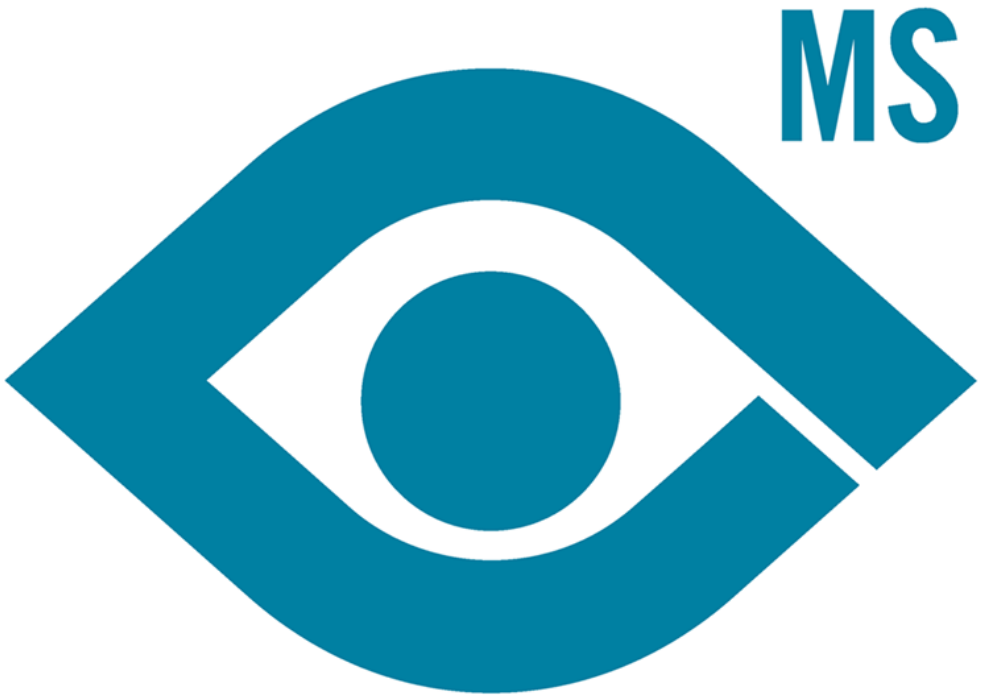
SCIEX
The Power of Precision

Natural Products HR-MS/MS Spectral Library

High Resolution Accurate Mass Libraries

Release Notes



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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 Natural Products HR-MS/MS Spectral Library 1.2 is an update to the Natural Products HR-MS/MS Spectral Library 1.1. This verified library includes High Resolution Accurate Mass Spectra for 1,295 natural products and traditional medicines. This library is released in the `lbp` format.

The library is compatible with:

- Data acquired with the SCIEX OS software 3.1 or later on a QTOF accurate mass system.

In the LibraryView software 1.4 or later and the SCIEX OS 3.1 software, use the library to do these tasks:

- Accurately identify compounds with more confidence in the reported results.
- Quickly search for compounds for both targeted and non-targeted screening.
- 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 get 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, 3.1 or later. • A licensed version of the LibraryView (SCIEX OS) software, 1.4 or later.
A licensed version of the LibraryView (SCIEX OS) software, 1.4 or later, is required to edit the library.

Supported Equipment

- ZenoTOF 7600 accurate mass system
- X500 QTOF accurate mass system
- TripleTOF accurate mass system
- 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

Natural Products HR-MS/MS Spectral Library 1.2

The Natural Products HR-MS/MS Spectral Library 1.2 contains of 1,295 high-resolution spectral data on natural products and traditional medicines. It is an updated version of the Natural Products HR-MS/MS Spectral Library 1.1.

Sometimes the LibraryView software 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.

Sometimes the SCIEX OS software stops responding when the Import compounds from LibraryView 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 Natural Products HR-MS/MS Accurate Mass Library

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

Note: Internet access is required to obtain the license.

Note: If the Natural Products HR-MS/MS Spectral Library 1.1 was installed, then download the Natural Products HR-MS/MS Spectral Library 1.2 and use the old license key.

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. If a license key is not available, then contact sciex.com/contact-us.

   The license key is distributed through an e-mail from SCIEX Now. If the license key is not available, then contact a sciex.com/request-support 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:

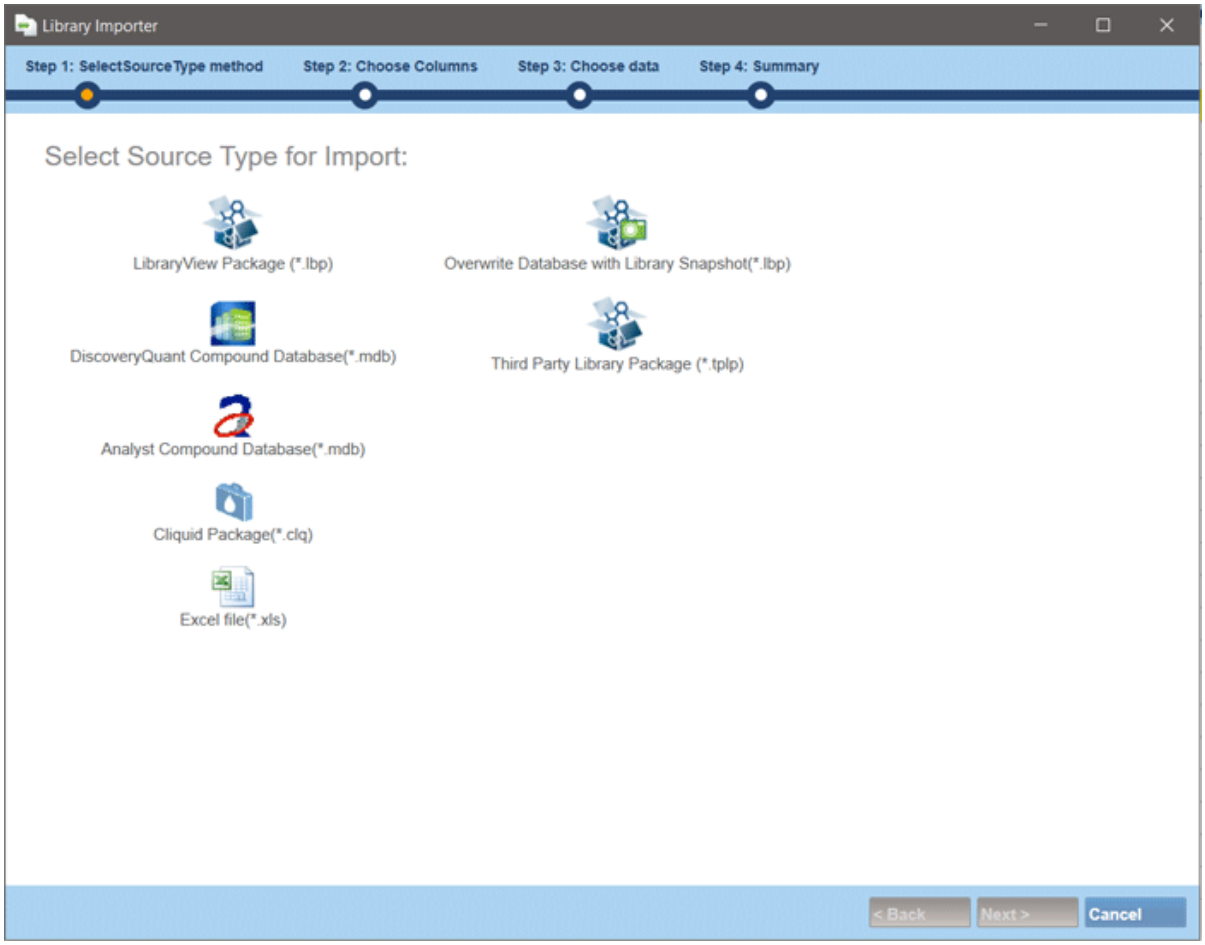
    - On a computer with version 1.4 of the LibraryView (SCIEX OS) software or later installed, save the license file in the `C:/Program Files/SCIEX/LibraryView/LibraryViewFramework/Server` folder.

    After the license is added, the library importer dialog opens automatically.

    Tip! As an alternative, to launch the library, run the `libraryviewpackager.exe` file located in the `C:/Program Files/SCIEX/LibraryView/LibraryViewFramework/Packager` folder.

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

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



12. Browse to the files extracted in step 3, and then select the `TCM MSMS Library 2.2 lbp` file.
13. To import all of the compounds, click **All** above the **Compound** column .

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

14. Click **Next**.

Note: If the import is cancelled 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.

15. For users with Natural Products HR-MS/MS Spectral Library 1.1, click **Overwrite All**. Refer to the section: Compound Conflicts.
16. Click **Finish**.
17. If the LibraryView software contains any previous libraries, then use the **Export** > **Library as snapshot (lbp)** feature to make a backup of all of the libraries before installation.

Note: If issues occur with any of the libraries, then it is faster to import the entire library as a snapshot than to use the `lbp` packages 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 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 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 the following:
    - 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. Do one of the following on the Library Importer dialog:
    - 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. Do one of the following on the Library Importer dialog:
   - 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**.

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**.

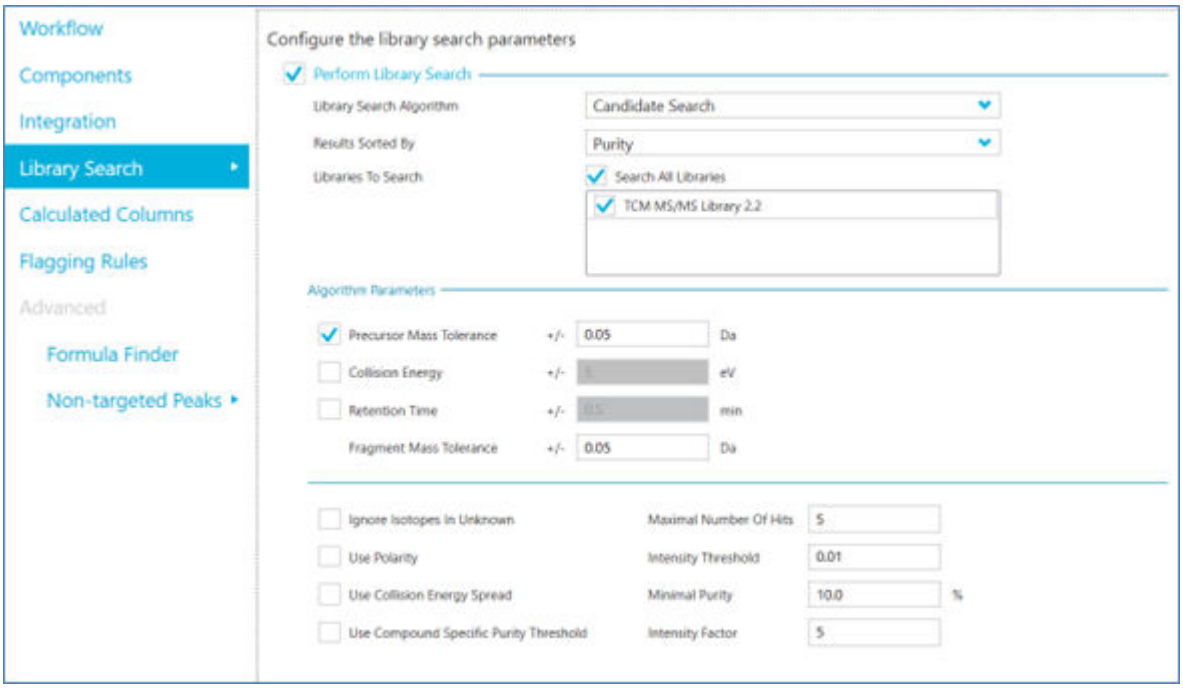
Note: To delete compound spectra, a licensed version of LibraryView software is required.

Recommended Library Search Settings

The Natural Products HR-MS/MS Spectral Library 1.2 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 decrease 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 Natural Products Library



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

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Documentation

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

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