Accurate Mass Metabolite HR-MS/MS Spectral Library 2.0

Release Notes

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Introduction 1

Features

The Accurate Mass Metabolite HR-MS/MS Spectral Library 2.0 replaces the Accurate Mass Metabolite Spectral Library and the Metabolite HR-MS/MS 1.0 Library. Ninety-three new metabolites were added to the Accurate Mass Metabolite HR-MS/MS Spectral Library 2.0. The additional LC-MS/MS spectra were obtained using a TripleTOF® 6600 system and the SCIEX X500R QTOF system.

The library is compatible with:

- Data processed using a combination of the MasterView™ 1.1 Software and the PeakView® 2.2 Software, on any TripleTOF® or any QTRAP® systems.
- Data acquired using SCIEX OS 1.4 or higher, on a SCIEX X500R QTOF system.

Use this library in the MasterView™ Software and in SCIEX OS to:

- Accurately identify compounds and increase confidence in the reported results.
- Enable rapid compound searches for targeted and non-targeted screening.
- Leverage the accurate mass and peak area reporting functionality.
- Compare a sample against a control for qualitative review, using the comparative profiling functionality.

Requirements

SCIEX OS	MasterView™ Software
An English version of: • Windows 7, 64-bit, operating system, with SP1. • Windows 10, 64-bit, operating system.	An English version of: • Windows 7, 64-bit, operating system, with SP1. • Windows 10, 64-bit, operating system.
The user must be logged on to the computer as a user with Administrator privileges.	The user must be logged on to the computer as a user with Administrator privileges.

SCIEX OS	MasterView™ Software
Internet access is required to obtain a license file for the library.	Internet access is required to obtain a license file for the Library.
A licensed version of the LibraryView™ Software, version 1.3 or higher, is required to edit the library.	• A licensed version of the LibraryView™ Software, version 1.0.3 or higher, is required to edit the library. • A licensed version of the PeakView® software, version 2.2 or higher.

Supported Equipment

- TripleTOF® 5600+ System
- TripleTOF® 6600 System
- SCIEX X500 QTOF accurate mass system
- QTRAP® system

Notes on Use and Known Issues 2

Notes on Use

Accurate Mass Metabolite HR-MS/MS Spectral Library 2.0

The Accurate Mass Metabolite HR-MS/MS Spectral Library 2.0 Library contains:

- an updated version of HR-MS/MS spectra for some of the metabolites distributed in the Accurate Mass Metabolite Spectral Library
- an updated version of HR-MS/MS spectra for some of the metabolites distributed in the Metabolite HR-MS/MS 1.0 Library
- HR-MS/MS spectra for 93 new metabolites that have been added to the Accurate Mass Metabolite HR-MS/MS Spectral Library 2.0

The spectra were acquired using a TripleTOF® 5600+ System, a TripleTOF® 6600 System, or a SCIEX X500R QTOF System.

Installation of a New Metabolite Library

Refer to Install a Licensed High Resolution Accurate Mass Library for instructions on installation.

Upgrade to an Existing Metabolite Library

- The Accurate Mass Metabolite HR-MS/MS Spectral Library 2.0 includes compounds with names that are similar to the compound names in the existing libraries. We recommend that users export and then remove the previous library before importing the new Accurate Mass Metabolite HR-MS/MS Spectral Library 2.0.
- If there are no custom-added spectra in the existing library, then create a backup of the library by exporting it as a LibraryView Package. Delete the existing library and empty the trash before importing the new Accurate Mass Metabolite HR-MS/MS Spectral Library 2.0.

To prevent the loss of customer added spectra, click **Edit Mode** in the LibraryView™ Software and do the following:

- Assign a unique name to existing compounds by adding "compound_lab name" to the compound name.
- Click **X** on the spectra entry in the LibraryView™ Software to delete all of the data from the compound and keep only the customer-appended spectra.

  Note: A licensed version of the LibraryView™ Software is required to delete compound spectra.

- Change the name of the existing library to create a version of the custom added spectra that can be kept indefinitely.

Isobaric compounds with the same HR-MS/MS pattern

Since the isobaric compounds have similar product ion spectra, they are differentiated by the retention time.

Known Issues

The LibraryViewServiceHost software occasionally stops responding

On the Windows 7, 64-bit, operating system, when the MasterView™ Software is opened from the PeakView® Software menu bar, the LibraryViewServiceHost service occasionally stops responding.

To resolve this issue, do the following:

1. In File 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.

The LibraryView™ Software occasionally stops responding when loading the library or results are not found when searching the library

To resolve these issues, do the following:

1. Make sure that the computer contains 32 GB RAM.
2. Start the computer again.
3. If the issue persists, then contact SCIEX Technical Support at sciex.com/request-support and request that the SQL databases be cleared and that the libraries be installed again.

SCIEX OS and the MasterView™ Software occasionally stop responding when the Import compounds from LV database feature is used

To resolve this issue, restart the software.

The **Import compounds from LV database** feature is used to import compound names and formulas from the library into SCIEX OS and the MasterView™ Software.

Installation 3

Install a Licensed High Resolution Accurate Mass Library

A licensed library can be installed from a DVD or from a zip application file downloaded from the SCIEX website. For each library compound, the application file can include compound names, CAS number, precursor *m/z*, mol file, collision energy, collision energy spread, and HR-MS/MS spectra (positive and negative).

Note: Internet access is required to obtain the license.

1. Log on to the computer as a 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 website.

   Tip! To prevent potential installation issues, save the file to a location other than the computer desktop and disconnect any external USB storage devices.
4. After the download is complete, right-click the downloaded file and then click **Extract All**.
5. Go to https://sciex.com/support/activate-software.
6. Click **login**.
7. Do one of the following:
   - Type the **Email Address** and **Password** of an existing account and then click **Log in**.
   - Click **Create An Account** and then follow the instructions provided.

   After the log on or account creation is completed, the Activate Software web page opens. The first name, last name, and e-mail address of the user are shown in the first three fields in the form.
8. Select the appropriate instrument in the **Select Your Instrument** field.

   Tip! If the instrument is not listed, then go to the SCIEX Now™ profile for the logged in user and add the instrument information.

9. In the Windows search field, type **ipconfig /all** to obtain the physical addresses, that is, the MAC addresses of the computer.

   A physical address, in the format "34-02-86-06-8A-05", is shown for each active adapter.

10. Type the physical addresses in the **Computer ID** field.

    Tip! A maximum of three physical addresses can be provided. Separate each address with a space. For example, 34-02-86-06-8A-05 34-02-86-06-8A-01 34-02-86-06-8A-09.

11. Type the license key from the license card in the **License Key** field.

    Note: The key begins with the letters AID. If a license key is not available, then contact sciex.com/request-support.

12. Click **Submit**.

    A message is shown indicating that an e-mail with the license file will be sent.

13. Save the license file to the appropriate location:

    - On a computer with the MasterView™ Software installed, save the license file in the C:/Program Files/AB Sciex/LibraryView/LibraryViewFramework/Server folder.
    - On a computer with the SCIEX OS installed, save the license file in the C:/Program Files/SCIEX/LibraryView/LibraryViewFramework/Server folder.

14. In the Windows search field, type **libraryviewpackager.exe** and then run the file.

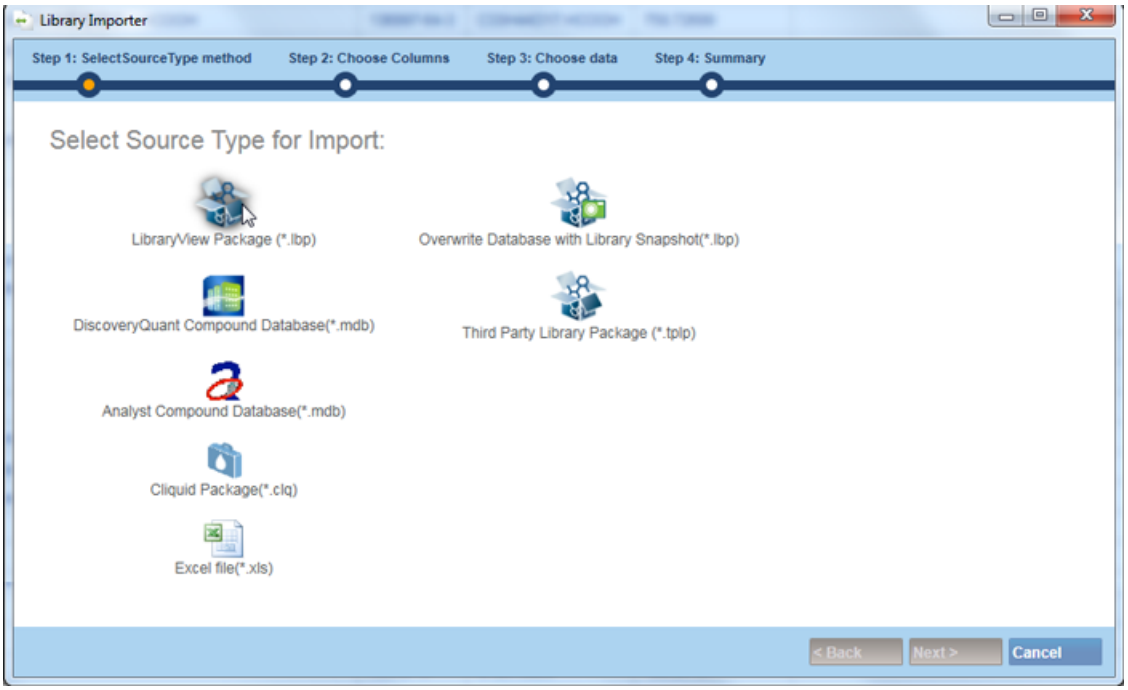
    Note: The **libraryviewpackager.exe** can also be accessed from one of the following locations, depending on the version of the LibraryView™ Software that is installed:

    - On a computer with MasterView™ software installed, the **libraryviewpackager.exe** file is located in the C:/Program Files/AB Sciex/LibraryView/LibraryViewFramework/Packager folder.
    - On a computer with SCIEX OS installed, the **libraryviewpackager.exe** file is located in the C:/Program Files/SCIEX/LibraryView/LibraryViewFramework/Packager folder.

    The Library Importer dialog opens.

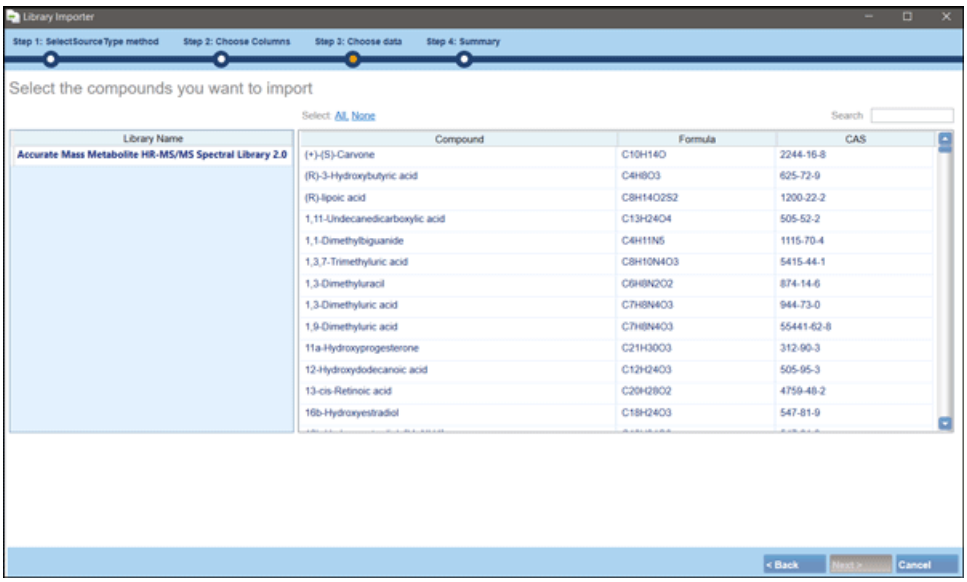
15. Click **LibraryView Package (.lbp)** on the Library Importer dialog.

Figure 3-1 Library Importer Dialog—Select Source Type for Import



16. Browse to the files extracted in step 4 or to the DVD and then select the Accurate Mass Metabolite HR-MS/MS Spectral Library 2.0 file.
17. Click **All** above the **Compound** column to import all of the compounds. Refer to Figure 3-2.

Figure 3-2 Library Importer Dialog—Select Compounds to Import



18. 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 will not revert the database to the pre-import state.

19. Resolve any conflicts, if required. Refer to Compound Conflicts.
20. Click **Finish** and then restart the computer.
21. If the LibraryView™ Software is installed, then create a backup of all of the libraries using the **Export > Library as snapshot (*.lbp)** feature after installation.

Note: If issues occur with any of the libraries, then the entire library can be imported as a snapshot more quickly than installing all of the libraries again using the lbp packages.

Compound Conflicts

When installing a library containing a group of compounds or installing individual compounds, the software searches 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 compound information. Compound information in the database is retained and the compound information from the package is discarded.

Conflict information is available to help the user make the correct choice.

View Compound Conflicts

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

Overwrite Compounds

To overwrite compounds, refer to Upgrade to an Existing Metabolite Library in Notes on Use.

1. Do one of the following on the Library Importer dialog:
   - Click **Overwrite All** 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 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 on the Library Importer dialog:
   - Click **Keep All Original** 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 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.

Recommended Library Search Settings

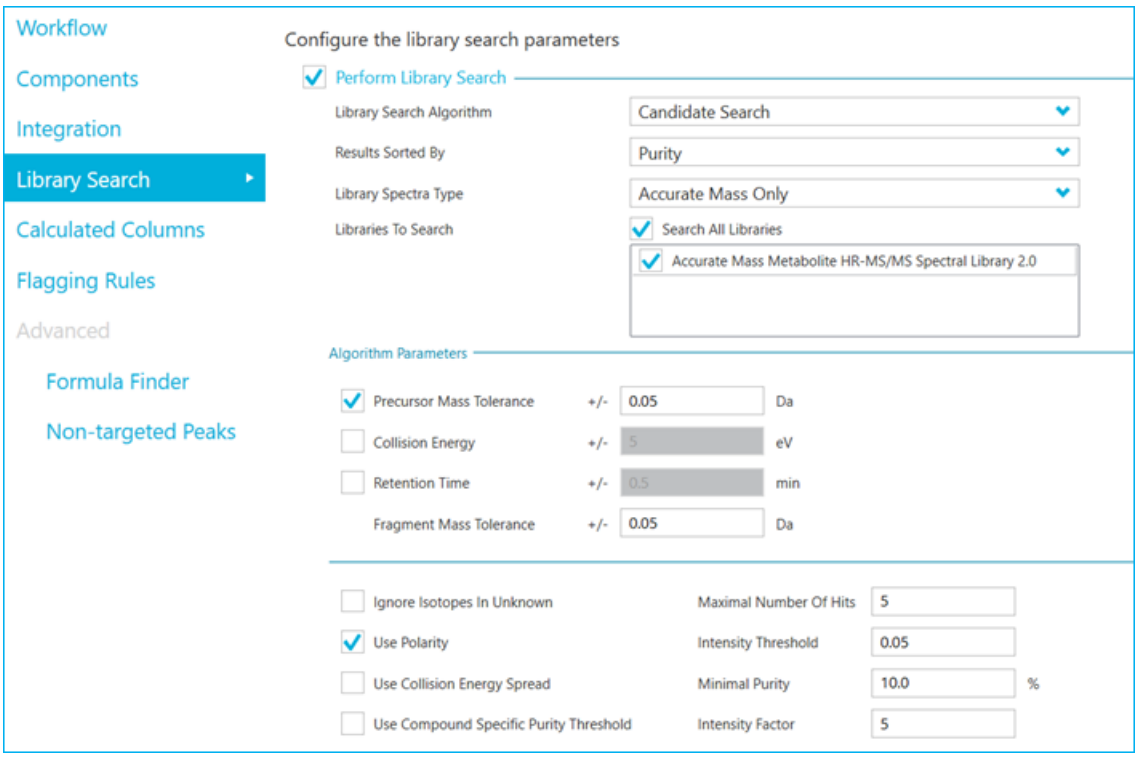
The Accurate Mass Metabolite HR-MS/MS Spectral Library 2.0 contains spectra from multiple instruments and spectra acquired at various Collision Energy (CE) settings. Therefore, the library search parameters must be carefully optimized to effectively search the library. Figure 3-3 shows the recommended library search settings for SCIEX OS.

Complete the following settings:

- Clear the **Collision Energy** check box, to prevent false negatives.
- Select the **Precursor Mass Tolerance** check box and then type 0.05 Da in the field provided.

- Set the **Fragment Mass Tolerance** to 0.05 Da.
- Reduce the **Intensity Threshold** to 0.02, if the fragment intensities fall below 0.05 (5%) of base peak.
- For QTRAP® system data, set **Precursor** and **Fragment Mass Tolerance** to 0.4

Figure 3-3 Recommended Search Settings for the Metabolite Library



For information about the library search parameters settings in the MasterView™ Software, refer to the *High Resolution Accurate Mass Libraries* Release Notes.

Contact Us

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- In Europe: Europe.CustomerTraining@sciex.com
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Online Learning Center

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