Release Notes

NIST26 MS/MS Library

High Resolution Accurate Mass Libraries

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Introduction 1

Features

The NIST26 MS/MS library is a compiled and curated tandem mass spectral database from the National Institute of Standards and Technology (NIST). The NIST26 MS/MS library contains 68,635 compounds, which is a 33% increase from the NIST23 MS/MS library. The NIST26 MS/MS library supports compound identification in human and plant metabolites, pollutants, contaminants, drugs, and other important compounds.

The NIST26 MS/MS library can be installed on the same computer where the SCIEX OS software 5.0 and the LibraryView software 1.8 are installed.

The NIST26 MS/MS library is compatible with data that was acquired with these systems:

- TripleTOF systems
- X500 QTOF systems
- ZenoTOF systems
- QTRAP systems

Use the NIST26 MS/MS library in the LibraryView software 1.8 and the SCIEX OS software 5.0 to do these tasks:

- Fast compound searches for nontargeted screening
- Compound identification that uses the accurate mass, isotopic ratio, and peak area in the SCIEX OS software
- Comparisons of a sample to a control for qualitative review with the comparative profile option in the SCIEX OS software

Requirements 2

- An English (US) version of Windows 11 LTSC 2024 is installed on one of these computers:
  - SCIEX Workstation - 5860
  - SCIEX Workstation Plus - 5860

  Note: An upgrade service is available to upgrade computers that have Windows 10 installed.
- A licensed version of the SCIEX OS software 5.0 is installed.
- A licensed version of the LibraryView software 1.8 is installed.
- Internet access is available to download the NIST26 MS/MS library.
- The user is logged on to the computer with Administrator privileges.

Notes on Use 3

The licensed NIST26 MS/MS library contains three sublibraries:

- High Res NIST library: 66,779 compounds
- Low Res NIST library: 66,562 compounds
- APCI NIST library: 623 compounds

To do the fastest search, select one sublibrary at a time.

To make sure that the search results are correct, use the High Res NIST library for high-resolution MS/MS data.

If the data processing setup is configured, then refer to the section: Recommended Settings for NIST26 MS/MS Library Searches.

Known Issues 4

Refer to the section: *Known Issues and Limitations* in the document: *LibraryView Software 1.8 Release Notes*.

Installation 5

Install the SCIEX OS Software 5.0

- To open the *Software Installation Guide*, click **Start** > **SCIEX OS** > **SCIEX OS Documentation** > **sciex-os-software-installation-guide-en**.

Install the LibraryView Software 1.8

1. If the LibraryView software contains other libraries, then to make a backup copy of all of the libraries, click **Export** > **LibraryView Database Snapshot Package (*.lbp)**.
2. To open the *Software Installation Guide*, click **Start** > **SCIEX** > **LibraryView Software Installation Guide**.

Install a Licensed Library

Note: Internet access is required to get the license.

1. Log on to the computer as a Windows user with Administrator privileges.
2. Go to sciex.com/products/spectral-library, and then download the required `zip` file.

   Tip! To prevent installation issues, save the file to the local computer, in a location other than the desktop.

3. After the download is completed, right-click the downloaded file, and then click **Extract All**. These files are included:
   - `apci_msms_nist.sdf`
   - `lr_msms_nist.sdf`
   - `hr_msms_nist.sdf`
   - `hr_msms_nist#2.sdf`
   - `hr_msms_nist#3.sdf`
4. Go to https://sciex.com/support/activate-software, and then log in with a SCIEX username and password.

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 correct system.

Tip! If the system is not in the list, then go to the SCIEX Now profile for the user who is logged on, and then add the system information.

6. To get the physical Media Access Control (MAC) addresses of the computer, in the Windows search field, type `ipconfig /all`.
   A physical MAC address is shown for each active adapter in the format 34-02-86-06-8A-05.
7. In the **Computer ID** field, type all of the physical addresses.

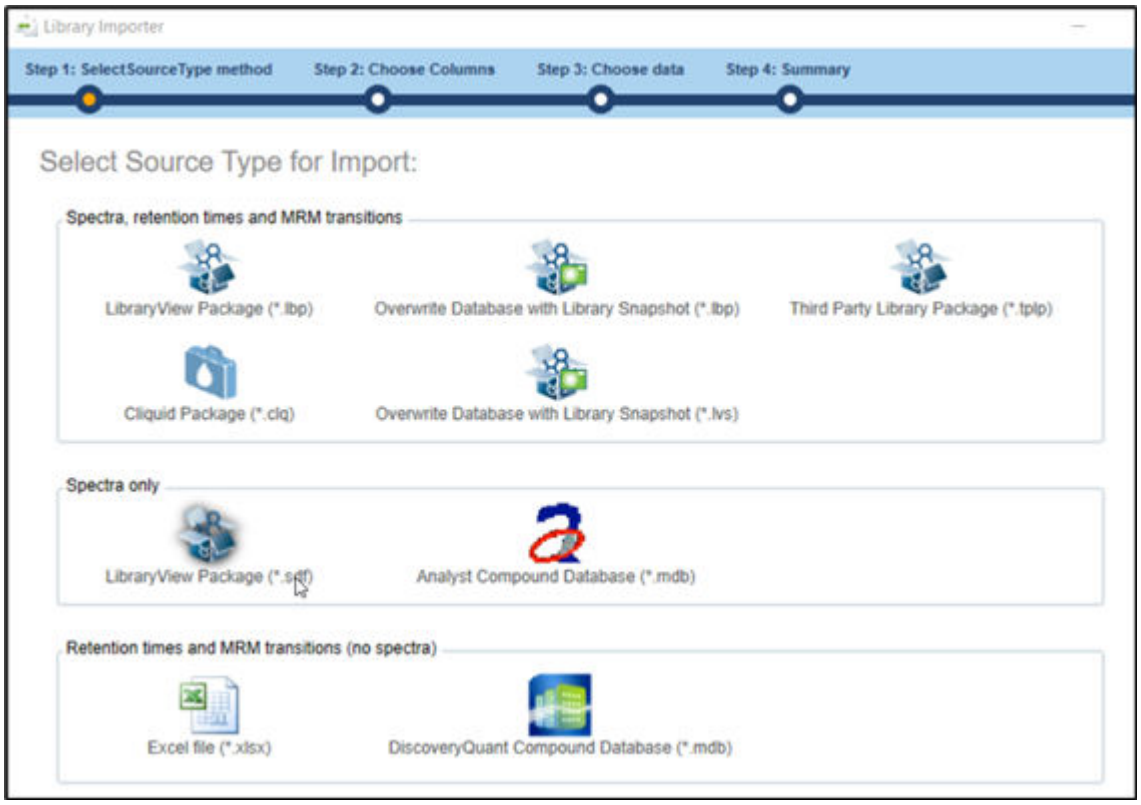
Tip! Supply a maximum of three physical MAC addresses. Use a space between each address. For example, 34-02-86-06-8A-05 34-02-86-06-8A-01 34-02-86-06-8A-09.

8. In the **License Key** field, type the license key.
   The license key is sent through an e-mail from SCIEX Now. If the license key is not available, then contact a sales representative at sciex.com/request-support.

Note: The key starts with the letters *AID*.

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. On a computer with the LibraryView software 1.8 installed, save the license file in the `C:/Program Files/SCIEX/LibraryView/LibraryViewFramework/Server` folder.
11. After the license is added, the Library Importer dialog opens.

Figure 5-1 Library Importer Dialog

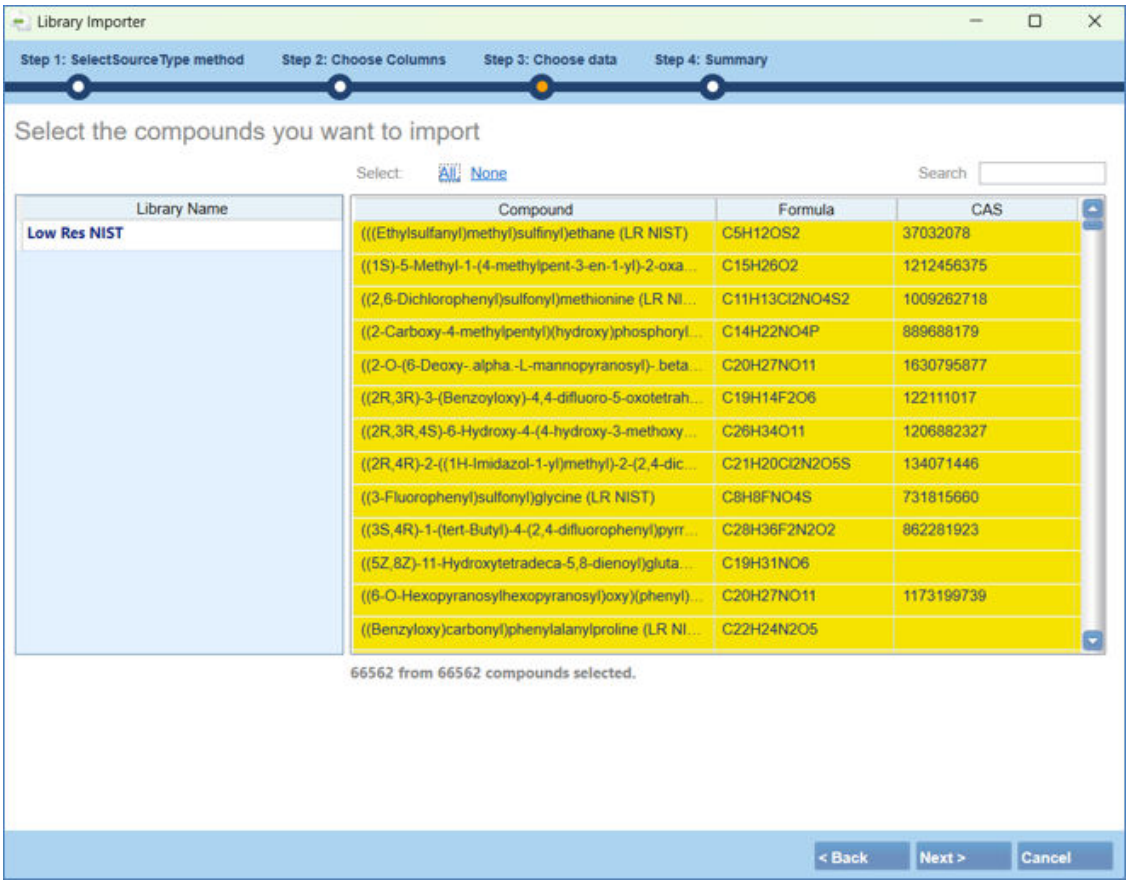


12. Click **LibraryView Package (*.sdf)**.

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

13. Browse to the files that were extracted in step 3, and then double-click the `lr_msms_nist.sdf` file.

Figure 5-2 `lr_msms_nist.sdf` File



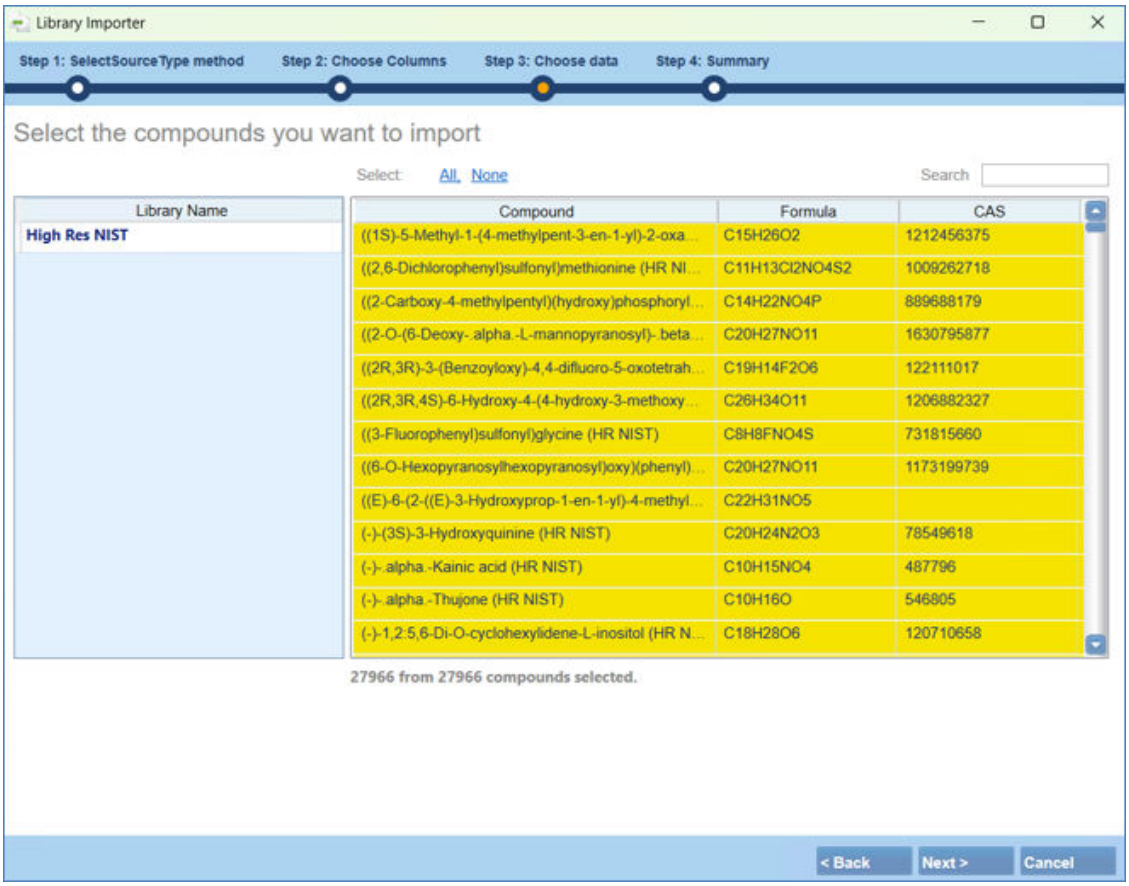
14. In the **Select** field, click **All**.
15. Click **Next**.
16. Click **Finish**.

Note: Each library might require more than 1 hour to install.

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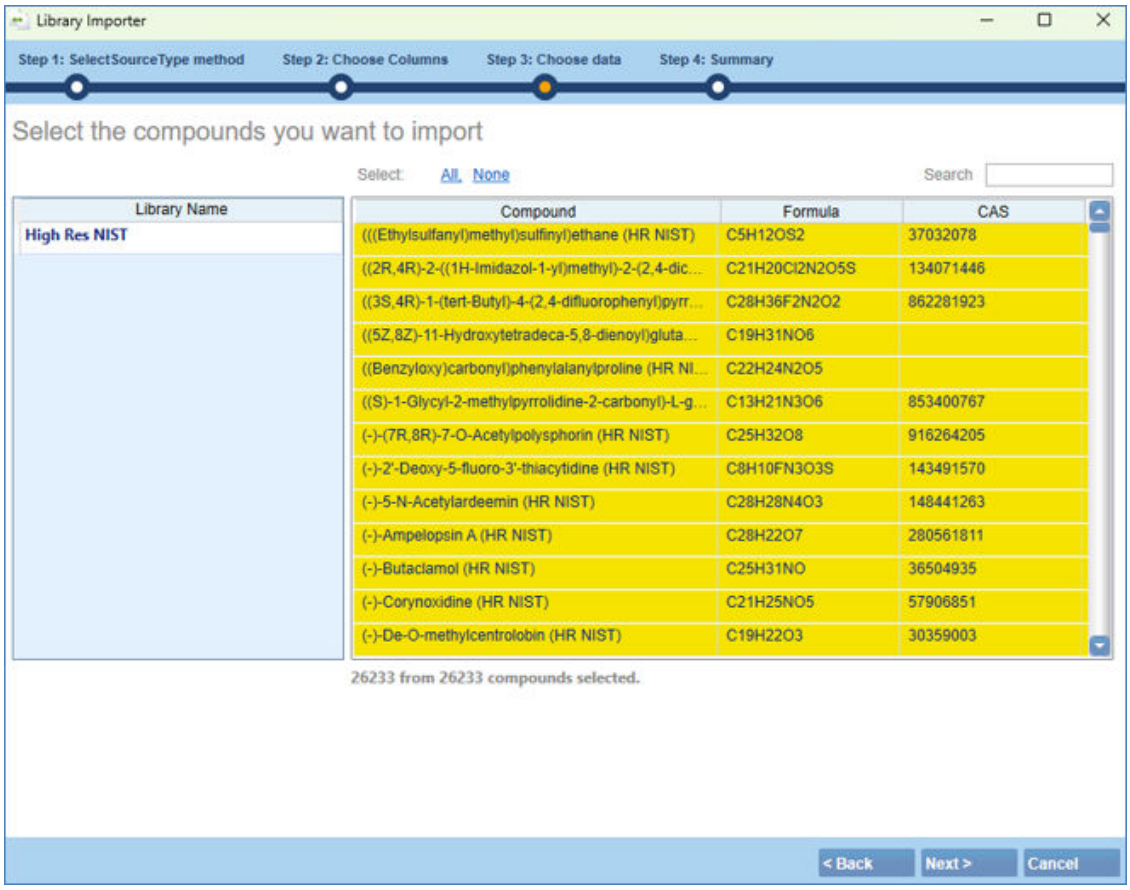
17. Browse to the files that were extracted in step 3, and then double-click the `hr_msms_nist.sdf` file.
18. Do step 14 to step 16.

Figure 5-3 `hr_msms_nist.sdf` File



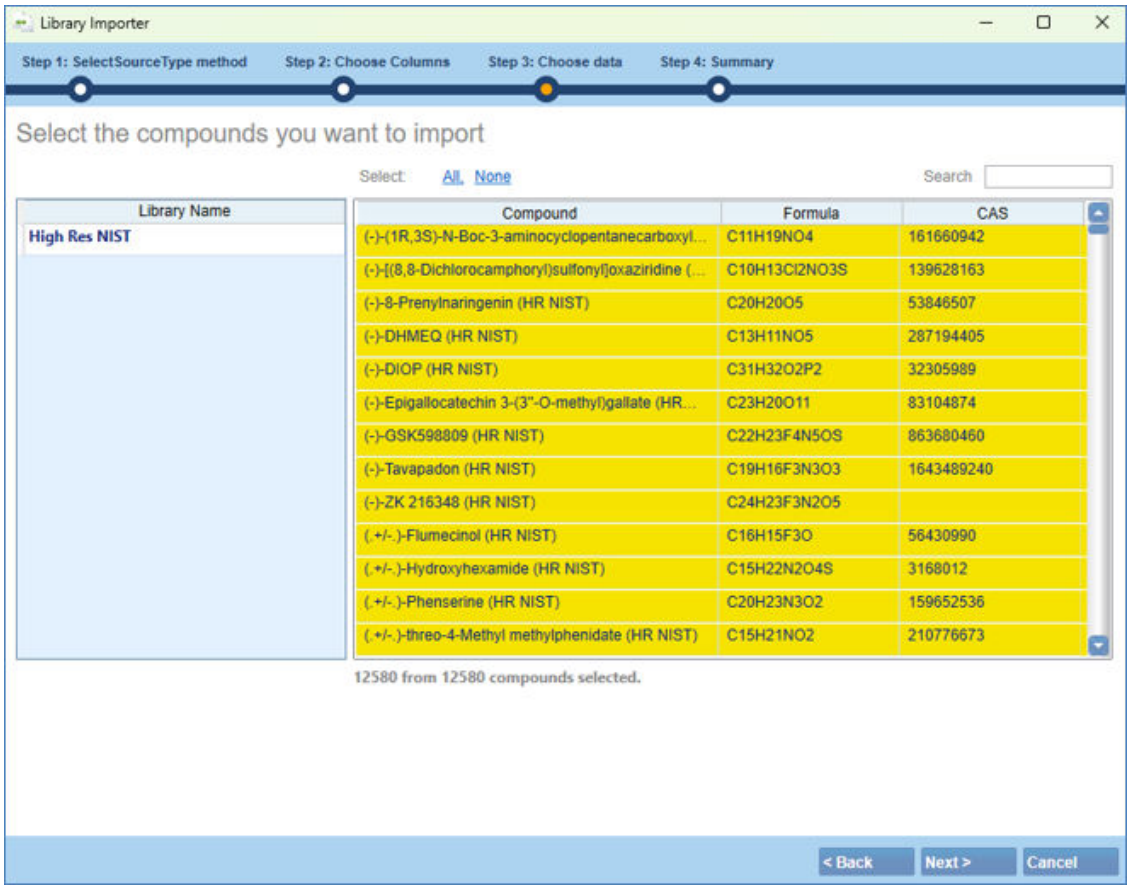
19. Browse to the files that were extracted in step 3, and then double-click the `hr_msms_nist#2.sdf` file.

Figure 5-4 `hr_msms_nist#2.sdf` File



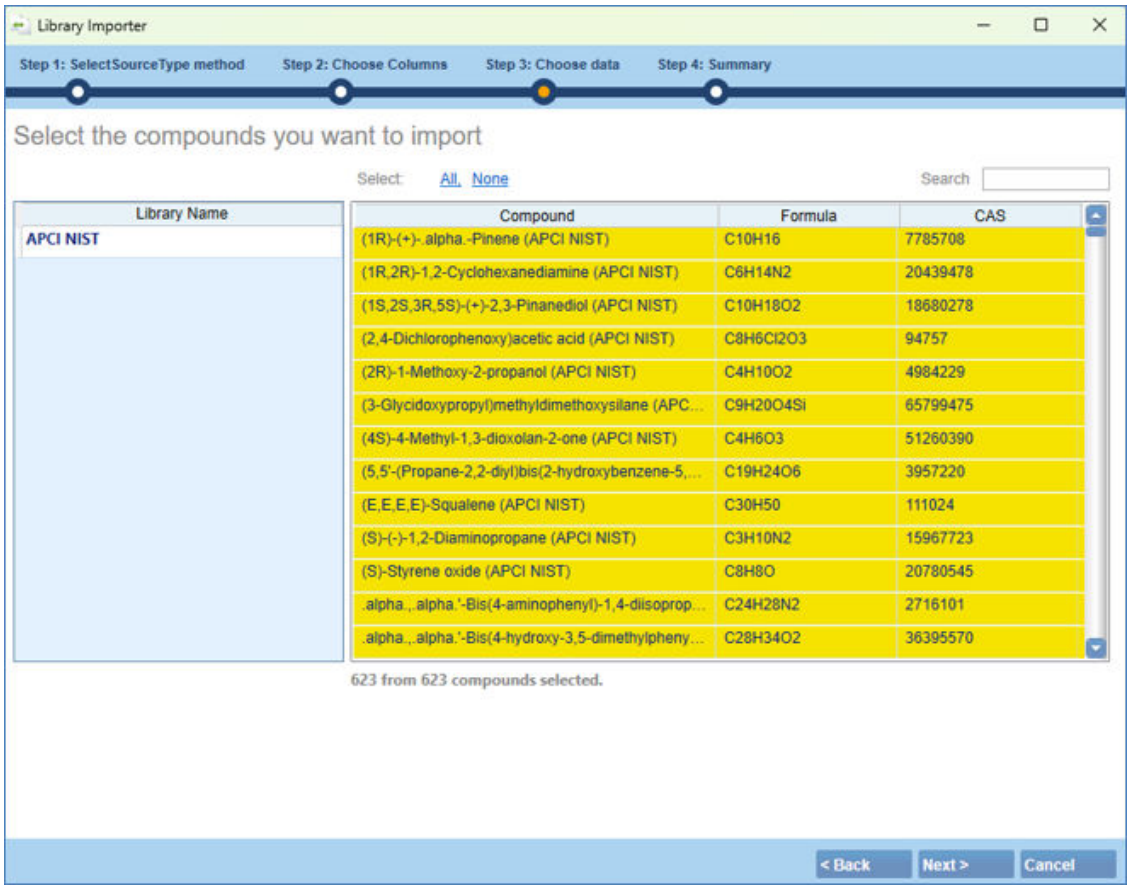
20. Do step 14 to step 16.
21. Browse to the files that were extracted in step 3, and then double-click the `hr_msms_nist#3.sdf` file.

Figure 5-5 `hr_msms_nist#3.sdf` File



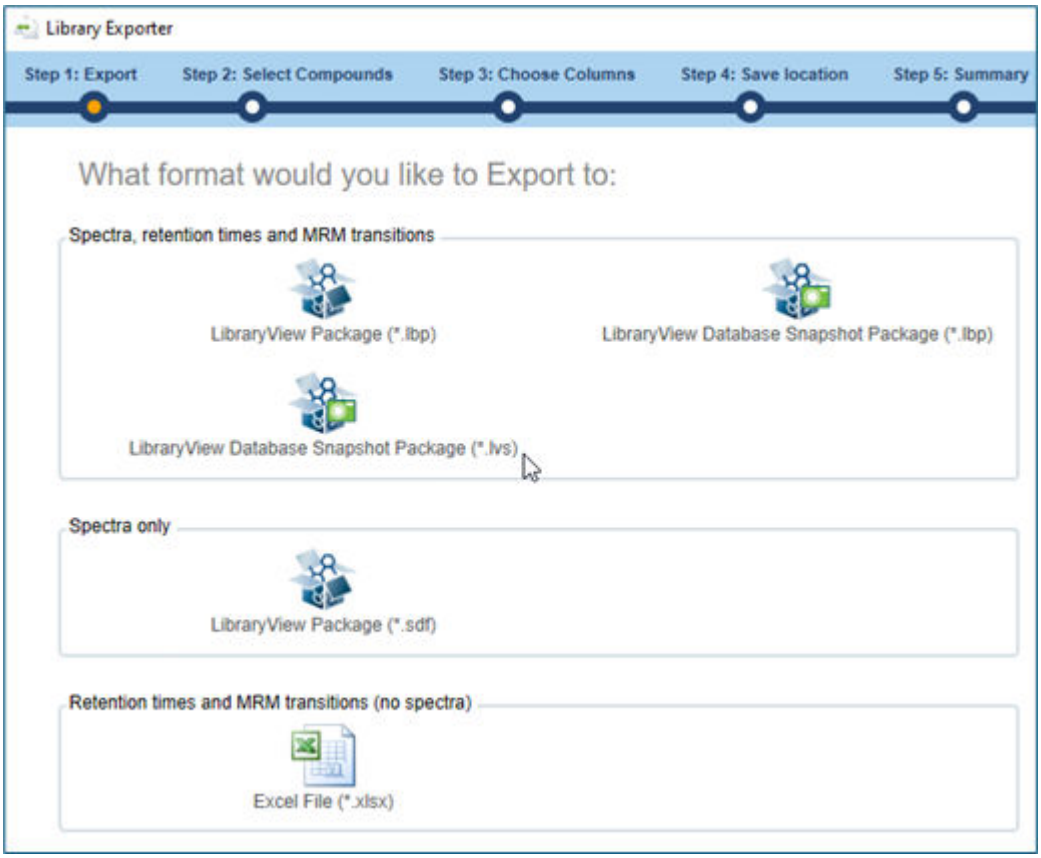
22. Do step 14 to step 16.
23. Browse to the files that were extracted in step 3, and then double-click the `apci_msms_nist.sdf` file.

Figure 5-6 `apci_msms_nist.sdf` File



24. Do step 14 to step 16.
25. After the installation is completed, to make a backup copy of all of the libraries, click **Export** > **LibraryView Database Snapshot Package (*.lvs)**.

Figure 5-7 Library Exporter Dialog



Note: If issues occur with a library, then import the full library as a snapshot. This alternative is faster than if the `sdf` packages are used to install all of the libraries again.

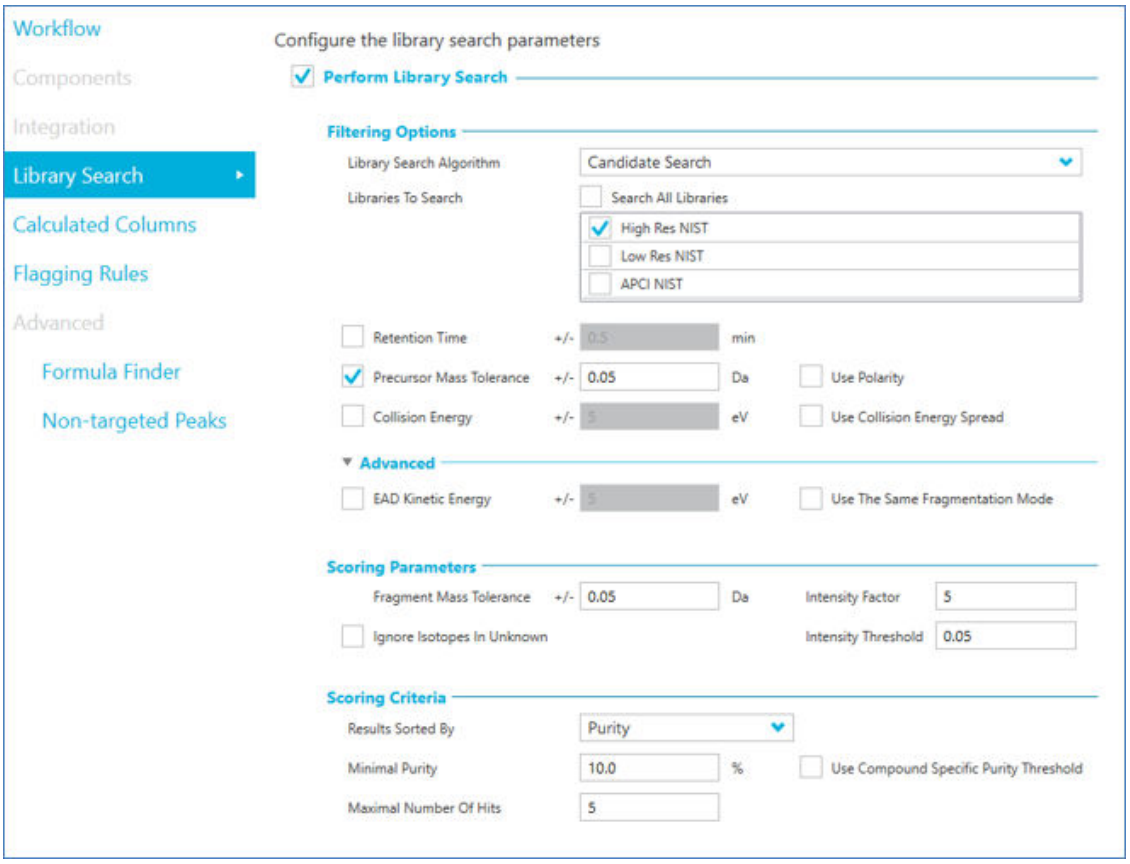
Recommended Settings for NIST26 MS/MS Library Searches 6

The NIST26 MS/MS library includes spectra from different instrument platforms and spectra merged from multiple spectra acquired at different settings for collision energy (CE). Thus, the library search parameters must be carefully optimized for satisfactory searches. Use the recommended values in the library search settings for the SCIEX OS software 5.0.

The figure that follows shows the default values on the Library Search tab. To do searches in the NIST26 MS/MS library, use these recommended settings:

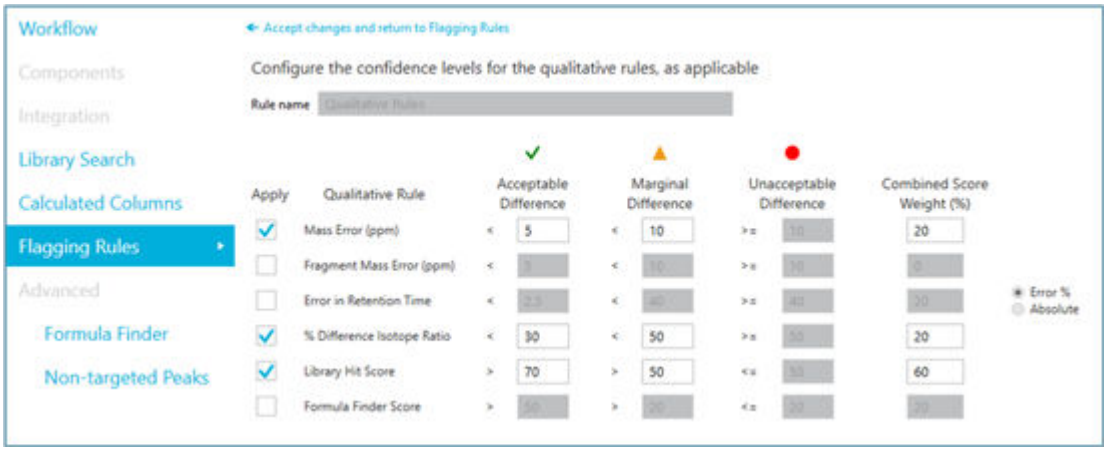
- Clear the **Collision Energy** check box to prevent false-negative results.
- Set **Precursor Mass Tolerance** to 0.05 Da to make the search faster.
- To adjust for the differences in relative intensity for different instruments, increase the **Intensity Factor** to 10.
- If required to get better search results for lower fragment signals, then decrease the **Intensity Threshold** to 0.02.

Figure 6-1 Library Search Tab



On the Flagging Rules tab, use the recommended settings in the figure that follows.

Figure 6-2 Flagging Rules Tab



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