	-1.31	9.802	9.802

Figure 5 Batch Summary Results with Retention Times Updated

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In this Book

This *Quick Start Guide* describes how to install and use the MassHunter Personal Forensic Toxicology Database. It also includes several familiarization exercises to help you get started.

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