SCIEX
The Power of Precision

All-In-One HR-MS/MS Spectral Library 2.1

High Resolution Accurate Mass Libraries

Release Notes

RUO-IDV-03-12490-A

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Contents

Introduction 1

Features

The All-in-One HR-MS/MS Spectral Library 2.1 is an update to the existing All-In-One HR-MS/MS Spectral Library 2.0. The 1,710 Extractable and Leachable (E&L) compounds extracted from the NIST Standard Reference Database are added as NIST E&L HR-MS/MS 1.0 to the All-in-One HR-MS/MS Spectral Library 2.1.

These libraries are compatible with:

- Data acquired using a combination of the MasterView™ 1.1 Software and the PeakView® 2.2 Software, on a TripleTOF® accurate mass system or a QTRAP® system.
- Data acquired using SCIEX OS 1.4 Software or higher on a SCIEX X500 QTOF accurate mass system.

Use these libraries in the MasterView™ Software and in SCIEX OS to perform these tasks:

- Help accurately identify compounds and increase confidence in the reported results.
- Enable rapid compound searches for targeted and non-targeted screening.
- Leverage the accurate mass, retention time, and peak area reporting functionality in both the MasterView™ Software and SCIEX OS.
- Compare a sample against a control for qualitative review using the comparative profiling option available in both the MasterView™ Software and SCIEX OS.

Requirements

SCIEX OS	MasterView™ Software
An English (US) version of: • Windows 7 (64-bit) operating system with SP1. • Windows 10 (64-bit) operating system.	An English (US) 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 each installed High Resolution Accurate Mass (HRAM) library.	Internet access is required to obtain a license file for each installed High Resolution Accurate Mass (HRAM) Library.
At least one of the following applications is required to install a library: • A licensed version of SCIEX OS, version 1.4 or higher. • A licensed version of the LibraryView™ Software, version 1.3 or higher.	At least one of the following software applications is required to install a library: • A licensed version of the PeakView® Software, version 2.2 or higher and a licensed version of the MasterView™ Software, version 1.1 or higher. • A licensed version of the LibraryView™ Software, version 1.0.3 or higher
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.

Supported Equipment

- A TripleTOF® accurate mass system
- A QTRAP® system
- A SCIEX X500 QTOF accurate mass system
- A Dell Precision T3600 computer or later model provided by SCIEX, with a minimum of 32 GB of RAM

Notes on Use, Known Issues, and Limitations 2

All-In-One HR-MS/MS Spectral Library 2.1

The All-in-One HR-MS/MS Spectral Library 2.1 is an update of the All-In-One HR-MS/MS Library 2.0. The new Extractable and Leachable (E&L) compounds extracted from NIST Library are added as NIST E&L HR-MS/MS 1.0 sub Library.

Customers without any All-In-One HR-MS/MS Spectral Library 2.0

Refer to Installation.

Customers with existing All-In-One HR-MS/MS Spectral Library 2.0

- The All-In-One HR-MS/MS Spectral Library 2.1 has similar compound names to All-In-One HR-MS/MS Spectral Library 2.0.
- Import the NIST E&L HR-MS/MS 1.0 as a LibraryView Package (lbp) when adding as a new sub library.
- Use the existing active licenses, HRAIO2.0.lic and NIST1.0.lic, to read the NIST E&L HR-MS/MS 1.0 library.
- If customer-appended spectra have not been appended to the existing library, then backup all of the libraries by exporting them as a LibraryView Database Snapshot Package and save the package to another location in the computer.
- Import All-in-One HR-MS/MS Spectral Library 2.1 as Overwrite Database using the Library Snapshot.
- Use the existing active licenses, HRAIO2.0.lic and NIST1.0.lic to read the new All-In-One HR-MS/MS Spectral Library 2.1.
- To prevent the loss of customer-appended spectra, do the following:
  1. Use a unique compound name and then append it with "compound_lab name". For example, Triazine_QC.
  2. Click X on the spectra entry in the LibraryView™ Software to delete all the data from the compound and to save only the customer-appended spectra.
  3. Change the library name of the permanent storage of the customer-appended spectra.

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

Isobaric compounds with the same MS/MS pattern

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

The LibraryViewServiceHost stops responding intermittently

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 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.

The LibraryView™ Software occasionally stops responding while it is loading the library or results are not found when during searches of the library

To resolve these issues, do the following:

1. Make sure that the computer has 32 GB RAM available.
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

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. The application file can include compound names, compound transition information, and compound library spectra.

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 contonue 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.
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 and then log in using a SCIEX username and password.

   Note: If the user does not have an existing account, then follow the on-screen instructions to create an account.

   The Activate Software page opens.
6. 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.

7. 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.

8. Type all of 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.

9. 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.

10. Click **Submit**.

    After the required information is submitted, a license file is sent to the e-mail address registered to the SCIEX.com account.

11. Save the license file to the appropriate location:

    - On a computer with version 1.0.2 or 1.0.3 of the LibraryView™ Software installed, save the license file in the C:/Program Files/AB Sciex/LibraryView/LibraryViewFramework/Server folder.
    - On a computer with version 1.3 or 1.4 of the LibraryView™ Software installed, save the license file in the C:/Program Files/SCIEX/LibraryView/LibraryViewFramework/Server folder.

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

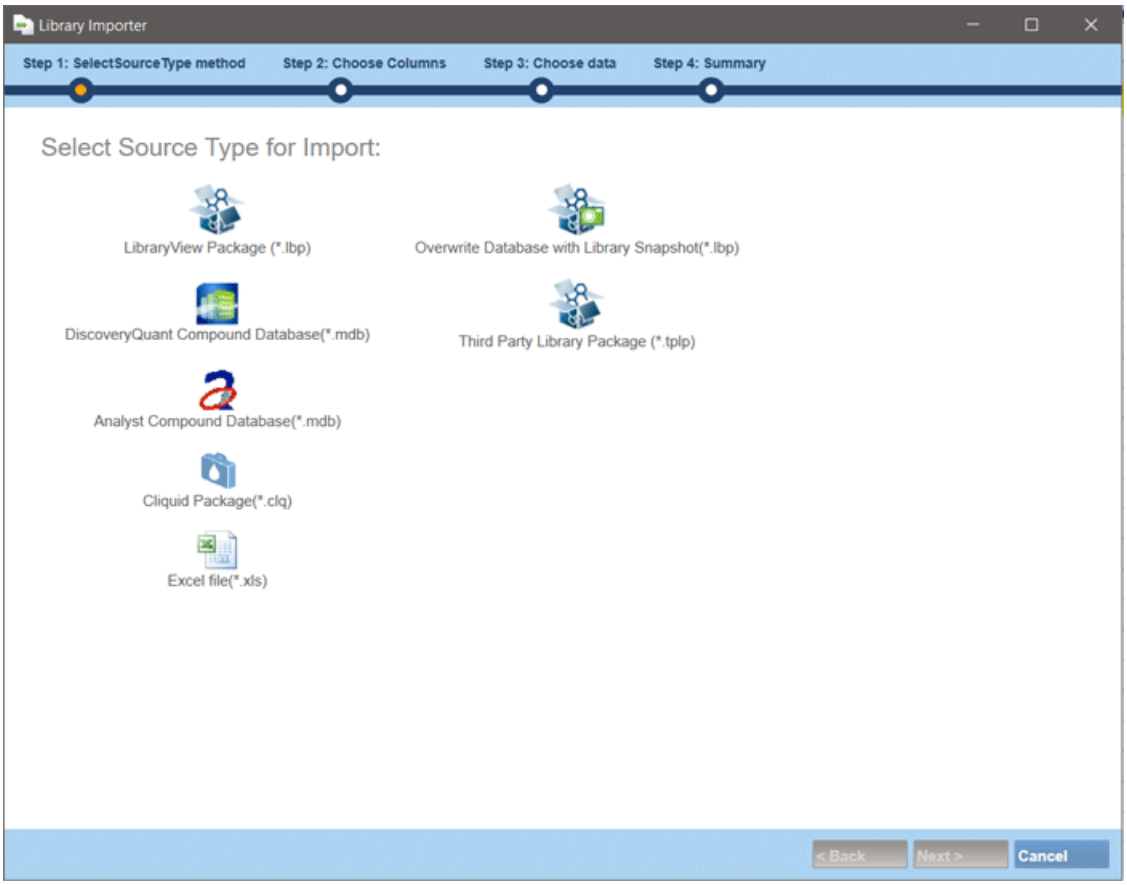
    Note: The **libraryviewpackager.exe** can also be accessed from one of the following locations, depending on the version of the LibraryView™ Software that is installed.

    - On a computer with version 1.0.2 or 1.0.3 of the LibraryView™ Software installed, the **libraryviewpackager.exe** file is located in the C:/Program Files/AB Sciex/LibraryView/LibraryViewFramework/Packager folder.
    - On a computer with version 1.3 or 1.4 of the LibraryView™ Software installed, the **libraryviewpackager.exe** file is located in the C:/Program Files/SCIEX/LibraryView/LibraryViewFramework/Packager folder.

    The Library Importer dialog opens.

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

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

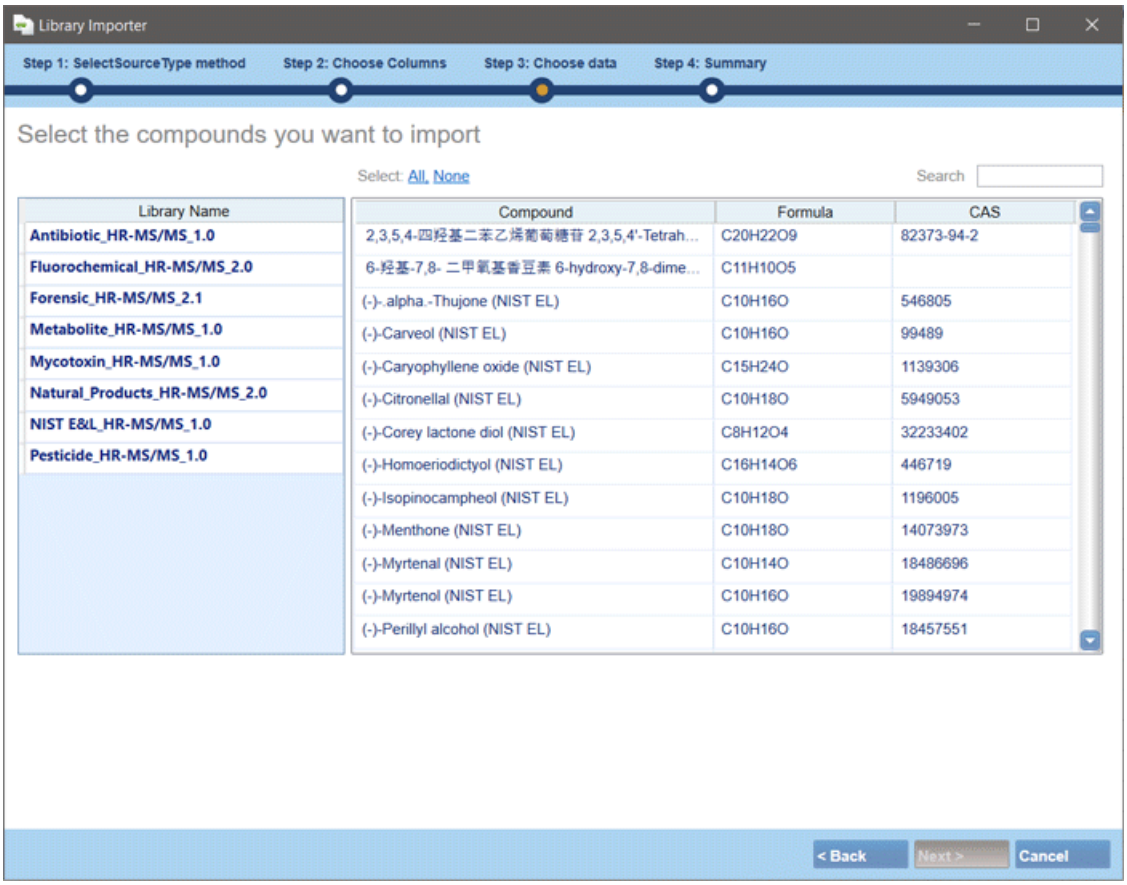


14. Browse to the files extracted in step 4 or to the DVD and then select the **All-In-One HR-MSMS Spectral Library 2.1.lbp** file.

15. Do one of the following:

    - Click **All** above the Compound column to import all of the compounds.

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



16. 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.

17. Resolve any conflicts, if required. Refer to Compound Conflicts.

18. Click **Finish**.

19. 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. On the Library Importer dialog, do one of the following:
   - 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

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.

Update Libraries that Contain Added Spectra

1. To prevent the loss of customer-appended spectra when libraries are updated, do the following:
   a. Append "compound_lab name" to the compound name.
   b. Click the 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.
   c. Import the new library.
2. Click **Finish** after all of the conflicts are resolved.

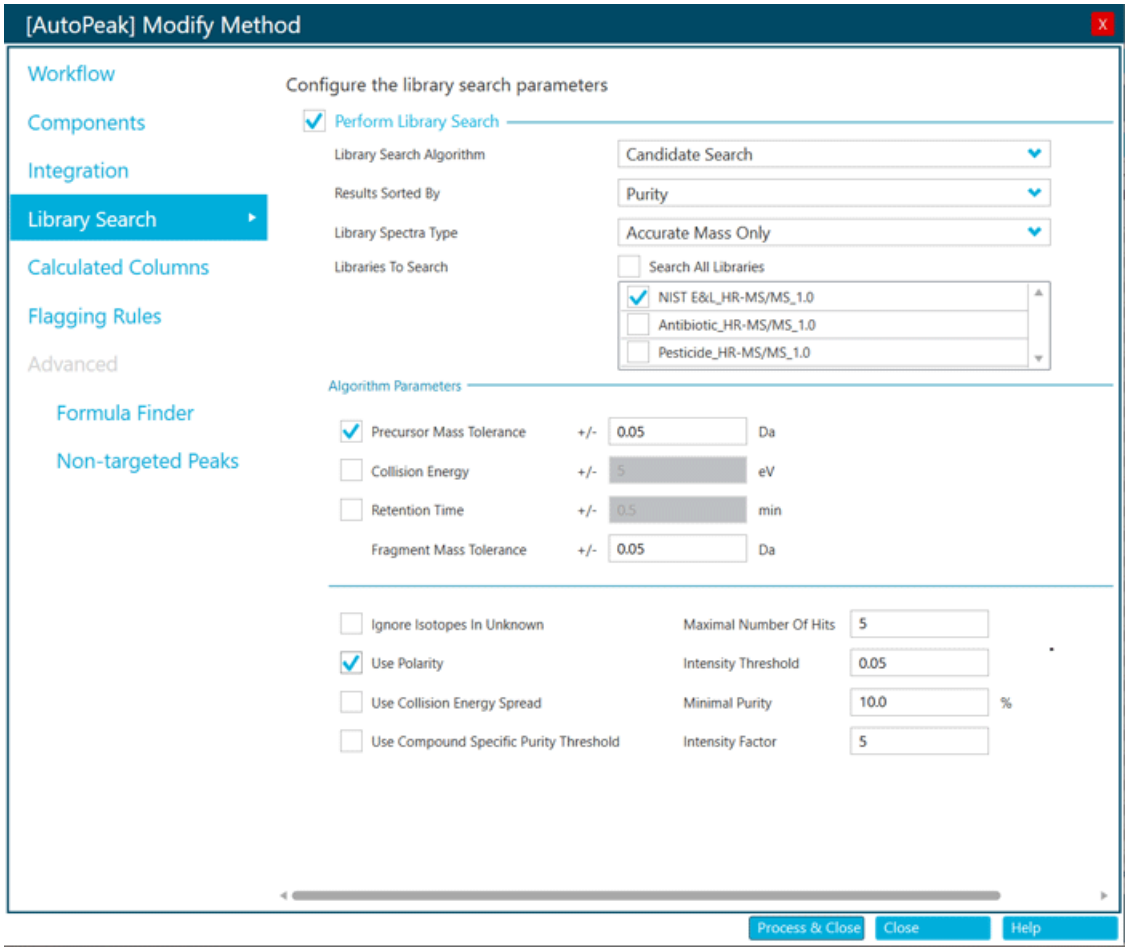
Note: A licensed version of LibraryView™ Software is required to delete compound spectra.

Recommended Library Search Settings

The All-In-One HR-MS/MS Library 2.1 contains spectra from multiple instrument platforms and spectra that is merged from multiple 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 the MasterView™ 1.1 Software and SCIEX OS 1.4. Complete the following settings:

- Deactivate the Collision Energy filtering to prevent false negatives.
- Set the Precursor Mass Tolerance to **0.05 Da** to accelerate the processing time.

Figure 3-3 Recommended Search Settings for the All-In-One HR-MS/MS Library 2.1



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

Contact Us

Customer Training

- In North America: NA.CustomerTraining@sciex.com
- In Europe: Europe.CustomerTraining@sciex.com
- Outside the EU and North America, visit sciex.com/education for contact information.

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- SCIEX University™

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SCIEX Support

SCIEX and its representatives maintain a staff of fully-trained service and technical specialists located throughout the world. They can answer questions about the system or any technical issues that might arise. For more information, visit the SCIEX website at sciex.com or contact us in one of the following ways:

- sciex.com/contact-us
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Note: For any questions or issues related to the StatusScope® Remote Monitoring Service, select **Instrument & Hardware** as the **Issue Type**.

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To find hardware product documentation, refer to the *Customer Reference* DVD that comes with the system or component.

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