High Resolution Accurate Mass Libraries

Release Notes

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Contents

Introduction 1

Features

High Resolution Accurate Mass (HRAM) libraries are designed for targeted library searching against HRAM product ion spectra. Each library contains HRAM MS/MS spectra for each compound included in the library.

These libraries are compatible with:

- Data acquired using a TripleTOF® accurate mass system.
- The combination of the MasterView™ 1.0 software and the PeakView® 2.1 software.
- The combination of the MasterView™ 1.1 software and the PeakView® 2.2 software.

Use these libraries to:

- Help accurately identify compounds and increase confidence in the reported results.
- Enable rapid searching in the MasterView™ software.
- Leverage the accurate mass, retention time, and peak area reporting functionality in the MasterView™ software.
- Compare a sample against a control for quick review using the comparative profiling option available in the MasterView™ software.

Contact Us

SCIEX Support

- sciex.com/contact-us
- sciex.com/support/request-support

Requirements

- An English (US) version of the Microsoft Windows 7 (32-bit or 64-bit) operating system with SP1 must be installed on the computer.
- A licensed version of the PeakView® 2.2 software combined with a licensed version of the MasterView™ 1.1 software must be installed on the computer.

  OR

  A licensed version of the PeakView® 2.1 software combined with a licensed version of the MasterView™ 1.0 software must be installed on the computer.
- The user must be logged on to the computer as a user with Administrator privileges to install a library.
- Internet access is required to obtain a license file for each installed High Resolution Accurate Mass Library.

Supported Equipment

- A TripleTOF® accurate mass system.
- A Dell Precision T3600 computer, or later model, provided by SCIEX.

Note: Older computer models might be compatible. However, they have not been tested and might result in degraded performance.

Notes on Use, Known Issues, and Limitations

Isobaric compounds with the same MS/MS pattern

Isobaric compounds with the same product ion spectra must be differentiated by their retention time.

The LibraryViewServiceHost stops responding intermittently

On the Microsoft Windows 7 (64-bit) operating system, when trying to open the MasterView™ software from the PeakView® software menu bar, the LibraryViewServiceHost service occasionally stops responding. To resolve this issue, do the following:

1. In Windows Explorer, right-click **Computer** and then click **Manage**.
2. In the Computer Management dialog, double-click **Services and Applications** and then double-click **Services**.
3. Right-click **LibraryViewServiceHost**, and then click **Start**.

This starts the LibraryViewServiceHost service again.

Installation 2

Install a Licensed High Resolution Accurate Mass Library

Note: The MasterView™ software, version 1.0 or 1.1, must be installed on the computer before a High Resolution Accurate Mass (HRAM) library can be installed. If MasterView™ software is not installed, then an error message is shown and the installation cannot be completed.

A licensed library can be installed from a DVD or from a .zip application file downloaded from the SCIEX Web site. The application file can include compound names, compound transition information, and compound library spectra.

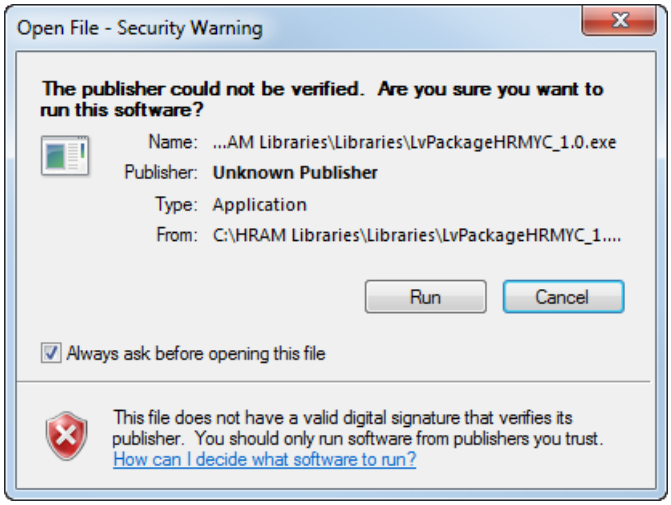
1. Log on to the computer as a Microsoft Windows user with administrator privileges.
2. Do one of the following:
   - If the library is being installed from a DVD, then load the DVD in the DVD drive and continue with step 5.
   - If the library is being installed from a downloaded file, then continue with step 3.
3. Download the required .zip file from the SCIEX Web site.

   Tip! To prevent potential installation issues, save the file to a location other than the computer desktop.

4. After the download is complete, right-click the downloaded file and then click **Extract All**.
5. Browse to the extracted files or the DVD and then double-click **LvPackageHR[libraryname_version].exe**.

   The Open File - Security Warning dialog opens.

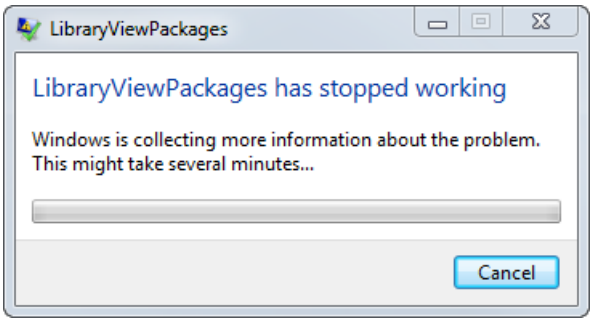
Figure 2-1 Open File - Security Warning Dialog



Tip! If the User Account Control dialog opens, then click **Yes**.

Note: If the LibraryViewFramework is not installed, then an error message is shown and the installation cannot be completed.

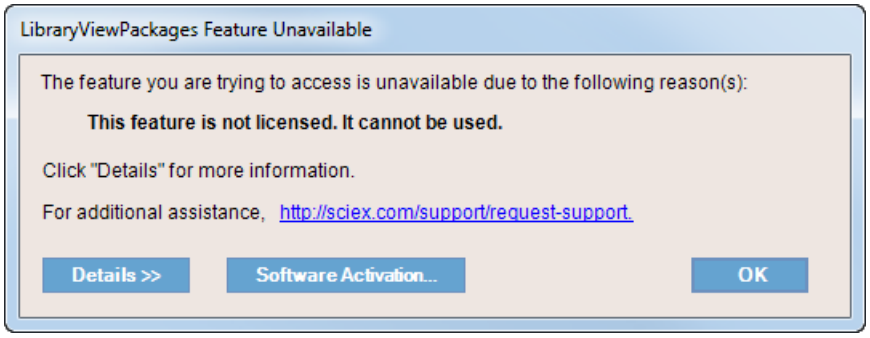
Figure 2-2 LibraryViewPackages Error Message



6. Click **Run** on the Open File - Security Warning dialog.

   The LibraryViewPackages Feature Unavailable dialog opens.

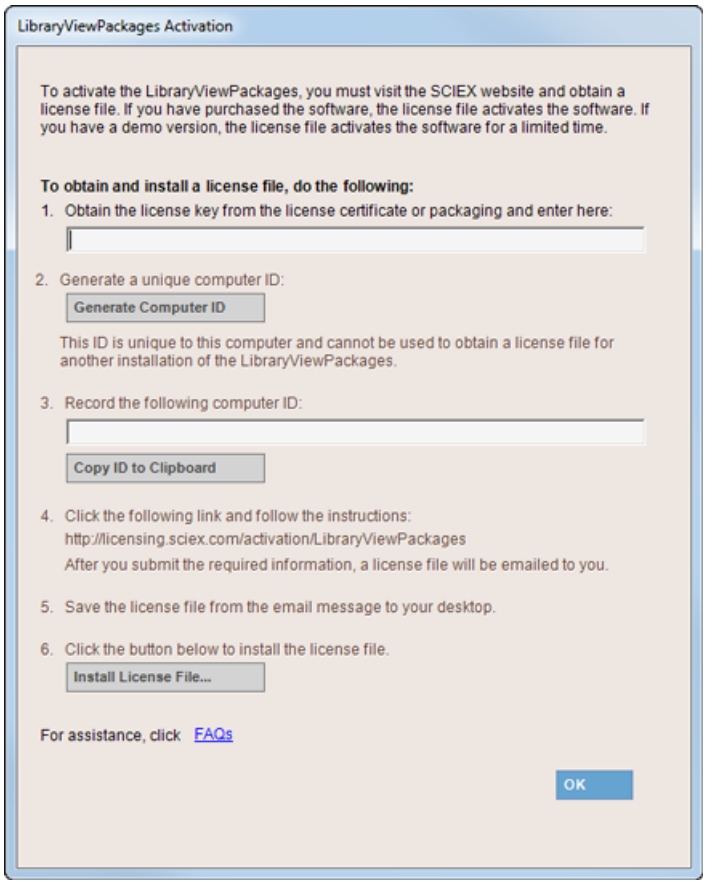
Figure 2-3 LibraryViewPackages Feature Unavailable Dialog



7. Click **Software Activation**.

   The LibraryViewPackages Activation dialog opens.

Figure 2-4 LibraryViewPackages Activation Dialog



8. Type the license key, exactly as shown, in the appropriate field.

If a license key is not available, then contact sciex.com/support/request-support .

9. Click **Generate Computer ID**.

   This creates a unique identifier for the workstation.

10. Click **Copy ID to Clipboard**.

11. Follow the instructions to obtain the license.

> **Note:** Internet access is required to obtain the license. If the computer does not have Internet access, then make a copy of the generated computer ID. On a computer with Internet access, go to the licensing page of the SCIEX Web site and then follow the instructions to obtain a license.

   After the required information is submitted, a license file is sent to all of the e-mail addresses provided.

12. Close the browser window.

13. When the e-mail containing the license file is received, copy the license file to the workstation desktop.

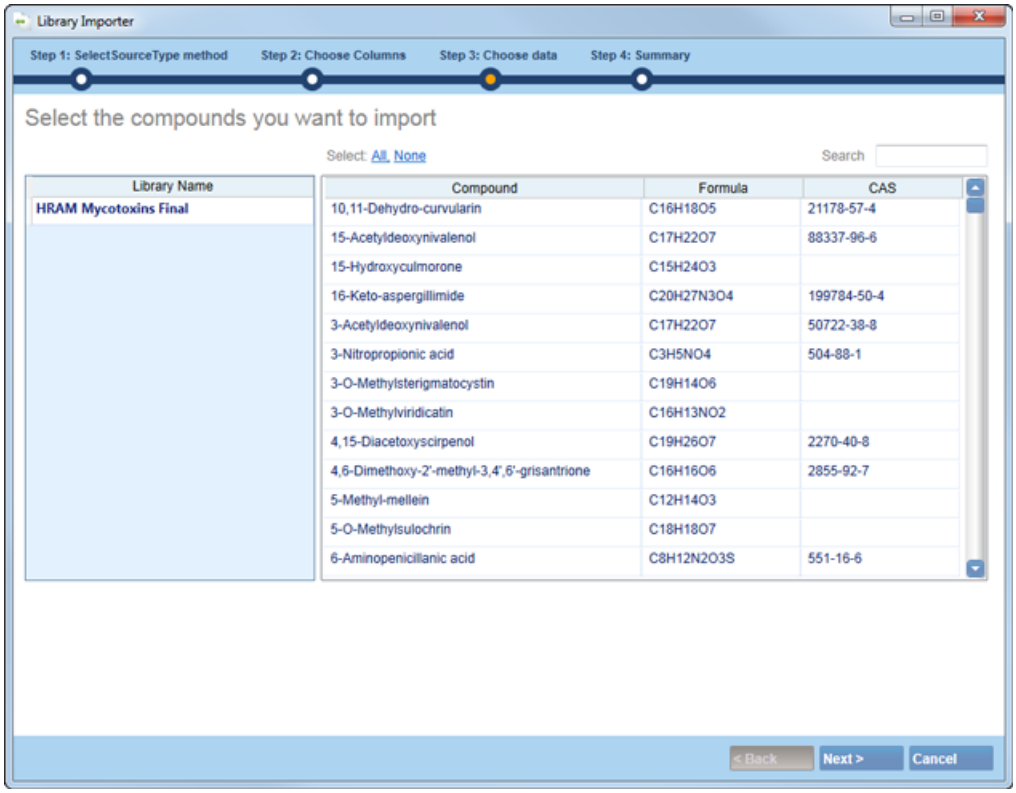
14. Click **Install License File** on the LibraryViewPackages Activation dialog.

   The Select the new license file to be installed dialog opens.

15. Browse to and select the license file and then click **Open**.

   Both the Select the new license file to be installed and the LibraryViewPackages Activation dialogs close and the Library Importer dialog opens.

Figure 2-5 Library Importer Dialog



16. Do one of the following:

- Click **All** above the **Compound** column on the Library Importer dialog to import all of the compounds.
- Click inside the appropriate row on the Library Importer dialog to import individual compounds.

Tip! To help locate compounds, use the **Search** field. As the search criteria is typed, the visible columns are searched and refreshed to show only the information that matches the criteria specified.

17. Click **Next**.

Note: If the user cancels the import before all of the compounds have been copied to the database, then any compounds that have already been imported remain in the database. The software does not revert the database to the pre-import state.

18. Resolve any conflicts, if required. Refer to Compound Conflicts on page 11.

19. Click **Finish**.

Compound Conflicts

When installing a library containing a group of compounds or installing individual compounds, the software checks the database for compounds with the same name or formula as a compound in the package. If compounds are found, then the software flags the corresponding compounds in the package and waits for user input to continue.

Users have the option to:

- Merge the compound information. New spectra, transitions, and retention times from the compound in the package are added to the compound information stored in the database.
- Overwrite the compound information. Compound information from the package replaces the compound information stored in the database.
- Keep the compound information. Compound information in the database is retained and the compound information from the package is discarded.

Conflict details are available to help the user make the correct choice.

View Compound Conflicts

1. Click **Resolve** on the Library Importer dialog beside the compound to view the details of the conflict.
2. Do one of the following:
   - Click **Keep Original** to keep the existing compound information and discard the new information.
   - Click **Use New** to replace the existing compound information with the new information.
3. Repeat steps 1 and 2 for each compound.
4. Click **Finish** after all of the conflicts are resolved.

Merge Compounds

1. Do one of the following:
   - Click **Merge** on the Library Importer dialog to merge new spectra, transitions, and retention times from individual compounds in the import package with the corresponding compound stored in the database.
   - Click **Merge All** on the Library Importer dialog to merge new spectra, transitions, and retention times from all of the compounds in the import package with the corresponding compounds stored in the database.
2. Click **Finish** after all of the conflicts are resolved.

Overwrite Compounds

1. Do one of the following:

   - Click **Overwrite All** on the Library Importer dialog to overwrite all of the compound information stored in the database with the corresponding compound information from the import package.
   - Click **Resolve** beside the appropriate compound on the Library Importer dialog and then click **Use New** to overwrite the compound information stored in the database with the corresponding compound information from the import package.

2. Click **Finish** after all of the conflicts are resolved.

Keep Original Compounds

1. Do one of the following:

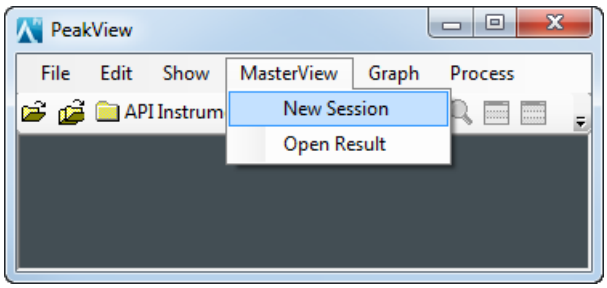
   - Click **Keep All Original** on the Library Importer dialog to keep all of the compound information stored in the database and discard the compound information from the import package.
   - Click **Keep Original** beside the appropriate compound on the Library Importer dialog to keep the individual compound information stored in the database and discard the compound information from the import package.

2. Click **Finish** after all of the conflicts are resolved.

Import a High Resolution Accurate Mass Library into the MasterView™ Software 3

1. Open the PeakView® software.
2. From the PeakView® software menu bar, click **MasterView > New Session.**

Figure 3-1 MasterView > New Session



The Select Samples dialog opens.

3. Expand the appropriate data folder and then do one of the following:
   - Drag the required samples from the **Available** pane to the **Selected** pane.
   - Select the required files and use the => to move samples from the **Available** pane to the **Selected** pane.

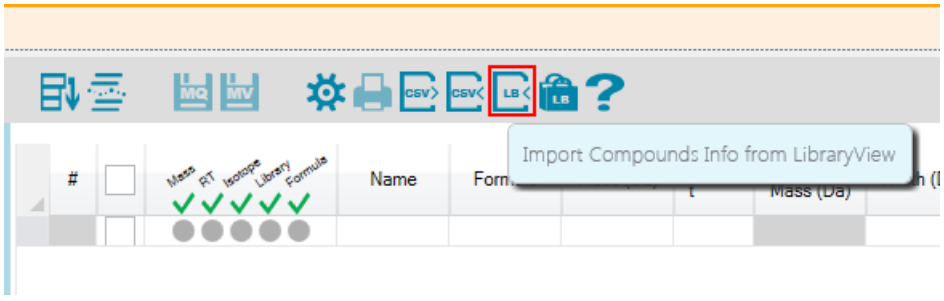
Tip! Use the <= to move samples from the **Selected** pane to the **Available** pane.

4. Click **OK**.

   The selected files open in the MasterView™ software.

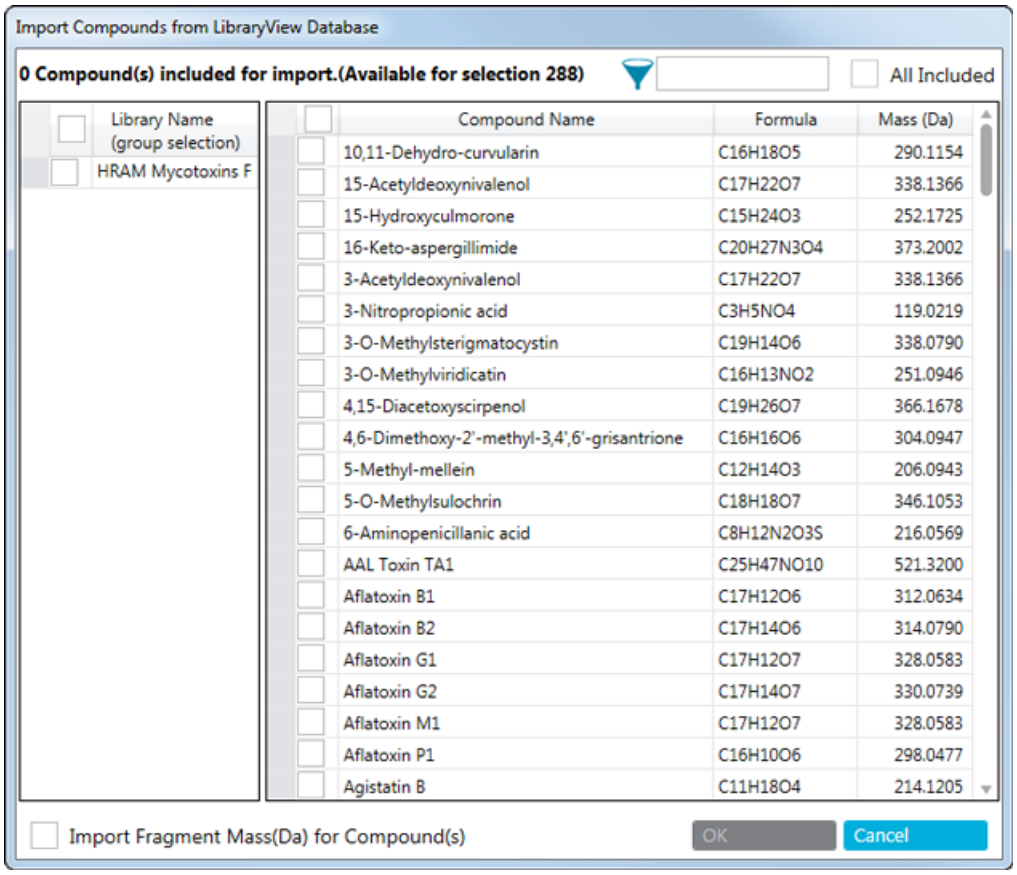
5. Click the **Import Compounds Info from LibraryView** icon.

Figure 3-2 Import Compounds Info from LibraryView Icon



The Import Compounds from LibraryView Database dialog opens.

Figure 3-3 Import Compounds from LibraryView Database Dialog



6. Do one of the following:

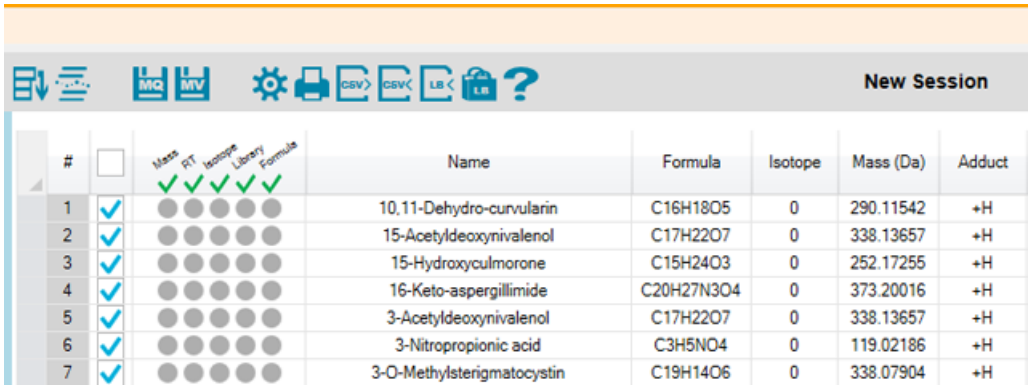
   - Select the check box to the left of the imported library name to import all of the compounds.
   - Select the check box to the left of each compound name to import individual compounds.

   Tip! To help locate compounds, use the **Search** field. As the search criteria is typed, the visible columns are searched and refreshed to show only the information that matches the criteria specified.

7. Click **OK**.

   The Import Compounds from LibraryView Database dialog closes and the selected compound information is shown in the MasterView™ software session pane.

Figure 3-4 MasterView™ Software Session Pane



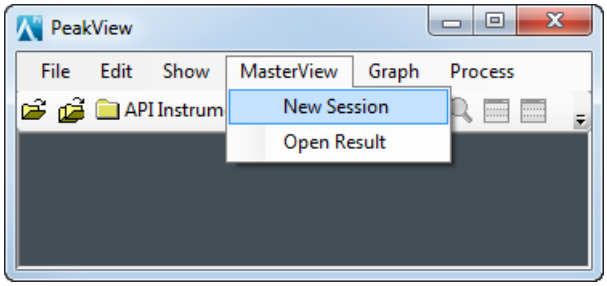
#	Name	Formula	Isotope	Mass (Da)	Adduct
1	10,11-Dehydro-curvularin	C16H18O5	0	290.11542	+H
2	15-Acetyldeoxynivalenol	C17H22O7	0	338.13657	+H
3	15-Hydroxyculmorone	C15H24O3	0	252.17255	+H
4	16-Keto-aspergillimide	C20H27N3O4	0	373.20016	+H
5	3-Acetyldeoxynivalenol	C17H22O7	0	338.13657	+H
6	3-Nitropropionic acid	C3H5NO4	0	119.02186	+H
7	3-O-Methylsterigmatocystin	C19H14O6	0	338.07904	+H

Targeted Library Searching in the MasterView™ Software 4

This section describes how to search data generated by any of the SCIEX TripleTOF® accurate mass systems using a targeted list of known compounds and a High Resolution Accurate Mass (HRAM) library with HRAM MS and MS/MS spectra.

1. Open the PeakView® 2.2 software.
2. From the PeakView® software menu bar, click **MasterView > New Session.**

Figure 4-1 MasterView > New Session



The Select Samples dialog opens.

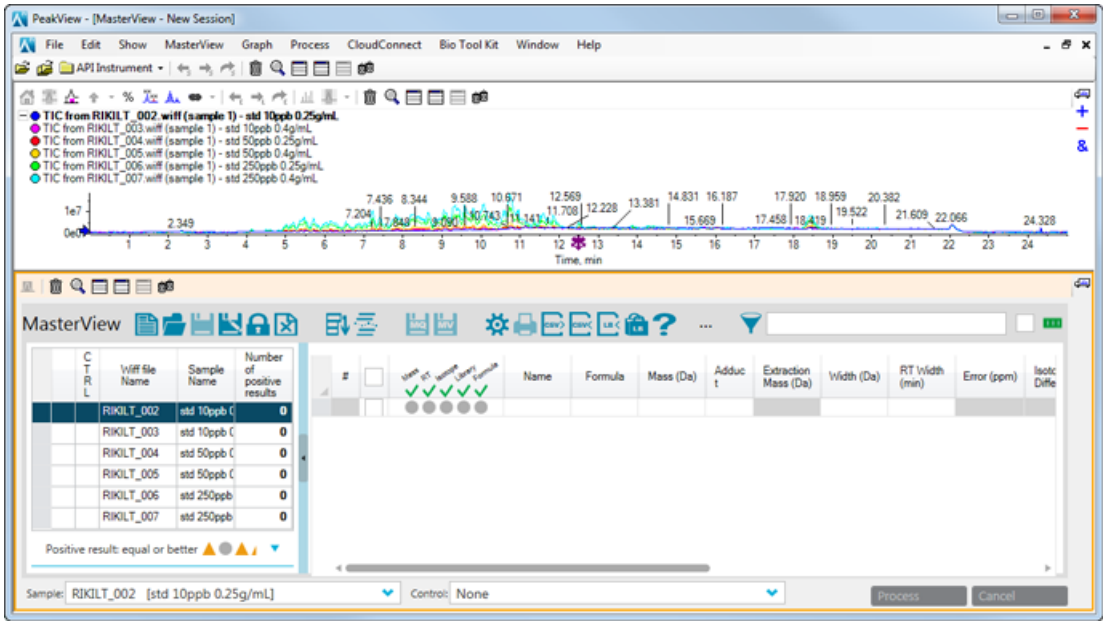
3. Expand the appropriate data folder and then do one of the following:
   - Drag the .wiff files containing the required samples from the **Available** pane to the **Selected** pane.
   - Select the .wiff files in the **Available** pane and then use the => to move the required samples to the **Selected** pane.

Tip! Use the <= to move samples from the **Selected** pane to the **Available** pane.

4. Click **OK**.

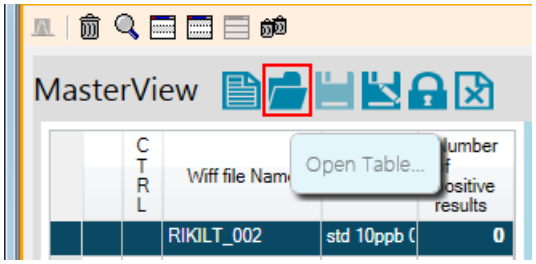
   The MasterView™ software New Session window opens.

Figure 4-2 MasterView - New Session Window



5. Click the **Open Table** icon.

Figure 4-3 Open Table Icon

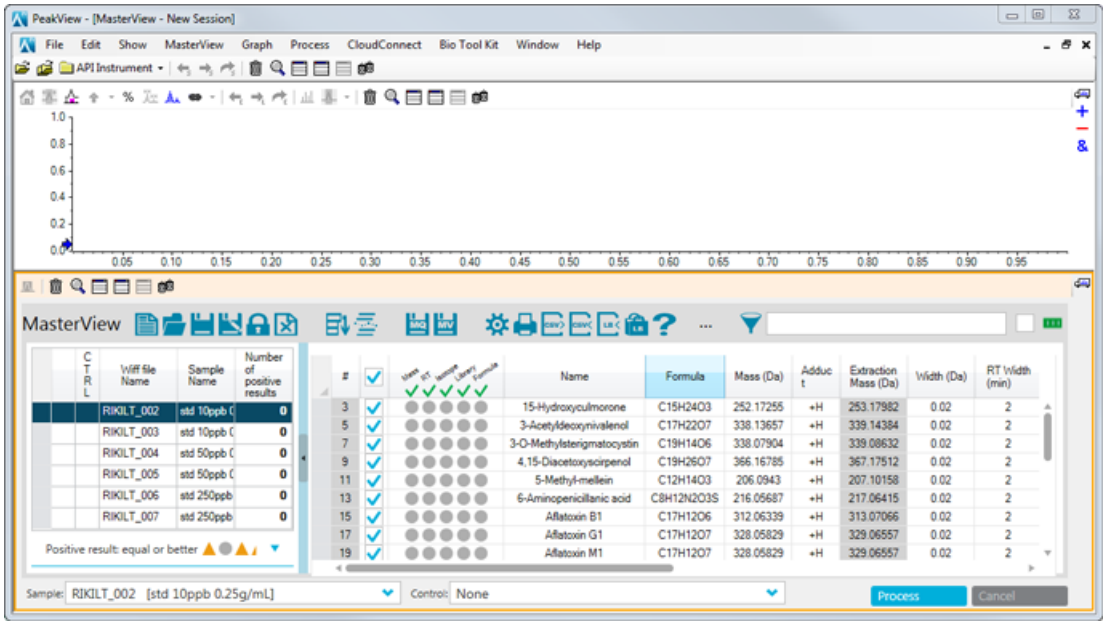


The Open dialog opens.

6. On the Open dialog, navigate to and select the appropriate .XIClist file and then click **Open**.

Note: The information from the .XIClist file is shown in the session table. Both positive and negative mode data can be included. For more information, refer to the MasterView™ software Help.

Figure 4-4 XIC List Open in a New Session Table



When the library is run for the first time, there is no retention time information. To populate the **Expected RT (min)** column, do the following:

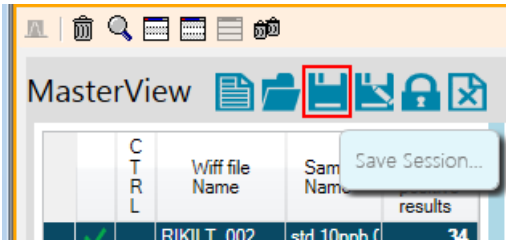
a. Select the first .wiff file and then click **Process**.

b. After processing is complete, copy the contents of **Found At RT (min)** column into the **Expected RT (min)** column.

> **Tip!** If the columns are not visible, click the **Settings** icon and then select the **Columns** tab. Make sure that the **Expected RT (min)** and **Found AT RT (min)** check boxes are selected and then click **OK**.

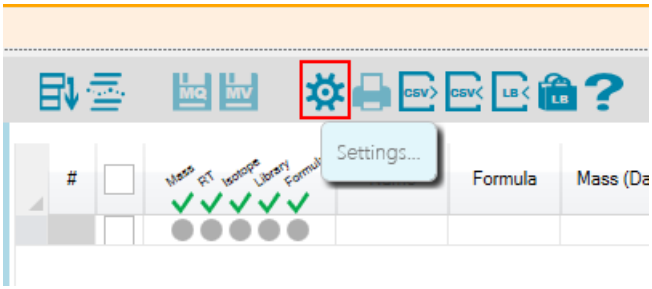
c. Click the **Save Session** icon to save the .XIClist, with the retention times, to use for future processing.

Figure 4-5 Save Session Icon



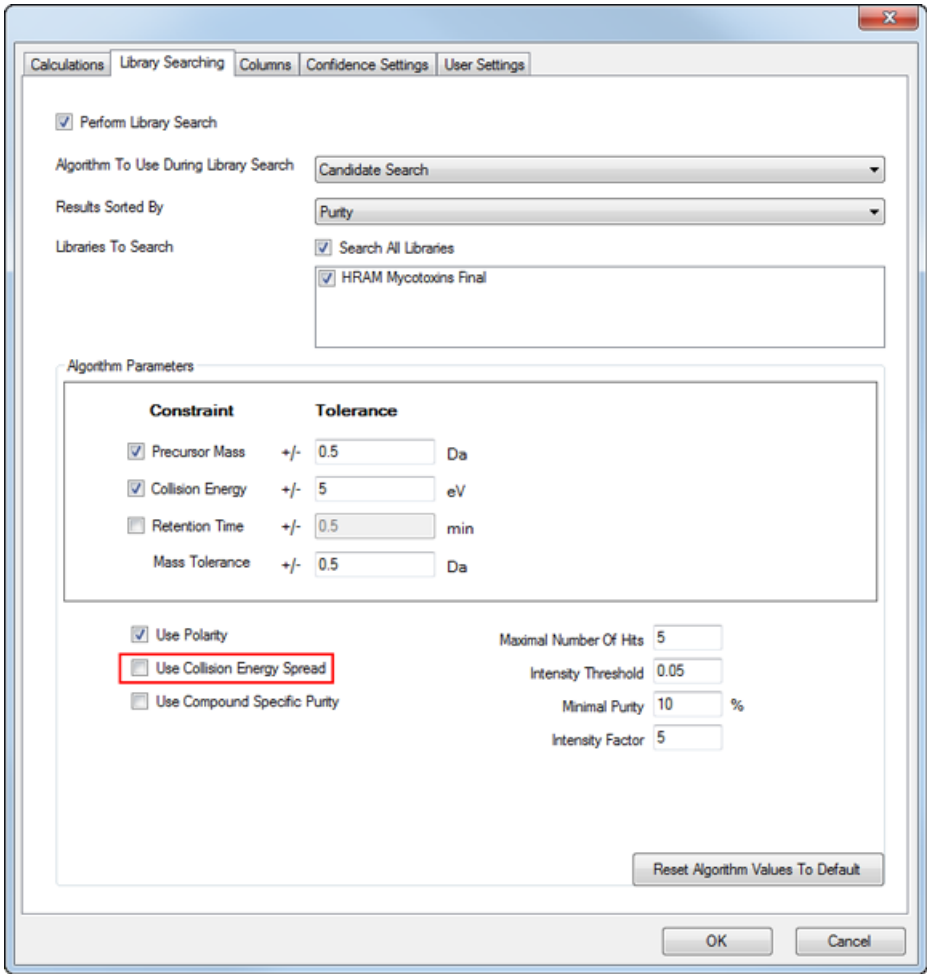
7. Click the **Settings** icon to edit the settings for data processing and library searching.

Figure 4-6 Settings Icon



8. In the settings dialog, select the **Library Searching** tab.
9. In the **Libraries To Search** section, select the installed library to make sure that the compounds searched for are matched in this library. The library is shown with the name that is assigned to it while it is imported in the MasterView™ software.
10. Clear the **Use Collision Energy Spread** check box.

Figure 4-7 Library Searching Tab



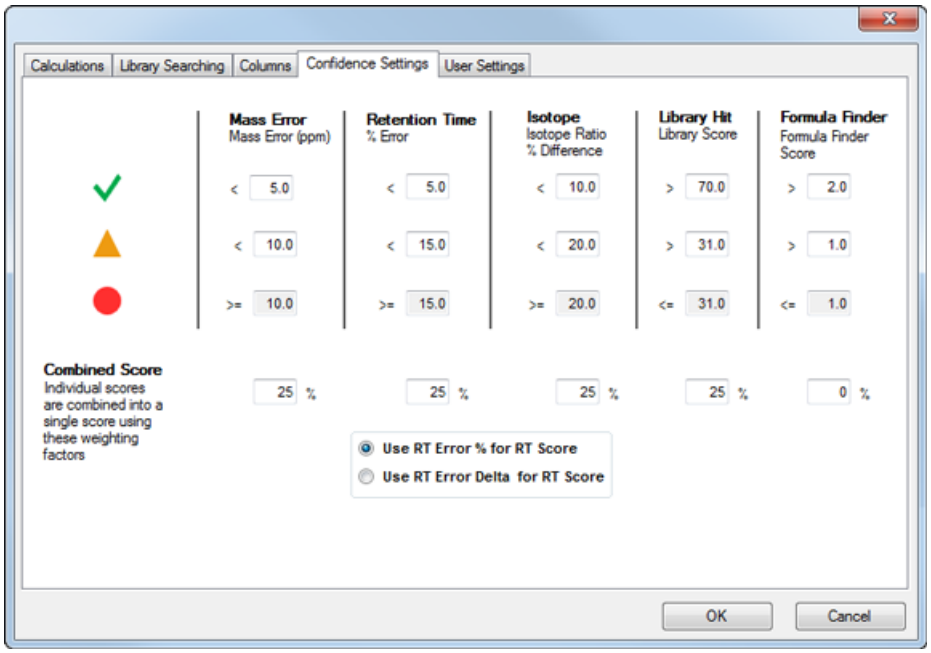
Note: For information about the different options in the settings dialog, refer to the MasterView™ software Help.

Note: Effective fragmentation of per- and polyfluoroalkyl substances in the Fluorochemical HR-MS/MS Library v1.0 requires higher collision energy (CE) than the 35 ±15 eV used for all other HR-MS/MS libraries. A CE of 60 eV was used to acquire most spectra in this library. This should be considered when setting up data acquisition methods for fluorochemicals. In addition, if data is not acquired at 60 eV, then the CE window in the MasterView™ software Library Searching settings should be increased to ± 25 eV. This approach should also be considered when searching for fluorochemicals using the All-in-One HR-MS/MS Library v1.1.

11. Click the **Confidence Settings** tab to define the criteria for acceptance of an identification based on a traffic light system.

The default settings are used in this example.

Figure 4-8 Confidence Settings Tab



12. Click **OK**.

Note: All settings are saved with the .XIClist file.

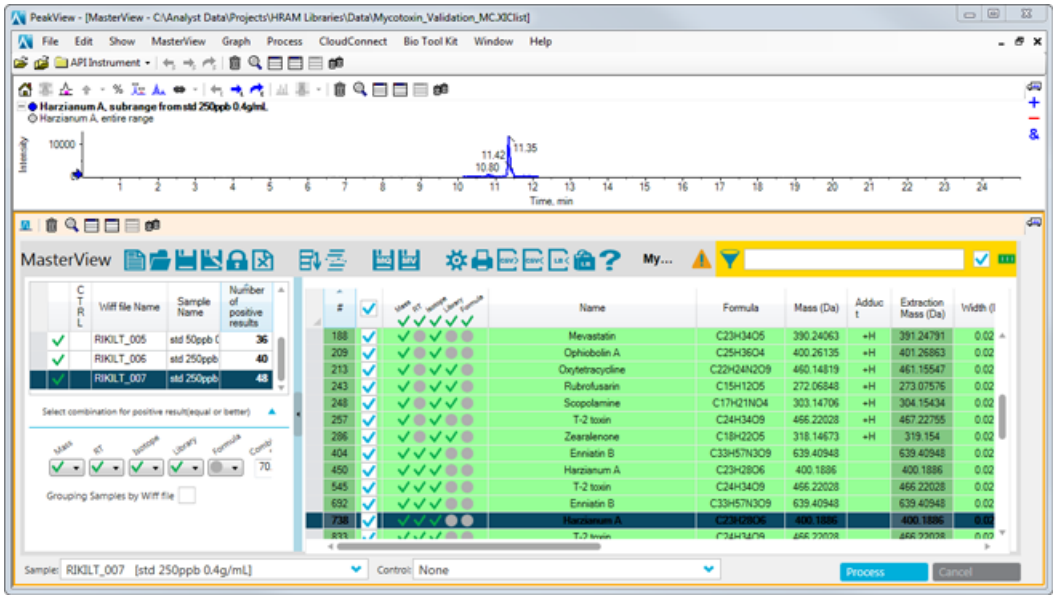
Note: To make sure that the isobaric compounds (compounds with the same accurate mass) are identified correctly, even if their product ion spectra are the same, specify the retention time in the XIClist in the MasterView™ software.

13. Click **Process**.

Using the information in the .XIClist file, the MasterView™ software calculates the XIC for each sample and then performs the library search against the imported compound information from the library for each sample.

Tip! The number of compounds identified as a positive hit is shown in the **Number of positive results** column in the left pane. The search results, including the confidence levels, are shown in the right pane. The XIC rows corresponding to the positive hits are highlighted.

Figure 4-9 Library Search Result

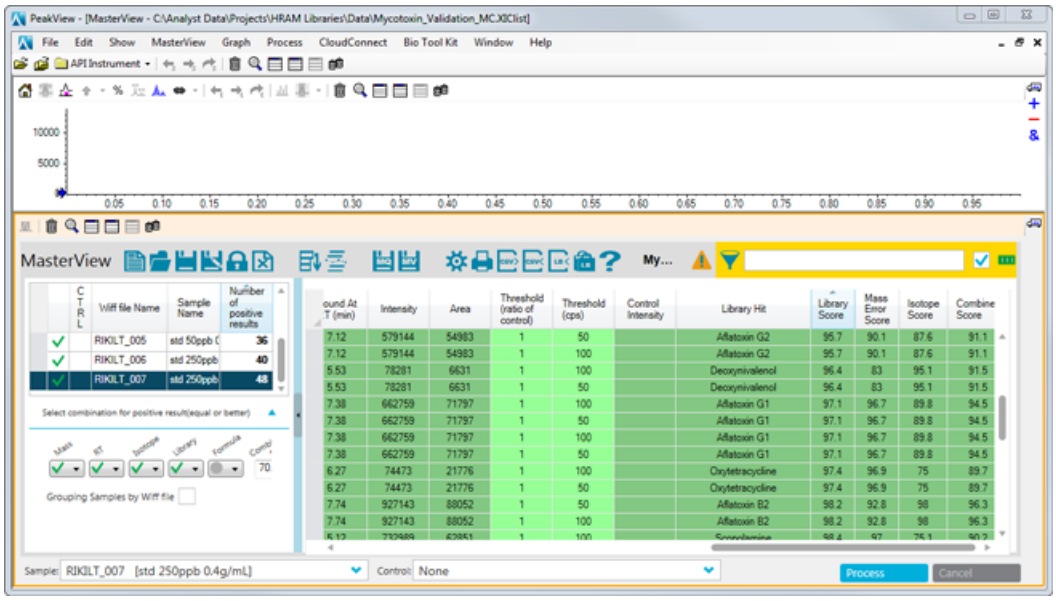


14. While reviewing the qualitative results of the library search, use the following information:

- Confidence in identification of compounds is visualized using the RT and library traffic lights.

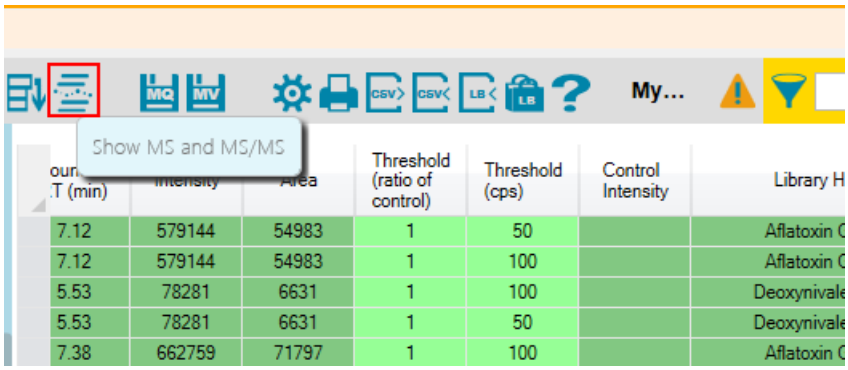
- Numeric values can be found in many columns, for example, the **Mass Error Score** and **Library Score** columns, and so on. Any of these columns can be used to sort results.

Figure 4-10 Library Search Results Sorted by Library Score



- The MS/MS spectrum can be visually compared to the library spectrum by clicking the **Show MS/MS** icon.

Figure 4-11 Show MS and MS/MS Icon



- Results can be reported using customizable report templates.

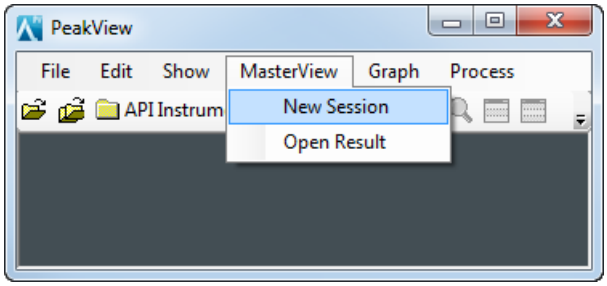
15. Click **Save Session**.

Non-Targeted Library Searching in the MasterView™ Software 5

This section describes how to search data generated by any of the SCIEX TripleTOF® accurate mass systems using a non-targeted list of known-unknown compounds and a High Resolution Accurate Mass (HRAM) library with HRAM MS and MS/MS spectra.

1. Open the PeakView® 2.2 software.
2. From the PeakView® software menu bar, click **MasterView > New Session.**

Figure 5-1 MasterView > New Session



The Select Samples dialog opens.

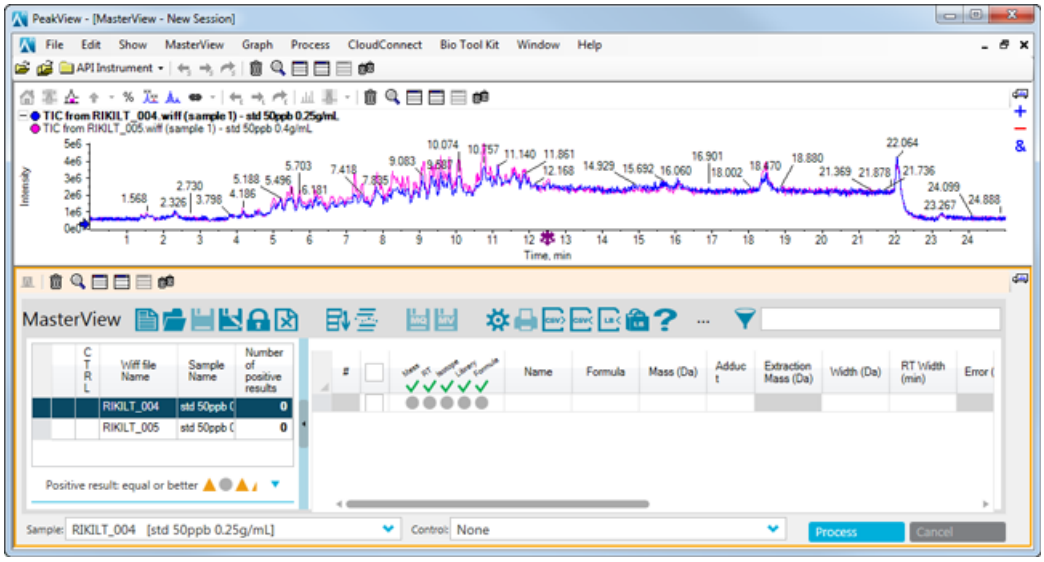
3. Expand the appropriate data folder and then do one of the following:
   - Drag the .wiff files containing the required samples from the **Available** pane to the **Selected** pane.
   - Select the .wiff files in the **Available** pane and then use the => to move the required samples to the **Selected** pane.

Tip! Use the <= to move samples from the **Selected** pane to the **Available** pane.

4. Click **OK**.

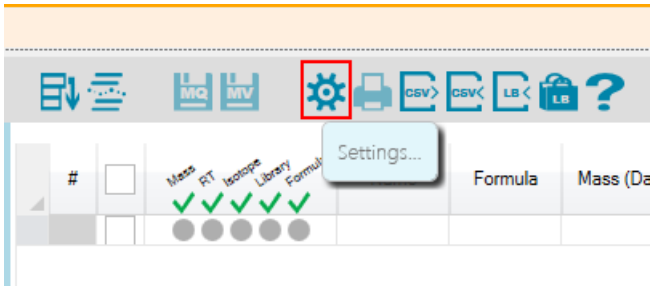
   The MasterView™ software New Session window opens.

Figure 5-2 MasterView - New Session Window



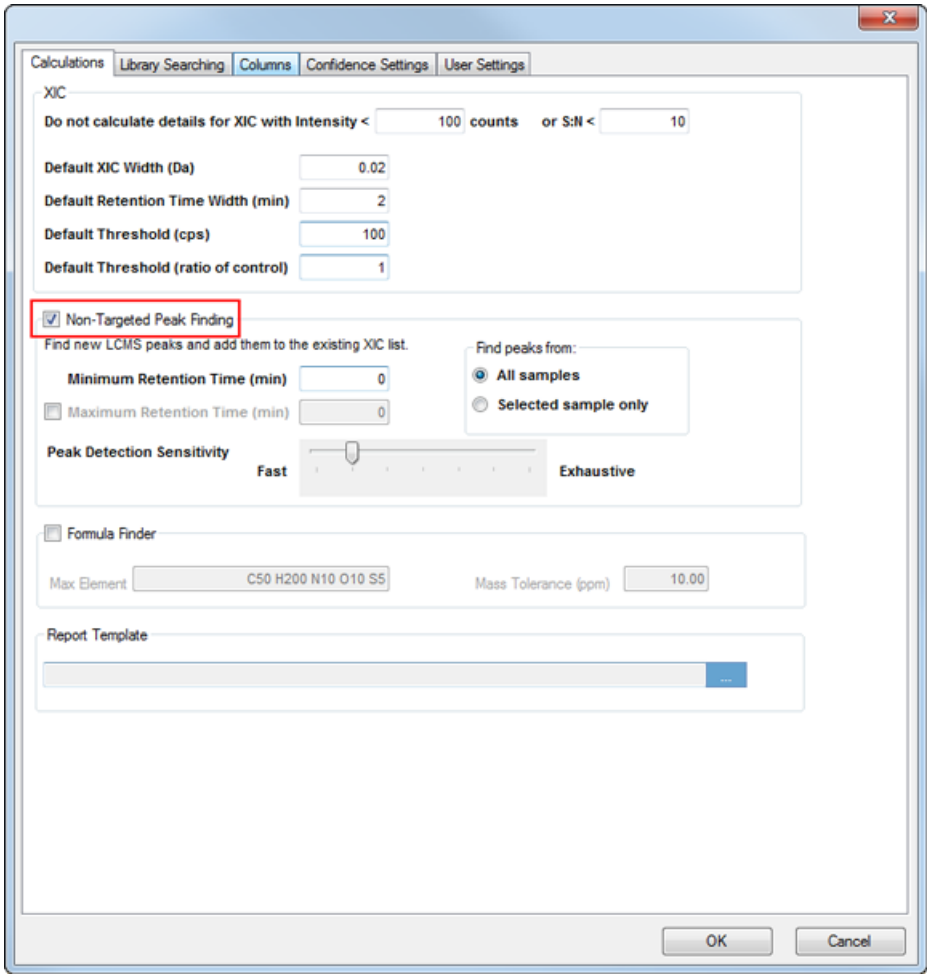
5. Click **Process**.
6. Click the **Settings** icon to edit the settings for data processing and library searching.

Figure 5-3 Settings Icon



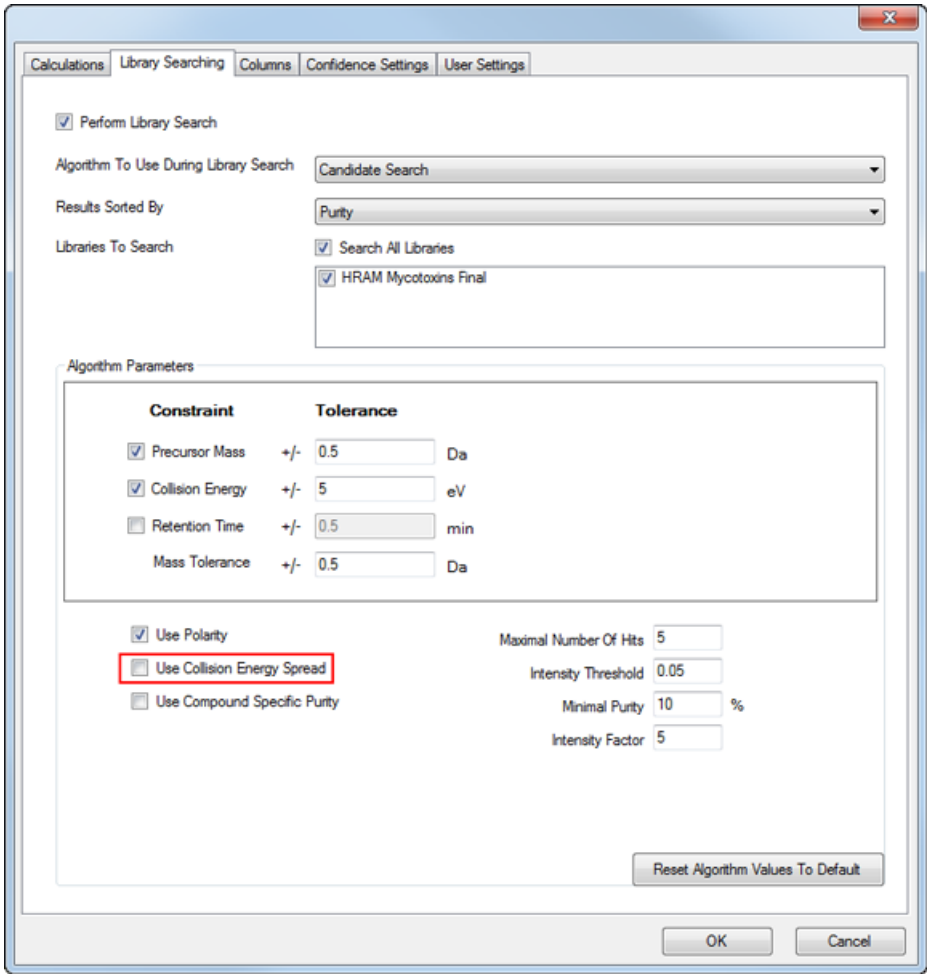
7. In the settings dialog, select the **Calculations** tab.
8. Select the **Non-Targeted Peak Finding** check box.

Figure 5-4 Calculations Tab



9. Click the **Library Searching** tab.
10. In the **Libraries To Search** section, select the installed library to make sure that the compounds searched for are matched in this library. The library is shown with the name that is assigned to it while it is imported in the MasterView™ software.
11. Clear the **Use Collision Energy Spread** check box.

Figure 5-5 Library Searching Tab



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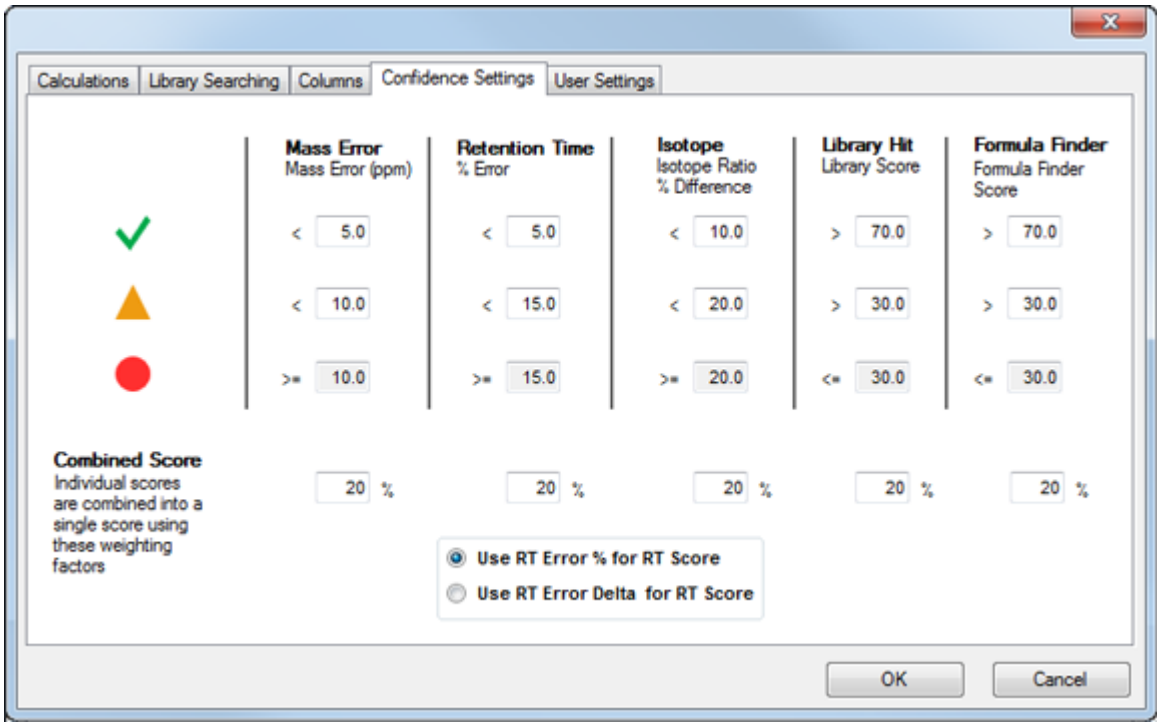
12. Click the **Confidence Settings** tab to define the criteria for acceptance of an identification based on a traffic light system.

The default settings are used in this example.

Figure 5-6 Confidence Settings Tab



13. Click **OK**.

Note: All settings are saved with the .XIClist file.

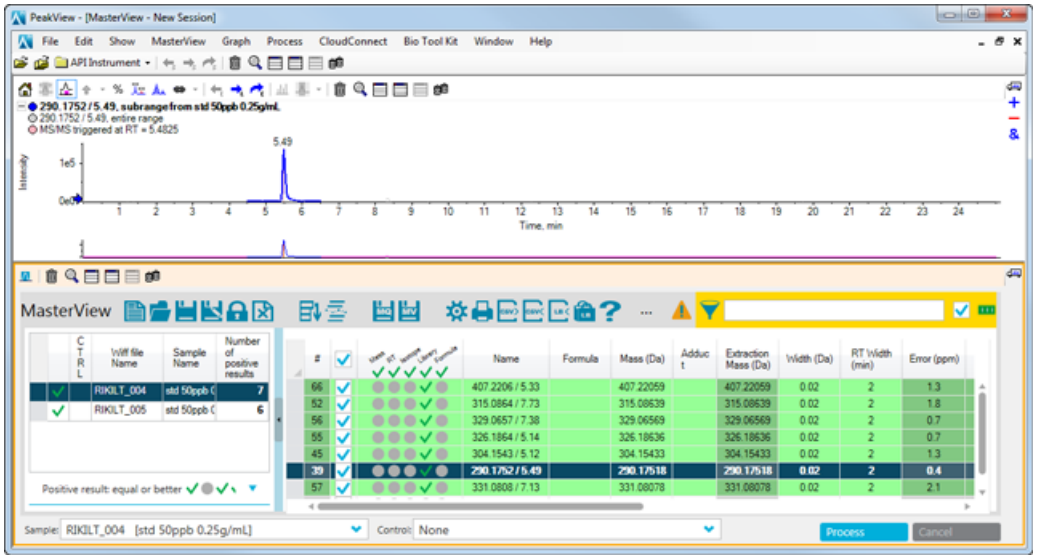
Note: To make sure that the isobaric compounds (compounds with the same accurate mass) are identified correctly, even if their product ion spectra are the same, specify the retention time in the XIClist in the MasterView™ software.

14. Click **Process**.

The MasterView™ software calculates the XIC for each sample included in the .wiff file and then performs the library search against the imported compound information from the library for each sample.

Tip! The number of compounds identified as a positive hit is shown in the **Number of positive results** column in the left pane. The search results, including the confidence levels, are shown in the right pane. The XIC rows corresponding to the positive hits are highlighted.

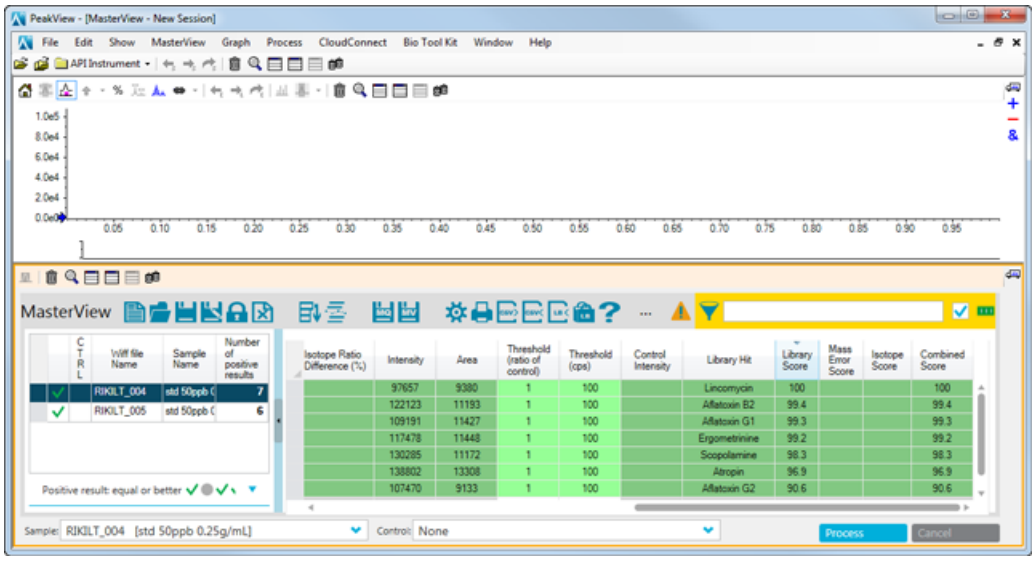
Figure 5-7 Library Search Result



15. While reviewing the qualitative results of the library search, use the following information:

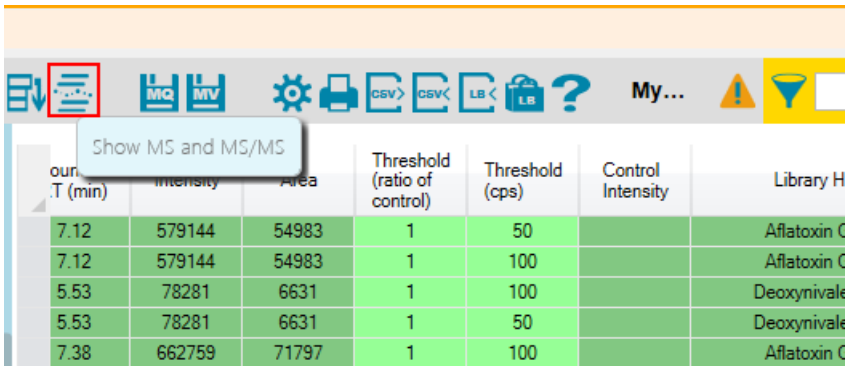
- Confidence in identification of compounds is visualized using the RT and library traffic lights.
- Numeric values can be found in many columns, for example, the **Library Score** column. Any of these columns can be used to sort results.

Figure 5-8 Library Search Results Sorted by Library Score



- The MS/MS spectrum can be visually compared to the library spectrum by clicking the **Show MS/MS** icon.

Figure 5-9 Show MS and MS/MS Icon



- Results can be reported using customizable report templates.

16. Click **Save Session**.

Revision History

Revision	Reason for Change	Date
A	First release of document.	October 2015