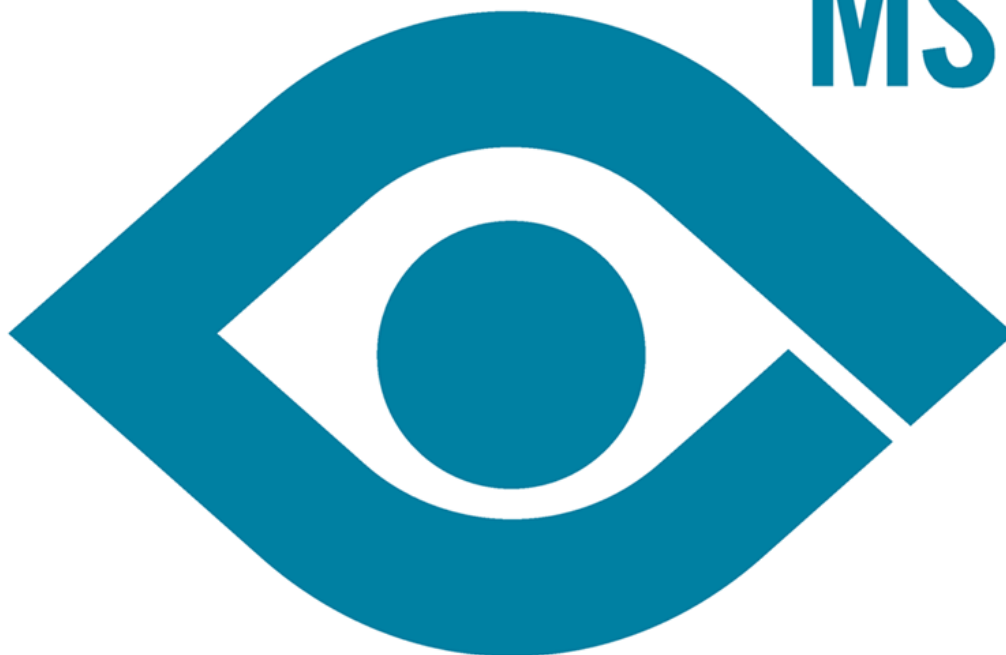


Accurate Mass Metabolite Spectral Library

Release Notes

MS



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Introduction and Features

The Accurate Mass Metabolite Spectral Library 1.0 is designed for targeted library searching against high resolution product ion spectra. The library contains accurate mass MS/MS spectra for each compound in the library.

- Compatible with data acquired using the TripleTOF® 5600/5600+ and TripleTOF 6600 systems.
- Compatible with MasterView™ 1.1 software with PeakView® 2.2 software combination and LibraryView™ 1.0 software. Compatible with MasterView 1.0 with PeakView 2.1 software combination.
- Helps to accurately identify compounds and confidence of reported result.
- Enables rapid searching in the MasterView software.
- Leverages the accurate mass, retention time, and peak area reporting functionality in the MasterView software.
- Fits well within the comparative profiling option in the MasterView software to compare a sample against a control for quick view.

Where to Get Help

Support

- support@absciex.com
- www.absciex.com
- Customer Documentation: techpubs@absciex.com

Requirements

- The Accurate Mass Metabolite Spectral Library requires an English version of the Microsoft Windows 7 (32- or 64-bit) operating system with SP1.
- PeakView® 2.2 software with MasterView™ 1.1 software combination or LibraryView™ 1.0 software already installed on the computer.
- A valid license file to use the Accurate Mass Metabolite Spectral Library.
- Internet access is required to obtain a license for the software.

Supported Equipment

- TripleTOF[®] 5600/5600+ and TripleTOF 6600 systems.
- Dell Precision T3600 or a later model provided by AB SCIEX is the recommended computer model.

Install the Library

The Accurate Mass Metabolite Spectral Library can be installed from a DVD or from a Web-downloadable package from the AB SCIEX website.

Installation using the Metabolite Spectral Library DVD

1. Log on to the computer as a Microsoft Windows user with Administrator privileges.
2. Insert the **Accurate Mass Metabolite Spectral Library 1.0 DVD** in the DVD drive.
3. Click **Install Accurate Mass Metabolite Spectral Library**.
4. Follow the on-screen instructions.
5. Follow the steps in [Import the Metabolite Spectral Library into the LibraryView Database](#).

Installation Using the Metabolite Spectral Library Web Download Package

1. Log on to the computer as a Microsoft Windows user with Administrator privileges.
2. Download the Accurate Mass Metabolite Spectral Mass Library Web-download package **AccurateMassMetaboliteSpectral-WebRelease.zip** on your system from <https://licensing.absciex.com/download/index>.
3. Extract the files from the compressed Web-download package to the local hard drive. On the Windows 7 operating system (OS), the unzip feature is available by default and an additional WinZip application is not required.

For Windows 7 OS, unzip the web download package using the following steps:

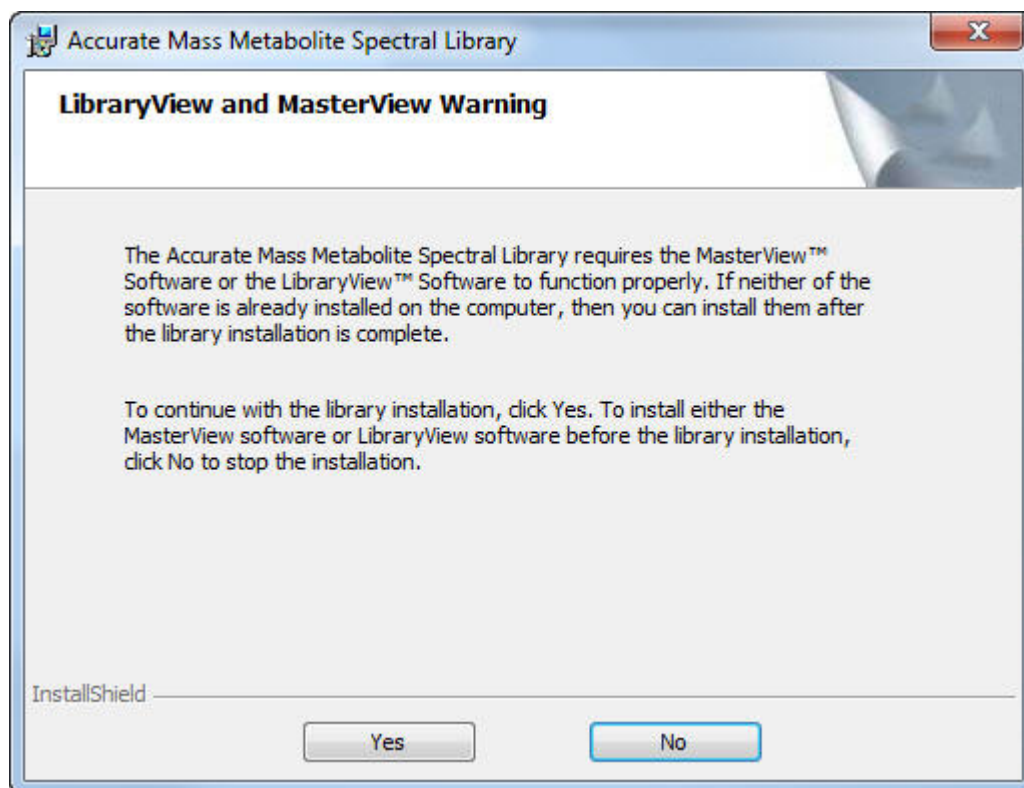
- a. Right-click the downloaded file **AccurateMassMetaboliteSpectral-WebRelease.zip**, and then click **Extract All**.
 - b. To make sure that all of the files are correctly extracted, select an accessible folder on the local computer or the network to extract the zipped files.
4. Navigate to the folder where the contents of the AccurateMassMetaboliteSpectral-WebRelease.zip file were extracted.

Accurate Mass Metabolite Spectral Library Release Notes

5. Double-click the **Accurate Mass Metabolite Spectral Library.exe** application.
6. Click **Yes** if the **User Account Control** dialog opens.

The installer checks for the presence of either of the prerequisite software, the LibraryView software or the MasterView software. Either of the software must be installed on the computer for the Accurate Mass Metabolite Spectral Library to work. If neither of the two software are found on the computer, then the following message is shown.

Figure 1-1 Warning Message



7. Click **Yes**.
The **InstallShield Wizard** opens.
8. Click **Next**.
The **License Agreement** dialog opens.
9. Accept the terms in the agreement.
10. Click **Next**.
11. Click **Install**.
The Metabolite Spectral Library installation begins.

12. Click **Finish** after the installation is completed.

The installer creates a folder for the Accurate Mass Metabolite Spectral Library in the **Start > All Programs > AB SCIEX > Accurate Mass Metabolite Spectral Library** . The library and user documentation are copied in that folder.

13. Follow the steps in [Import the Metabolite Spectral Library into the LibraryView Database](#).

Import the Metabolite Spectral Library into the LibraryView Database

Before importing the Metabolite Spectral Library into the LibraryView Database, make sure to install either the MasterView™ 1.1 or LibraryView™ 1.0 software on the computer. Refer to the installation guide for these software.

1. Click **Accurate Mass Metabolite Spectral Library** option in **Start > All Programs > AB SCIEX > Accurate Mass Metabolite Spectral Library** .

Tip! If the LibraryView Package has stopped working message is shown, then do the following:

- a. Close the program.
- b. Right-click the **Accurate Mass Metabolite Spectral Library** option in **Start > All Programs > AB SCIEX > Accurate Mass Metabolite Spectral Library** and then, click **Run as administrator**.

The LibraryView Package starts extracting.

2. Click **Yes** if the **User Account Control** dialog opens.
3. On the **LibraryViewPackages Feature Unavailable** dialog, click **Software Activation**.
4. In the **LibraryViewPackages Activation** dialog, type the license key for the package.

Note: If the license key field is already populated, delete the existing entry and then type the license key for the Metabolite Spectral Library.

5. Click **Generate Computer ID**.

This creates a unique identifier for the workstation.

6. Click **Copy ID to Clipboard**.
7. Click the <http://licensing.absciex.com/activation/LibraryViewPackages> link.
8. Follow the instructions to obtain the license.

Note: If the workstation does not have Internet access, make copies of the license key and the generated computer ID and then go to a computer that has Internet access. Go to <http://licensing.absciex.com/activation/LibraryViewPackages> and then follow the instructions to obtain the license.

After the required information is submitted, a license file is emailed to all email addresses provided.

9. Close the browser window.
10. When the e-mail containing the license file is received, copy the license file to the workstation desktop.
11. In the **LibraryViewPackages Activation** dialog, click **Install License File**.
12. On the **Select the new license file to be installed** dialog, browse to and then select the license file.
13. Click **Open**.

Both the **Select the new license file to be installed** and **LibraryViewPackage Activation** dialogs close.
14. Click **OK** in the License installed successfully message.
15. In the **Library Importer** dialog, do one of the following:
 - To import all compounds, select the **All** option.
 - To import individual compounds, select the required compound name in the right pane.
 - To import a library and the associated compounds, select the required library name in the Library Name pane. For this example, click the **Metabolites** library name to import all of the compounds of the Accurate Mass Metabolite Spectral Library.

Note: Compounds stored in the library are automatically selected in the compound list.

16. Click **Next**.

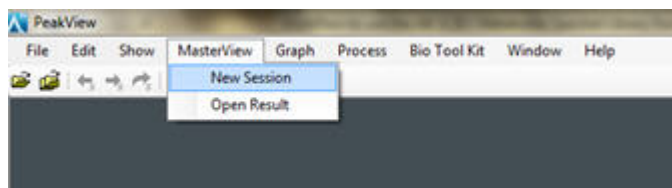
All of the compounds in the selected library start to be imported.
17. Resolve any conflicts, if required. Refer to Compound Conflicts in the *MasterView Software Help* or *LibraryView Software Help*.
18. Click **Finish**.

Import the Metabolite Spectral Library into the MasterView Software

1. Launch the **PeakView 2.2** software.

2. Select **MasterView** > **New Session** from the **PeakView** software menu.

Figure 1-2 New Session Option in the MasterView Software



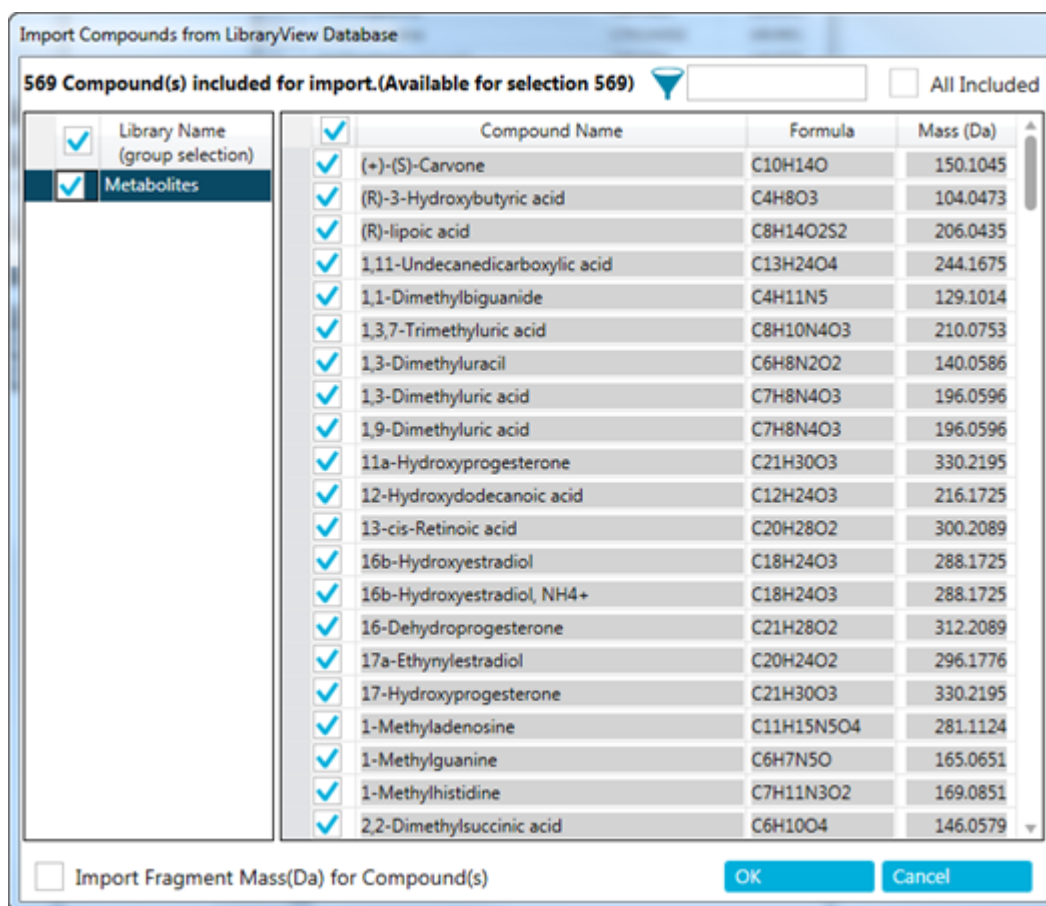
3. Using the **Select Samples** dialog, open appropriate data files.
4. Click the **Import Compounds Info From LibraryView** icon.

Figure 1-3 Import Compounds from LibraryView Database



5. In the **Import Compounds from LibraryView Database** dialog, click **Metabolites** check box to import all the compounds in the library. Refer to *Import Compound Information from the LibraryView Software Database* in the MasterView Software Help.

Figure 1-4 Import Compounds from LibraryView Database Dialog



6. Click **OK**.

The **Import Compounds from LibraryView Database** dialog closes, and the compound information is shown in the session pane.

Import the Metabolite Spectral Library into the LibraryView™ Software

The LibraryView™ 1.0 software is already installed on the computer.

Note: When the Accurate Mass Metabolite Spectral Library is imported into the LibraryView Database, the library automatically becomes available in the LibraryView software.

Notes on Use, Known Issues, and Limitations

Isoelemental compounds with the same MS/MS pattern

Isoelemental compounds with the same MS/MS pattern need to be differentiated by their retention time.

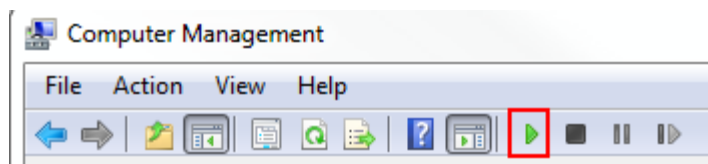
The LibraryView service stops responding intermittently

On Microsoft Windows 7 (64-bit) operating system, when trying to start the MasterView software from the PeakView software, the LibraryView service stops responding intermittently. To resolve this issue, do the following:

1. In **Windows Explorer**, right-click **Computer** and then click **Manage**.
2. In the **Computer Management** window, click **Services and Applications** and then double-click **Services**.
3. Right-click **LibraryViewServiceHost**, and then click **Start**.
4. Click **LibraryViewServiceHost** and then click **Play** on the toolbar.

This will help to start the LibraryView service again.

Figure 1-5 Computer Management Window



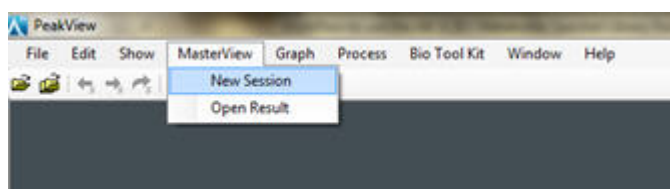
Workflow to use the Metabolite Spectral Library Searching in the MasterView Software

2

This section describes the steps to search the TripleTOF[®] 5600/5600+ and TripleTOF[®] 6600 systems data using a targeted list of known compounds and a metabolite library with high resolution MS and MS/MS spectra.

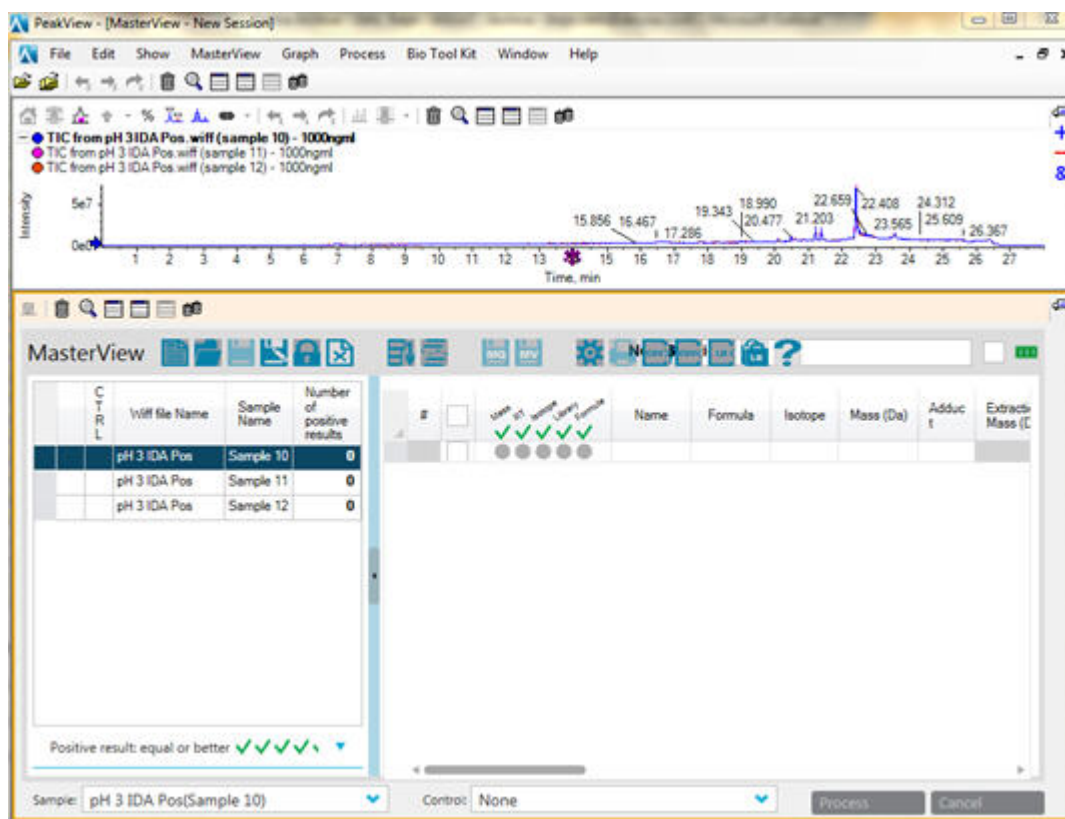
1. Start the **PeakView 2.2** software.
2. Click **MasterView > New Session** from the **PeakView** software menu.

Figure 2-1 New Session option in MasterView



3. Using the **Select Samples** dialog, open the appropriate data files.

Figure 2-2 MasterView - New Session Window



4. Open an XIC list (.XIClist file) related to either positive or negative mode data. For more information, refer to the MasterView Software Help.

Figure 2-3 Open XIC List

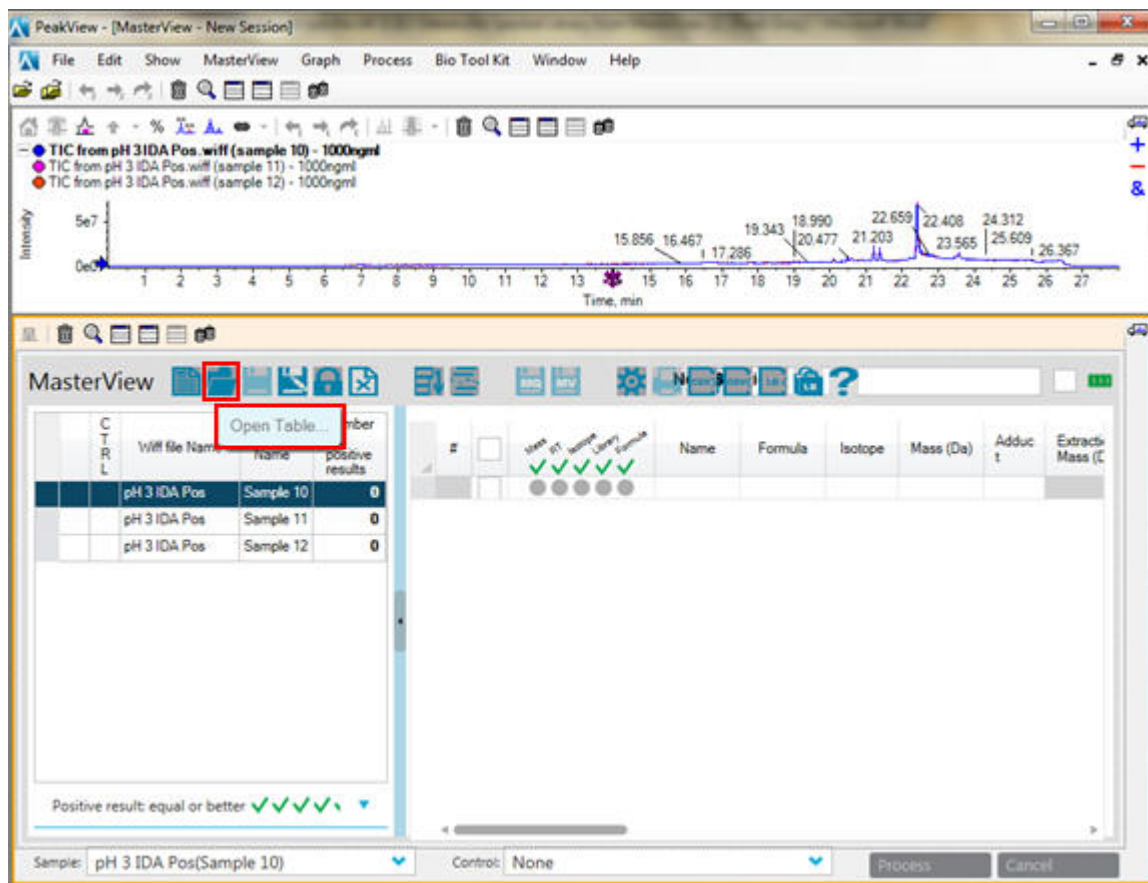
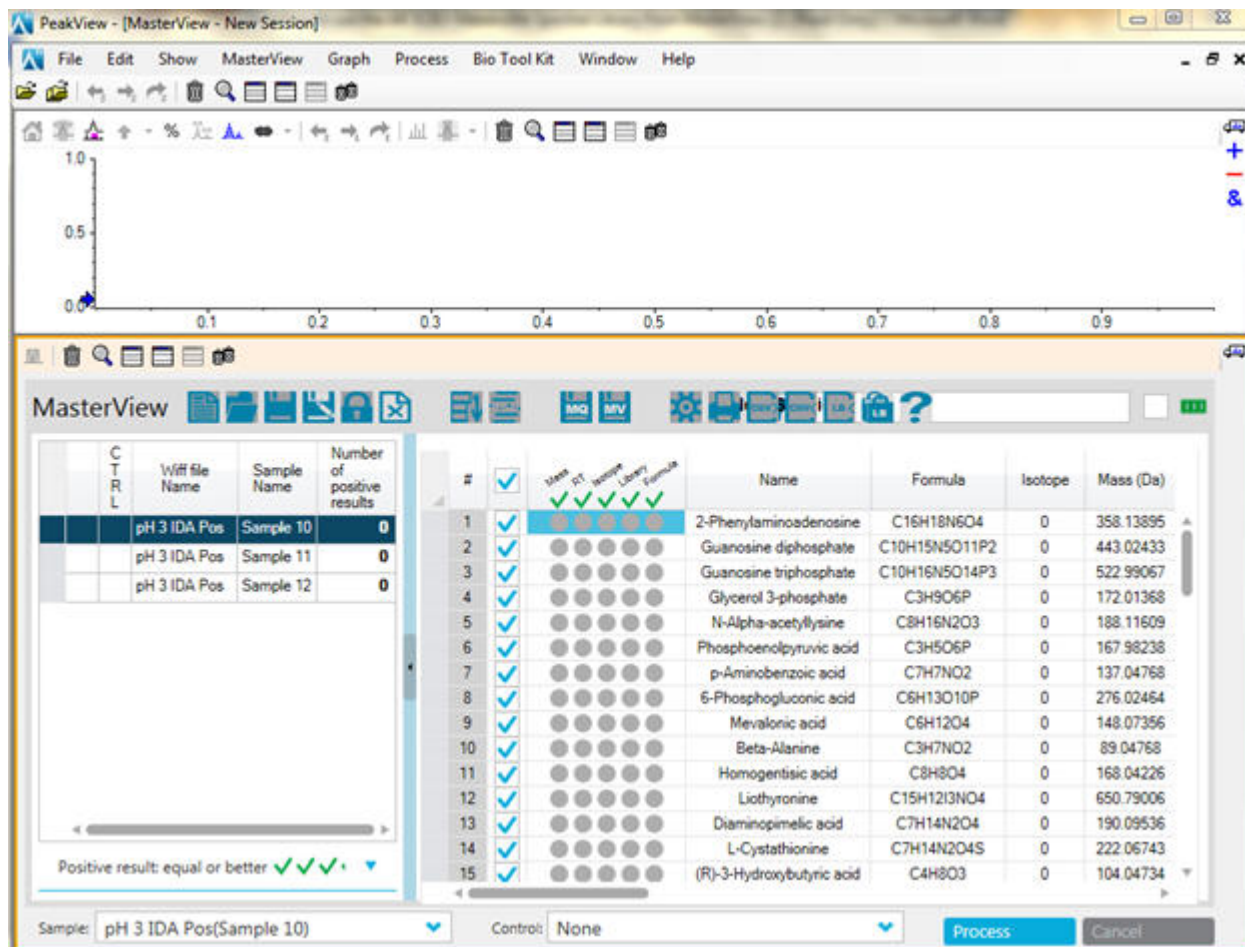


Figure 2-4 XIC List Open in Session Table



The XIC list information is shown in the session table. When the library is run for the first time, there is no retention time information. To populate the **Expected RT** column, do the following:

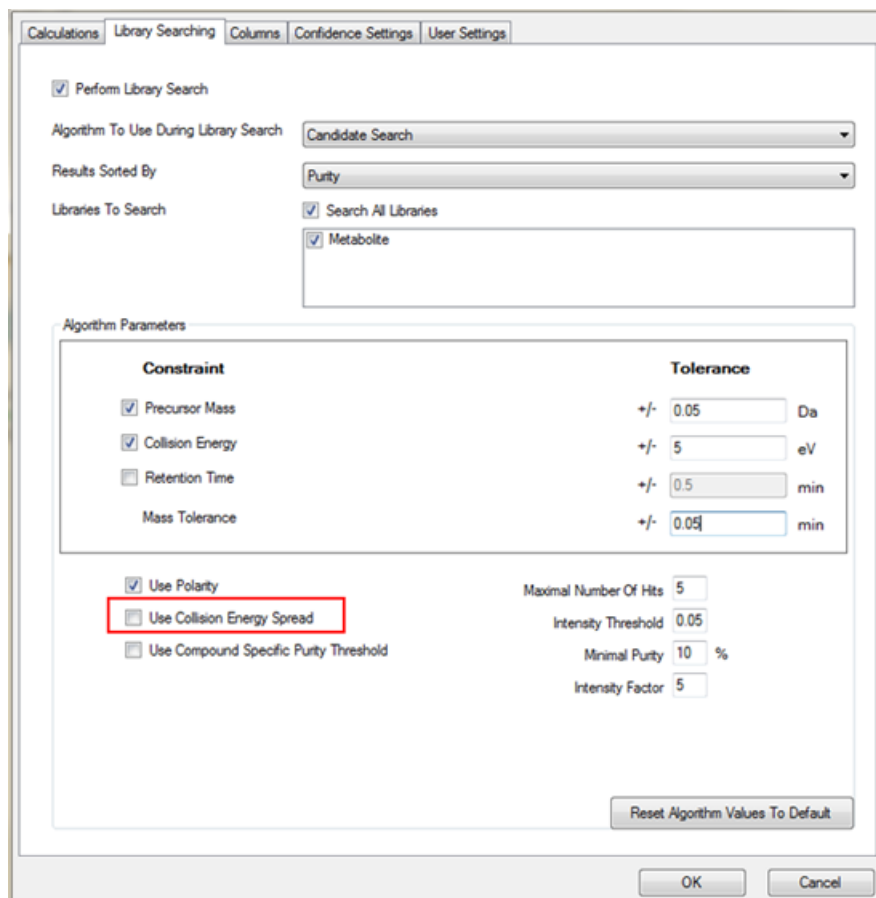
- a. Process the first dataset.
 - b. Copy the contents of **Found At RT** column and then paste into the **Expected RT** column.
 - c. Save that XIC list and use it in future to process because it now includes the retention times.
5. Click **Settings** to edit the settings for data processing and library searching.

Figure 2-5 Settings Icon



6. In the **settings** dialog, select the **Library Searching** tab.
7. In the **Libraries to Search** section, click the Metabolite Spectral 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.
8. Clear the **Use Collision Energy Spread** check box.

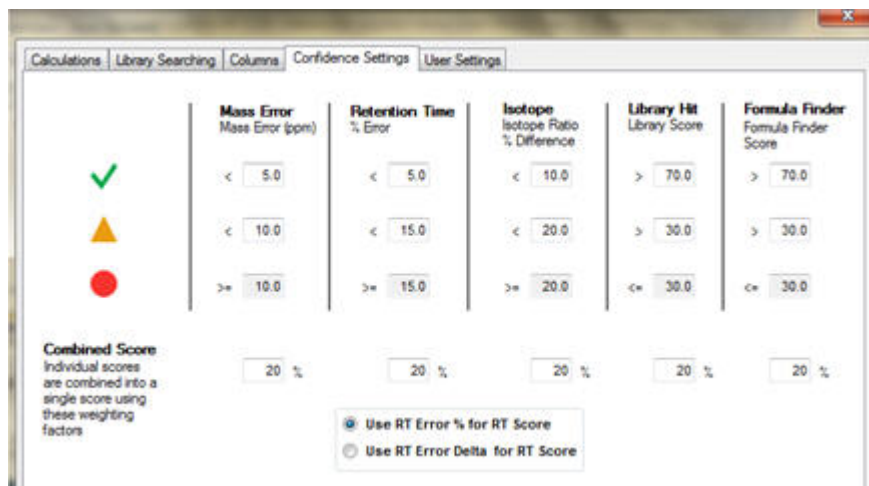
Figure 2-6 Library Searching Tab



Note: For information about the different options in the **Settings** dialog, refer to the MasterView Software Help.

- Click the **Confidence Settings** tab to define the criteria for acceptance of an identification based on a traffic light system. Use the default settings for this example.

Figure 2-7 Confidence Settings Tab



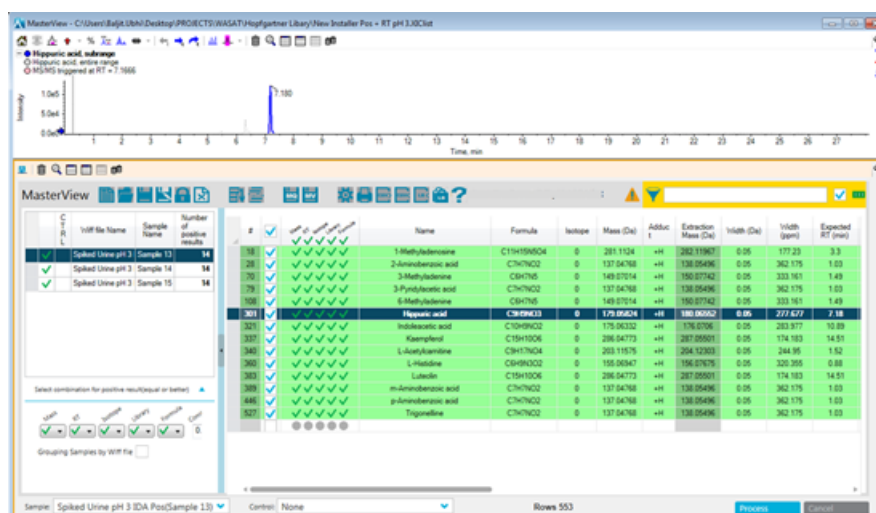
Note: All settings are saved with the XIC list.

Note: To make sure that the isoelemental compounds (compounds with the same accurate mass) are identified correctly, even if their MS/MS is the same, specify the retention time in the XIC list in the MasterView software.

- Click **Process**.

Using the information in the XIC list, the MasterView software calculates the XIC for each sample included in the .wiff file and then performs the library searching against the Metabolite Spectral library for each sample. The number of compounds identified as a positive hit is shown in the sample pane. The search results, including the confidence level, are shown in the session pane. The XIC rows corresponding to the positive hits are highlighted.

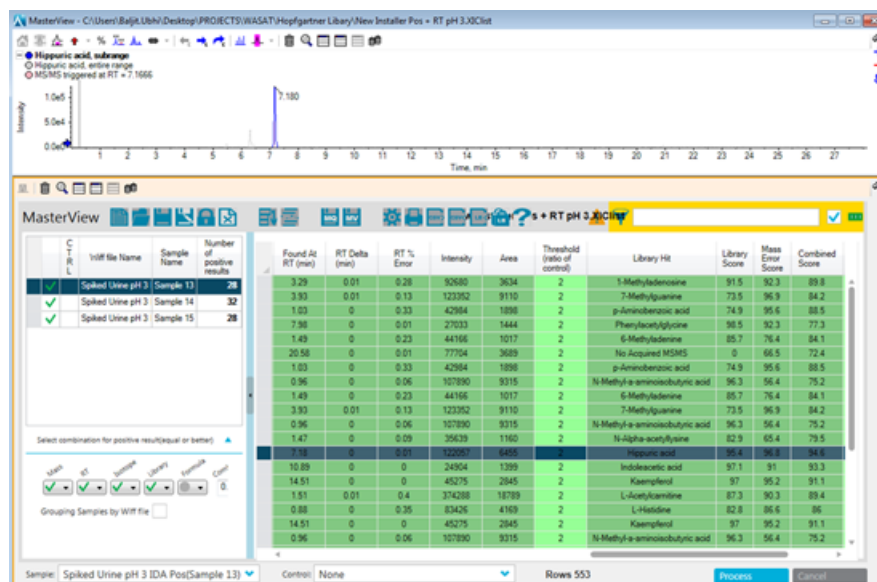
Figure 2-8 Library Search Result



11. 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 light.
- Numeric values can be found in the RT % Error and Library Score column. Any of these columns can be used to sort results.

Figure 2-9 Library Search Results: Use Library Score column to sort results



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

Figure 2-10 Show MS and MS/MS option



12. While reviewing the quantitative results of the library search, use the following information:

- Results can be reported using customizable report templates.
- Additional library searching and reporting functionality is available in the LibraryView™ software.

Revision History

Revision	Reason for Change	Date
A	First release.	December 2014