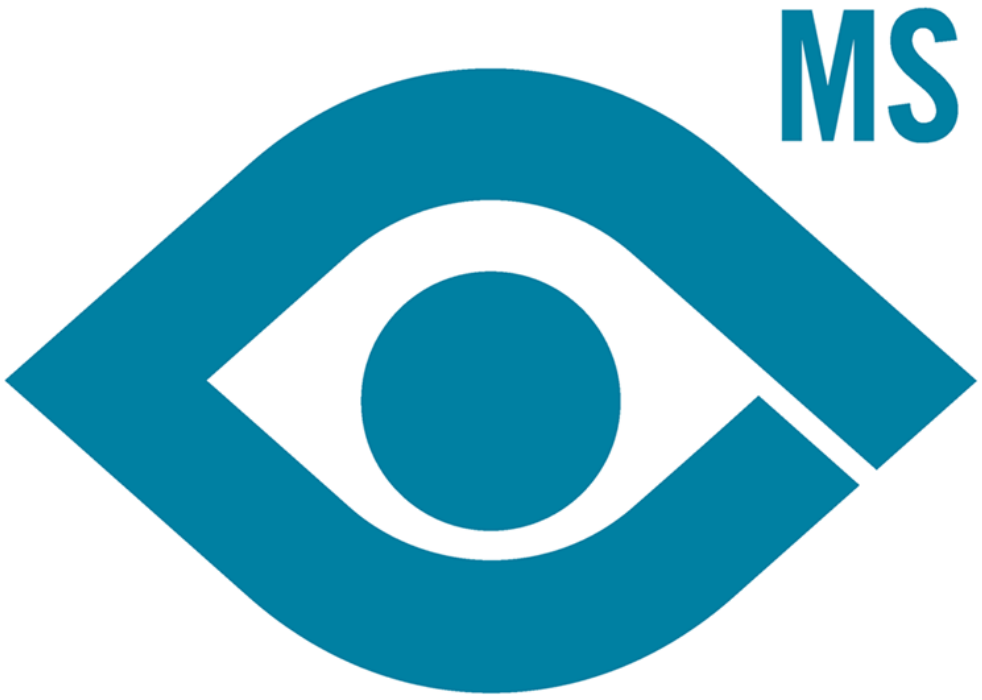
SCIEX
The Power of Precision

Forensic HR-MS/MS Spectral Library 2.2

High Resolution Accurate Mass Libraries

Release Notes



RUO-IDV-03-15764-A

October 2023

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(GEN-IDV-09-10816-E)

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AB Sciex Pte. Ltd.
Blk33, #04-06 Marsiling Industrial Estate Road 3
Woodlands Central Industrial Estate, Singapore 739256

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Introduction 1

Features

The Forensic HR-MS/MS Spectral Library 2.2 is an update to the existing Forensic HR-MS/MS Spectral Library 2.1. This verified library includes the High Resolution Accurate Mass Spectra for 1,747 forensic drugs and metabolites frequently tested in forensic samples, including blood and urine. Approximately, 261 drug entities, the chemical names, chemical formulas, and CAS No. have been updated with curated information in the Forensic HR-MS/MS Spectral Library 2.2 library.

These libraries are compatible with:

- Data acquired with the SCIEX OS software 2.1 or later on a QTOF accurate mass system or on a QTRAP system.

In the LibraryView 1.4 or later and the SCIEX OS software, use the libraries to do these tasks:

- Quickly and accurately identify compounds, with more confidence in the reported results.
- Quickly search for compounds for both targeted and non-targeted screening.
- Leverage the accurate mass, retention time, and peak area reporting functionality in the LibraryView software and SCIEX OS software.
- Use the comparative profiling option that is available in the SCIEX OS software to compare a sample to a control for qualitative review.

Requirements

SCIEX OS Software
An English (US) version of: • Windows 10 (64-bit) operating system.
The user must be logged on to the computer as a user with Administrator privileges.
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 the SCIEX OS software, 2.1 or later. • A licensed version of the LibraryView software, 1.4 or later.

SCIEX OS Software
A licensed version of the LibraryView software, 1.4 or later, is required to edit the library.

Supported Equipment

- A ZenoTOF 7600 accurate mass system
- An X500 QTOF accurate mass system
- A TripleTOF accurate mass system
- A QTRAP system
- A Dell Precision T3600 computer, or a later model, supplied by SCIEX, with a minimum of 32 GB of RAM

Notes on Use, Known Issues, and Limitations 2

The LibraryView software occasionally stops responding while it is loading the library, or results are not found during searches of the library

To correct 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 continues, 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.

The SCIEX OS software occasionally stop responding when the Import compounds from LV database feature is used

The Import compounds from LibraryView software database feature is used to import compound names and formulas from the library to the SCIEX OS software.

Installation 3

Install a Licensed Forensic HR-MS/MS Accurate Mass Library

A licensed library can be installed from a `zip` file downloaded from the SCIEX website. The `zip` file can contain 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. 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.
3. After the download is complete, right-click the downloaded file, and then click **Extract All**.
4. Go to https://sciex.com/support/activate-software, and then log on with a SCIEX username and password.

   Note: To create an account, follow the on-screen instructions to create an account.

   The Activate Software page opens.
5. Select the applicable instrument in the **Select Your Instrument** field.

   Tip! If the instrument is not listed, then go to the SCIEX Now profile for the logged-on user, and add the instrument information.
6. In the Windows search field, type `ipconfig /all` to get the physical (MAC) addresses of the computer.
   A physical address, in the format `34-02-86-06-8A-05`, is shown for each active adapter.
7. Type all of the physical addresses in the **Computer ID** field.

   Tip! A maximum of three physical addresses can be typed. Separate the addresses with a space. For example, 34-02-86-06-8A-05 34-02-86-06-8A-01 34-02-86-06-8A-09.
8. In the the **License Key** field, type the license key.

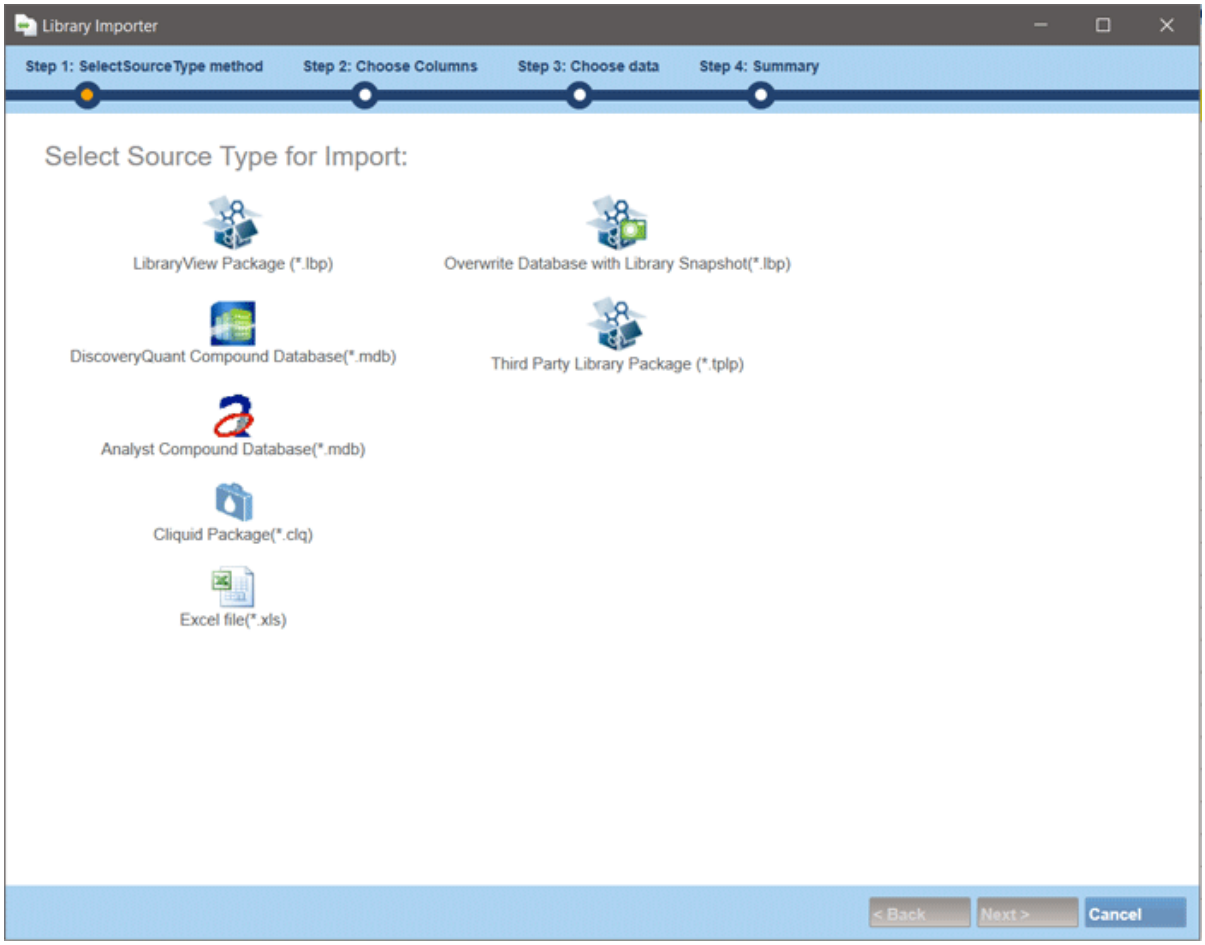
The license key might be distributed through an e-mail from SCIEX Now. If the license key is not available, then contact a SCIEX sales representative.

Note: The key begins with the letters AID.

9. Click **Submit**.
   After the required information is submitted, a license file is sent to the e-mail address registered to the SCIEX Now account.
10. Save the license file to the correct location:
    - On a computer with version 1.4 of the LibraryView (SCIEX OS software) software installed, save the license file in the `C:/Program Files/SCIEX/LibraryView/LibraryViewFramework/Server` folder.
11. As an alternative, the user can also do the following:
    a. To launch the library, run the `libraryviewpackager.exe` file located in the `C:/Program Files/SCIEX/LibraryView/LibraryViewFramework/Packager` folder.

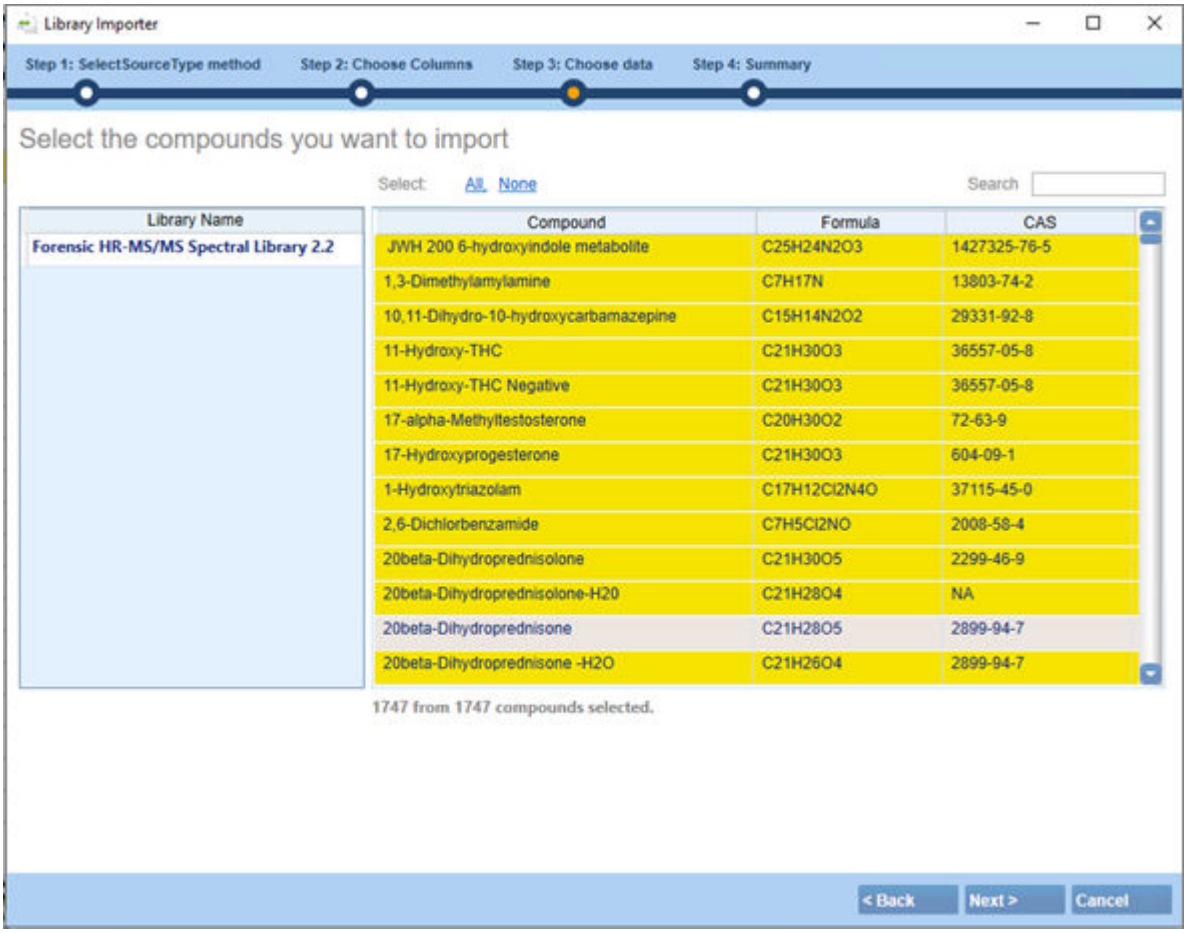
    The Library Importer dialog opens.
12. Click the **LibraryView Package (*lbp)** option on the Library Importer dialog.

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



13. Browse to the files extracted in step 3, and then select the `Forensic HR-MS/MS Spectral Library 2.2.lbp` file.
14. To import all of the compounds, click **All** above the **Compound** column .

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



15. Click **Next**.

Note: If the import is canceled before all of the compounds have been copied to the database, then any compounds that have already been imported stay in the database. The database will not go back to the pre-import state.

16. For users with Forensic HR-MS/MS Spectral Library 2.1, click **Overwrite All**. Refer to the section: Compound Conflicts.
17. Click **Finish**.
18. If the LibraryView software is installed, then use the **Export** > **Library as snapshot (lbp)** feature to make a backup of all of the libraries after installation.

Note: If issues occur with any of the libraries, then importing the entire library as a snapshot is faster than installing all of the libraries again using the lbp packages.

Compound Conflicts

When individual compounds or a library with a group of compounds is installed, the software searches the database for compounds with the same name or formula as each compound in the package. If compounds with the same name are found, then the software flags the compound in the package and shows a prompt to the user.

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 that is stored in the database.
- Overwrite the compound information. Compound information from the package replaces the compound information that is stored in the database.
- Keep compound information. Compound information in the database is kept and the compound information from the package is discarded.

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

See Compound Conflicts

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

Merge Compounds

1. On the Library Importer dialog, do one of the following:
    - 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**
    - 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, click **Merge All** .
2. After all of the conflicts are resolved, click **Finish**.

Overwrite Compounds

1. Do one of the following 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 **Overwrite All**.
   - To overwrite the compound information stored in the database with the corresponding compound information from the import package, click **Resolve** beside the applicable compound and then click **Use New**.
2. After all of the conflicts are resolved, click **Finish**.

Keep Original Compounds

1. Do one of the following 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 All Original**.
   - To keep the individual compound information stored in the database and discard the compound information from the import package, click **Keep Original** beside the applicable compound.
2. After all of the conflicts are resolved, click **Finish**.

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. Import the new library.
2. After all of the conflicts are resolved, click **Finish**.

Note: to delete compound spectra, a licensed version of LibraryView software is required.

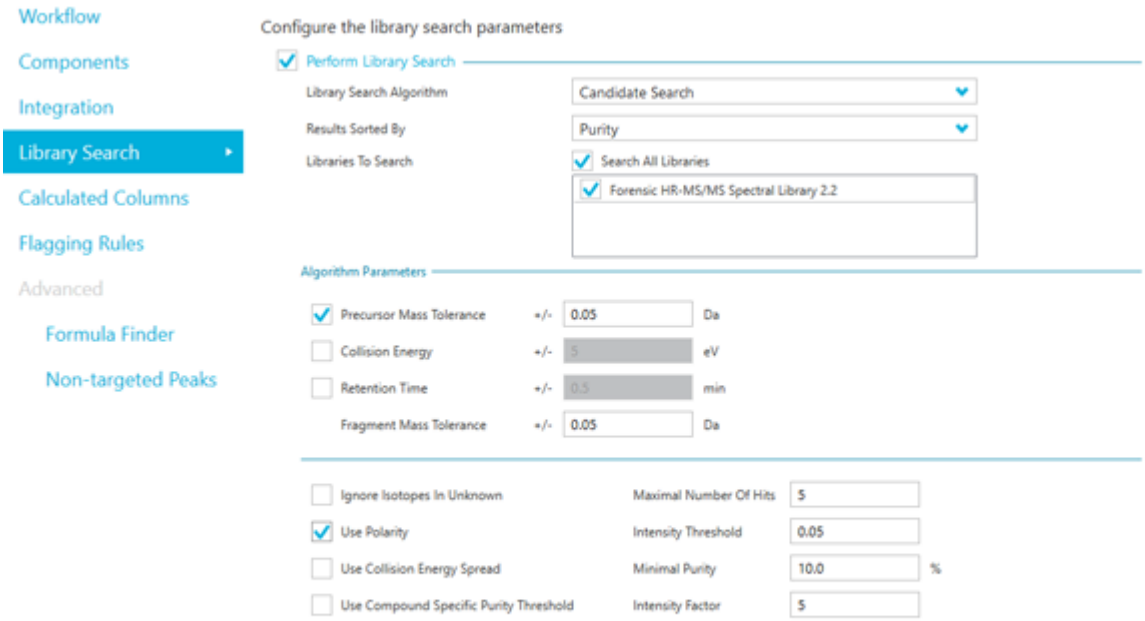
Recommended Library Search Settings

The Forensic HR-MS/MS Spectral Library 2.2 contains spectra from multiple instrument platforms and spectra acquired at different collision energy (CE) settings. Optimize the library search parameters carefully to effectively search the library. For the recommended library search settings for the SCIEX OS software, refer to the figure: Figure 3-3. Complete the following settings:

- Deactivate the collision energy filtering to prevent false negatives.

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

Figure 3-3 Recommended Search Settings for the Accurate Mass E&L Open Access Library



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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
- sciex.com/request-support

Note: For any questions or issues related to the StatusScope remote monitoring service, select **Instrument & Hardware** as the **Issue Type**.

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This version of the document supercedes all previous versions of this document.

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To find software product documentation, refer to the release notes or software installation guide that comes with the software.

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