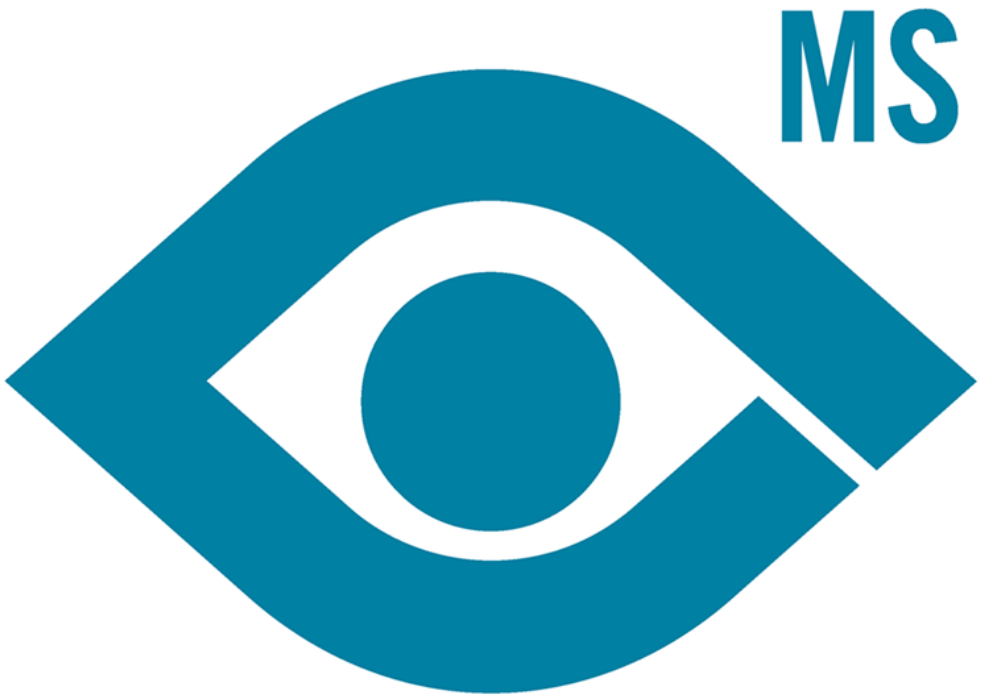
Release Notes

All-In-One HR-MS/MS Spectral Library 2.1.1

High Resolution Accurate Mass Libraries



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Contents

Introduction 1

Features

The All-in-One HR-MS/MS Spectral Library 2.1.1 supplies a collection of high-resolution spectral data that are organized into seven sub-libraries. These sub-libraries include antibiotics, pesticides, fluorochemicals, forensic compounds, natural products, mycotoxins, and metabolites. This diverse coverage supports a wide range of analytical applications, which lets users confidently identify compounds across different research and testing domains.

These libraries are compatible with

- Data acquired on TripleTOF systems or QTRAP systems.
- Data acquired with the SCIEX OS software 3.4.5 or later on X500 QTOF systems or ZenoTOF systems

Use these libraries in the LibraryView software 1.7 or later or in the SCIEX OS software 3.4.5 to do these tasks:

- Accurately identify compounds and increase confidence in the reported results.
- Do rapid compound searches for targeted and non-targeted screening.
- Use the accurate mass, retention time, and peak area reporting functionality in the SCIEX OS software.
- Compare a sample against a control for qualitative review with the comparative profiling option that is available in the SCIEX OS software.

Requirements

SCIEX OS Software
An English (US) version of: • Windows 10 (64-bit) operating system. • Windows 11 LTSC 2024.
The user must be logged on to the computer as a user with Administrator privileges.
Internet access is required to get a license file for each installed High Resolution Accurate Mass (HRAM) library.

SCIEX OS Software
A minimum of one of these applications is required to install a library: • A licensed version of the SCIEX OS software 3.4.5 or later. • A licensed version of the LibraryView software (SCIEX OS software), version 1.7 or higher.
A licensed version of the LibraryView software 1.7 or later, is required to edit the library.

Supported Equipment

- ZenoTOF systems
- X500 QTOF systems
- QTRAP systems
- TripleTOF systems
- A Dell Precision T3600 computer, or later model, supplied 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 2.1.1

The All-in-One HR-MS/MS Spectral Library 2.1.1 is an update to version 2.1. The NIST E&L HR-MS/MS 1.0 sub-library, which includes 1,710 Extractable and Leachable (E&L) compounds, has been removed. The updated library will have seven sub-libraries with a total of 3,978 compounds

Customers without All-In-One HR-MS/MS Spectral Library 2.0/2.1

Refer to Installation.

Customers with All-In-One HR-MS/MS Spectral Library 2.0/2.1

- Use the active license, HRAIO2.0.lic, to read the new All-In-One HR-MS/MS Spectral Library 2.1.1.
- The NIST E&L 1.0 sub-library is not supported. Customers with AIO 2.1 must remove the full NIST E&L sub library.
- Customers with AIO 2.0 should make a backup of their libraries. Customers can export the libraries as a LibraryView Database Snapshot Package and then save the package to a different location on the computer.

  Use Library Snapshot and the Overwrite Database feature to import the All-in-One HR-MS/MS Spectral Library 2.1.1.

Isobaric compounds with the same MS/MS pattern

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

Intermittently, the LibraryViewServiceHost does not respond

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 procedure starts the LibraryViewServiceHost service again.

The LibraryView software occasionally does not respond while the library is loaded, or results are not found during searches of the library

To correct these issues, do this:

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.

Installation 3

Install a Licensed High Resolution Accurate Mass Library

A licensed library can be installed from a zip file that is downloaded from the SCIEX website. The file can include compound names, compound transition information, and compound library spectra.

Note: Internet access is required to get 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 installation issues, save the file to the local computer, in a different location than the 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 use a SCIEX username and password to log in.

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

   The Activate Software page opens.
5. In the **Select Your Instrument** field, select the applicable instrument.
6. In the Windows search field, type **ipconfig /all** to get 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.
7. In the **Computer ID** field, type all of the physical addresses.

   Tip! A maximum of three physical addresses can be supplied. Divide 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.
8. In the **License Key** field, type the license key from the license card.

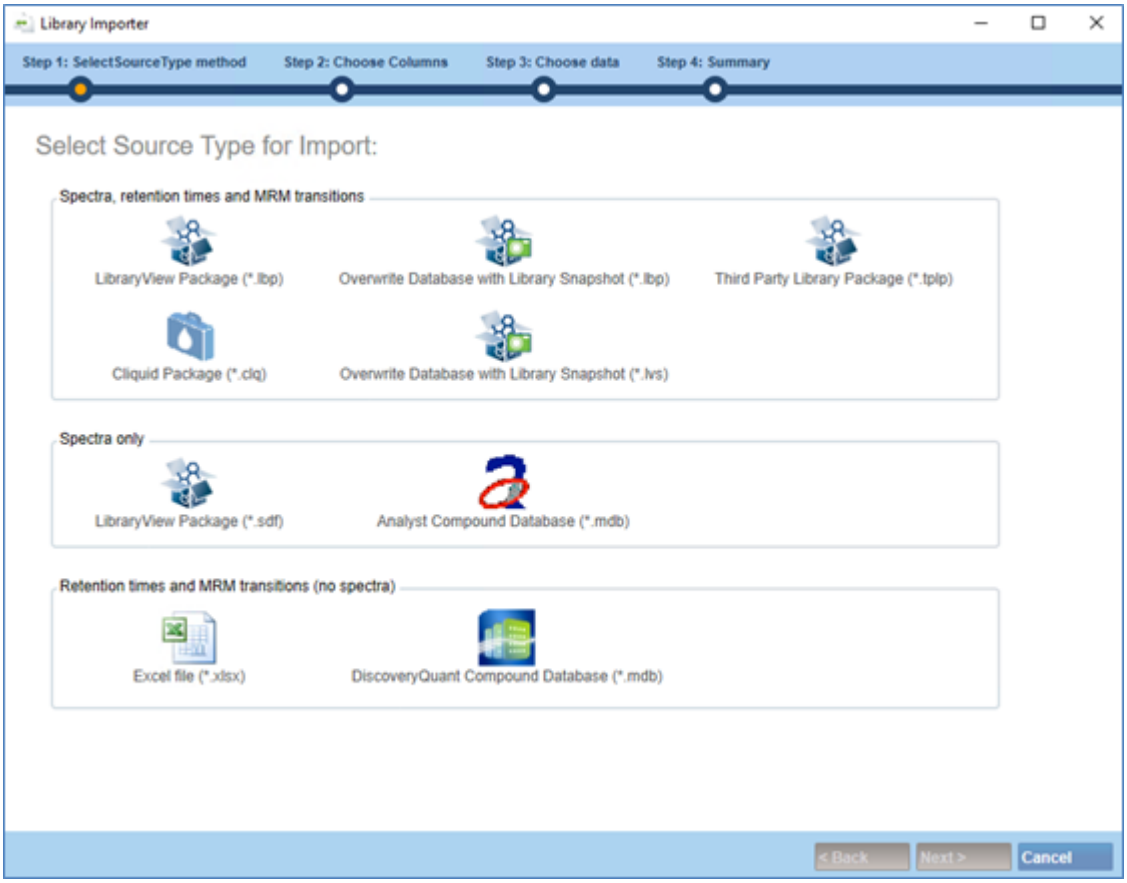
   Note: The key begins with the letters AID. If a license key is not available, then contact sciex.com/request-support.

9. Click **Submit**.
   After the required information is submitted, a license file is sent to the e-mail address that is registered to the SCIEX.com account.
10. Save the license file in the folder `C:/Program Files/SCIEX/LibraryView/LibraryViewFramework/Server`.
11. In the Windows search field, type **libraryviewpackager.exe**, and then run the file.

    Note: On a computer with the LibraryView software 1.7 installed, the **libraryviewpackager.exe** file is in the folder `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.

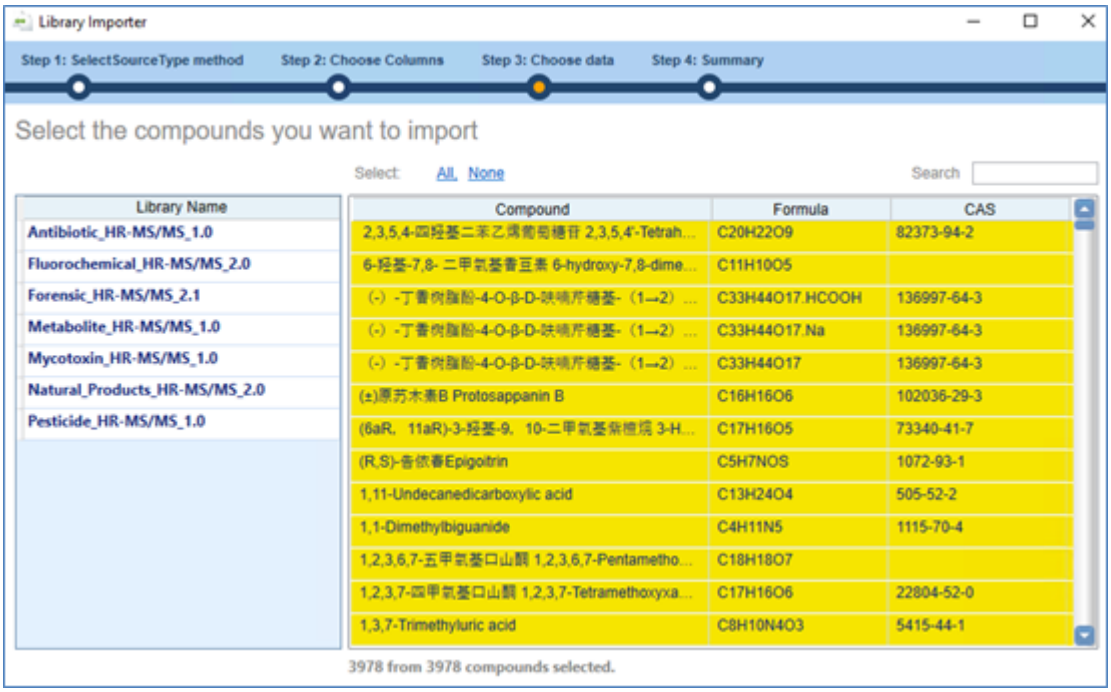
Figure 3-1 Library Importer Dialog—Select Source Type for Import



13. Browse to the files that were extracted in step 3 or to the DVD, and then select the **All-In-One HR-MSMS Spectral Library 2.1.1.lbp** file.

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

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



15. 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 stay in the database. The software will not change the database back to the pre-import state.

16. Resolve any conflicts, if required. Refer to Compound Conflicts.
17. Click **Finish**.
18. If the LibraryView software is installed, then after installation, use the **Export** > **Library as snapshot (lbp)** feature to make a backup of all of the libraries.

Note: If issues occur with any of the libraries, then the full library can be imported as a snapshot more quickly than if the lbp packages are used to install all of the libraries again.

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 identifies 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 kept in the database.
- Overwrite the compound information. Compound information from the package replaces the compound information that is kept 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 these steps:
   - To keep the compound information that is in the database and discard the new information, click **Keep Original**.
   - To replace the compound information that is in the database 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 these steps:
   - To merge new spectra, transitions, and retention times from individual compounds in the import package with the related compound information that is in the database, click **Merge**
   - To merge new spectra, transitions, and retention times from all of the compounds in the import package with the related compound information that is in the database, click **Merge All**.
2. After all of the conflicts are resolved, click **Finish**.

Overwrite Compounds

1. On the Library Importer dialog, do one of these steps:
   - To overwrite all of the compound information that is in the database with the related compound information from the import package, click **Overwrite All**.

- To overwrite the compound information that is in the database with the related 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. On the Library Importer dialog, do one of these steps:

   - To keep all of the compound information that is in the database and discard the compound information from the import package, click **Keep All Original**.
   - To keep the individual compound information that is in the database and discard the compound information from the import package, click **Keep Original** beside the applicable compound.

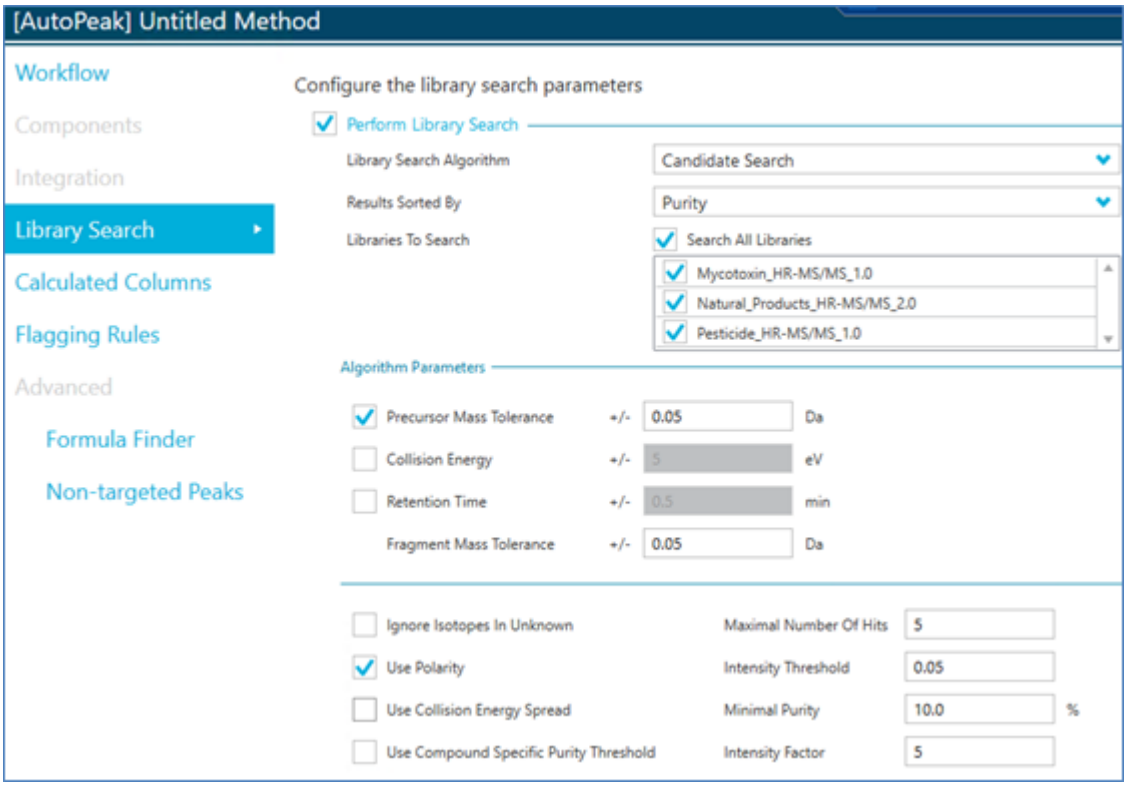
2. After all of the conflicts are resolved, click **Finish**.

Recommended Library Search Settings

The All-In-One HR-MS/MS Library 2.1.1 contains spectra from multiple instrument platforms and spectra that is merged from multiple spectra acquired at various Collision Energy (CE) settings. Thus, the library search parameters must be carefully optimized for the best search results. The figure that follows shows the recommended library search settings for the SCIEX OS software 1.7. Update these settings:

- To prevent false negatives, deactivate the Collision Energy filtering.
- To increase the processing time, set the Precursor Mass Tolerance to **0.05 Da**.

Figure 3-3 Recommended Search Settings for the All-In-One HR-MS/MS Library 2.1.1



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