Release Notes

NIST23 MS/MS Library

High Resolution Accurate Mass Libraries

TPUB-CUST-16042-A

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Contents

Introduction 1

Features

The National Institute of Standards and Technology (NIST) MS/MS library is a compiled and curated database that contains 51,501 small molecule compounds. The library also features biological peptides. It offers a comprehensive range of compounds under different fragmentation conditions, such as positive and negative modes from ion trap up to MS4 and beam-type collision cells like QTOF, Higher-energy Collisional Dissociation (HCD), and Triple Quad system.

NIST 23 Library is compatible with:

- Data acquired with the SCIEX OS software on a X500 QTOF system or ZenoTOF 7600 accurate mass system.
- Data acquired with the Analyst TF sotware 1.7.1 or later on any TripleTOF system.
- Data acquired with the Analyst software 1.6.2 or later on any QTRAP system.
- LibraryView, version 1.7 that supports the structured data files (sdf) format of NIST 23 libraries.
- The SCIEX OS software 3.4.5 and LibraryView software 1.7 installed on the same computer.

Use the LibraryView software 1.7 and the SCIEX OS software 3.4.5 to do these tasks:

- Do rapid compound searches for targeted and non-targeted screening.
- Leverage and filter the accurate mass, isotopic ratio, and peak area in the SCIEX OS software for compound identification.
- Compare a sample to a control for qualitative review with the comparative profile option that is available in the SCIEX OS software.

Requirements 2

- An English (US) version of Windows 10 or higher (64-bit) operating system must be installed.
- The user must be logged on to the computer as a user with Administrator privileges.
- An internet access is required to download the NIST23 MSMS Library.
- A licensed version of the SCIEX OS software, version 3.4.5 or higher must be installed.
- A licensed version of the LibraryView software 1.7 or higher.

Supported Equipment 3

- Mass spectrometer:
  - A ZenoTOF 7600 system
  - A TripleTOF accurate mass system
  - A QTRAP system
  - An 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 4

The licensed NIST23 MSMS Library contains three sub-libraries:

- High Res NIST: 49,590 compounds
- Low Res NIST: 49,865 compounds
- APCI NIST: 561 compounds

For optimum efficiency in searches, SCIEX recommends to select one relevant sub-library for the library search. Use the High Res NIST library for high-resolution MS/MS data to make sure of accurate and reliable search results.

For beam-type systems like QQQ, HCD, and QTOF, the MS2 spectra are a result of dissociation in a collision cell of a selected precursor ion. For ion trap systems, the MS2 spectra are a result of dissociation in the trap after isolation of the precursor ion. Data may also be specified as MS3 and MS4 spectra that is gotten from a precursor ion isolated for subsequent iterations of MS/MS.

The NIST23 library supports targeted and untargeted workflows during data analysis. If components are imported from the library database, then issues like mismatched mass ranges or excessively long compound list names might occur. In such cases, remove these compounds from the component table.

If the data processing setup is configured, then refer to the section: Recommended Library Search Settings for optimal results.

Known Issues and Limitations 5

Refer to the document: *LibraryView Software 1.7 Release Notes*

Installation 6

Install the SCIEX OS Software 3.4.5

For software installation guide, click **Start** > **SCIEX OS** > **SCIEX OS Documentation** > **sciex-os-software-installation-guide-en**.

Install the LibraryView Software 1.7

For customer documentations, click **Start** > **SCIEX** > **LibraryView Software Installation Guide**

Note: If the LibraryView software contains other libraries, then use the **Export** > **LibraryView Database Snapshot Package (*.lbp)** feature to make a backup copy of all the libraries before installation.

Install a Licensed NIST23 MSMS Library

A licensed library can be installed from a `zip` file that is downloaded from the SCIEX website. The file can contain 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 location other 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 then log in with a SCIEX username and password.

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

   The Activate Software page opens.
5. Select the correct system in the **Select Your Instrument** field.

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. In the Windows search field, type `ipconfig /all` to get the physical Media Access Control (MAC) addresses of the computer.
   a. A physical MAC 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! Supply a maximum of three physical addresses. 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.

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

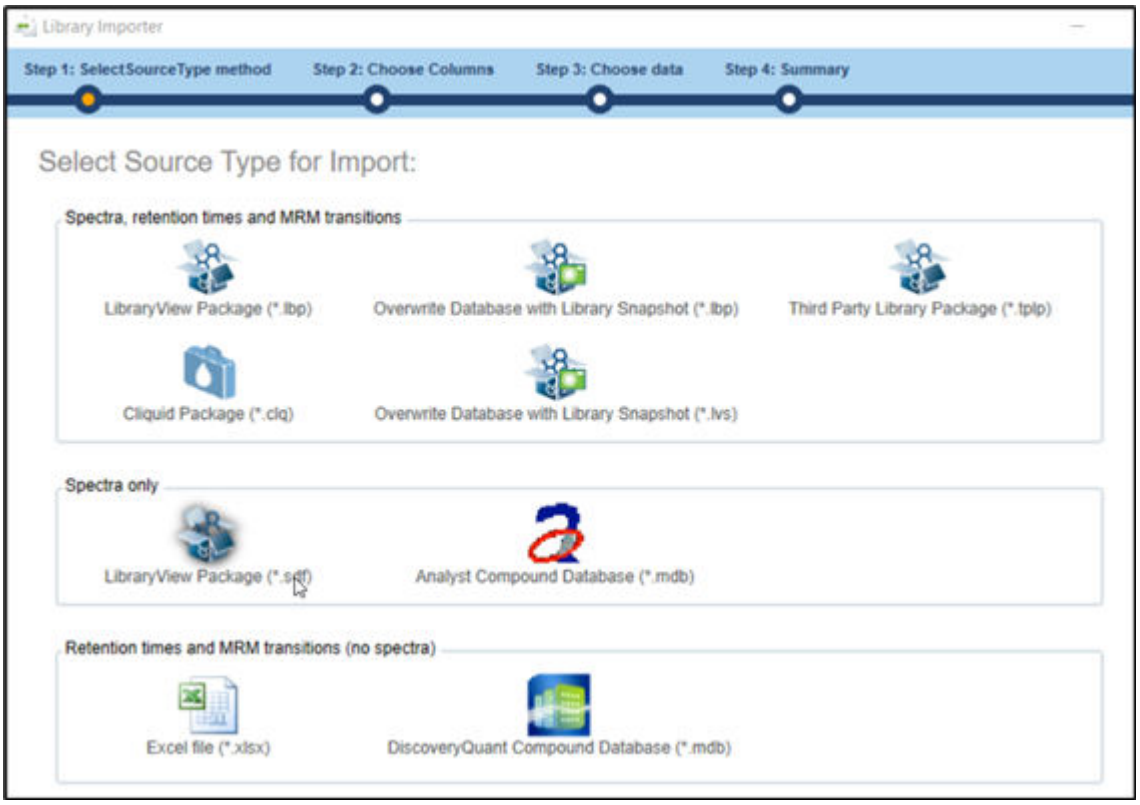
Note: The key starts with the letters AID.

9. Click **Submit**.
   After the required information is submitted, a license file is sent to the email address registered to the sciex.com account.
10. Save the license file to the required location:
11. On a computer with the LibraryView software 1.7 installed, save the license file in the `C:/Program Files/SCIEX/LibraryView/LibraryViewFramework/Serverfolder`.
    After the license is added, the library importer dialog opens automatically.

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

12. On the Library Importer dialog, click **LibraryView Package (*.sdf)** option.

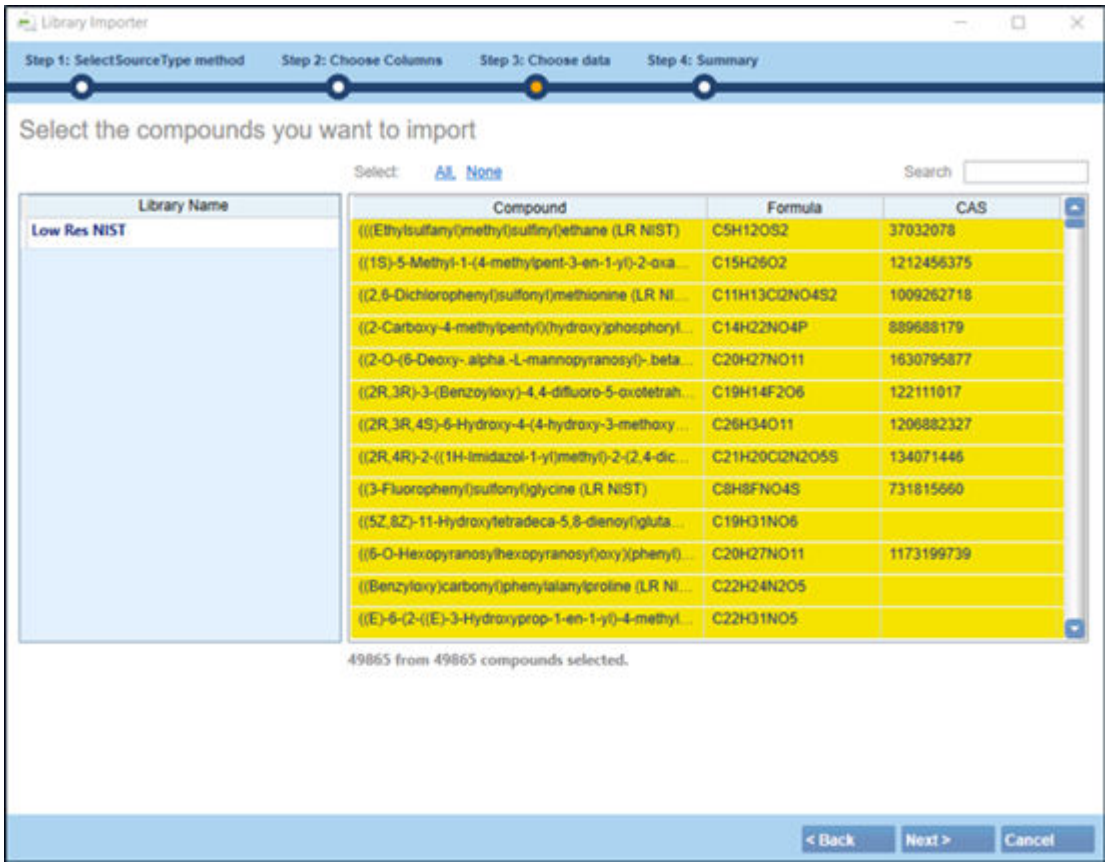
Figure 6-1 Library Importer Dialog: Select Source Type for Import



13. Browse to the files that were extracted in step 3, and then select the `Low Res NIST.sdf` file.
14. Do one of these steps:
    - Click **All** above the Compound column to import all of the compounds. Refer to the figure: Figure 6-2.
    - To import individual compounds, click in the correct row.

Tip! To find compounds, use the **Search** field. As the search criteria is typed, the visible columns are searched and refreshed to show only the information that matches the criteria included in this document.

Figure 6-2 Library Importer Dialog: Select Compounds to Import

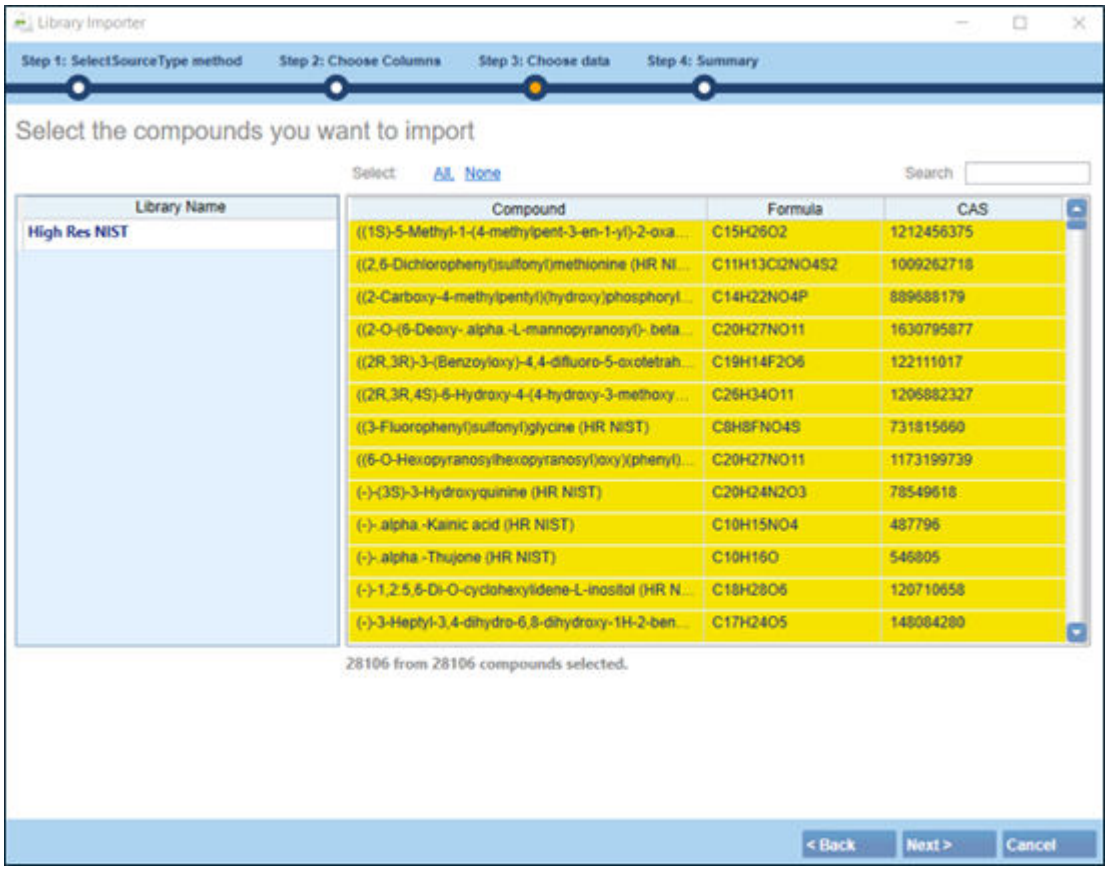


15. Click **Next**.
16. Click **Finish**.

Note: Each library might take up to an hour to install, because of the large size of the library.

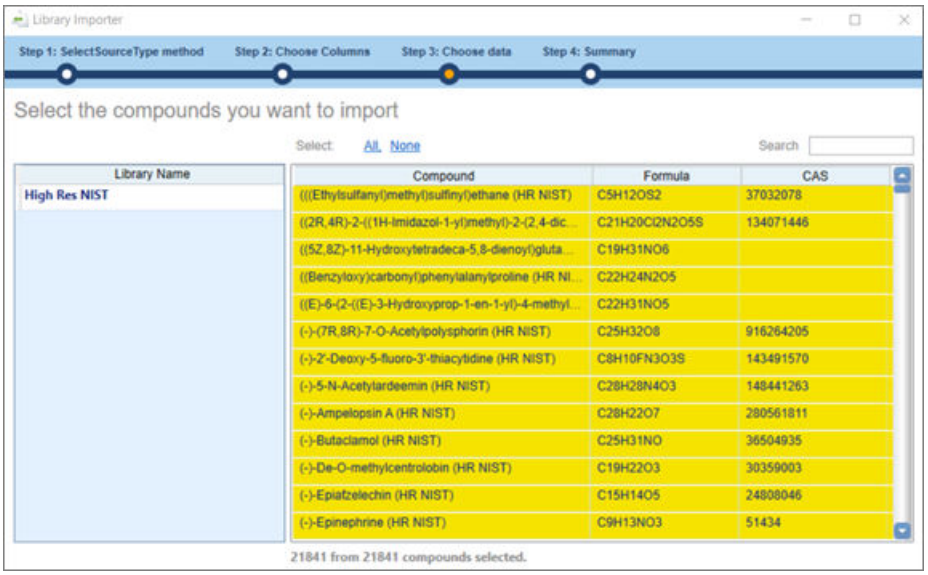
17. Browse to the files that were extracted in step 3, and then double-click `High Res NIST.sdf`.
18. Do step 14 to step 16.

Figure 6-3 Library Importer Dialog: High Res NIST



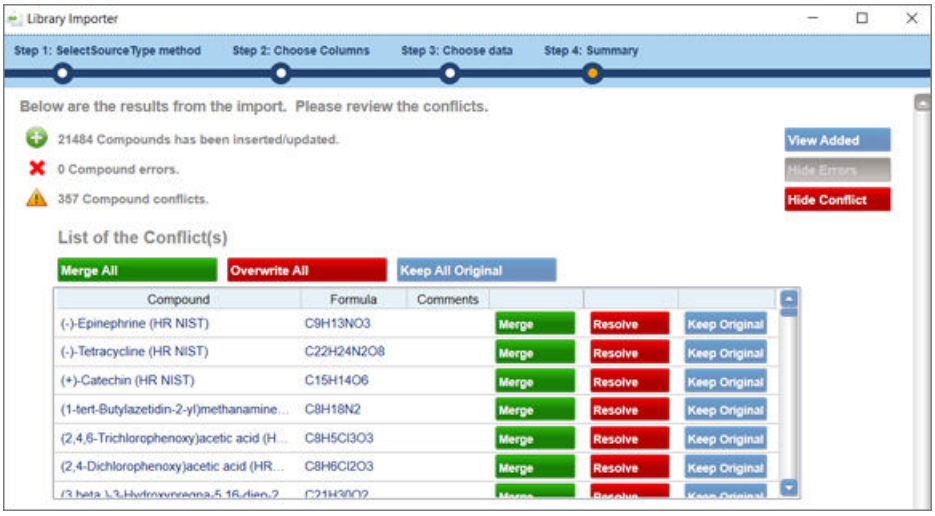
19. Browse to the files that were extracted in step 3, and then double-click `High Res NIST 2`.

Figure 6-4 Library Importer Dialog: High Res NIST 2



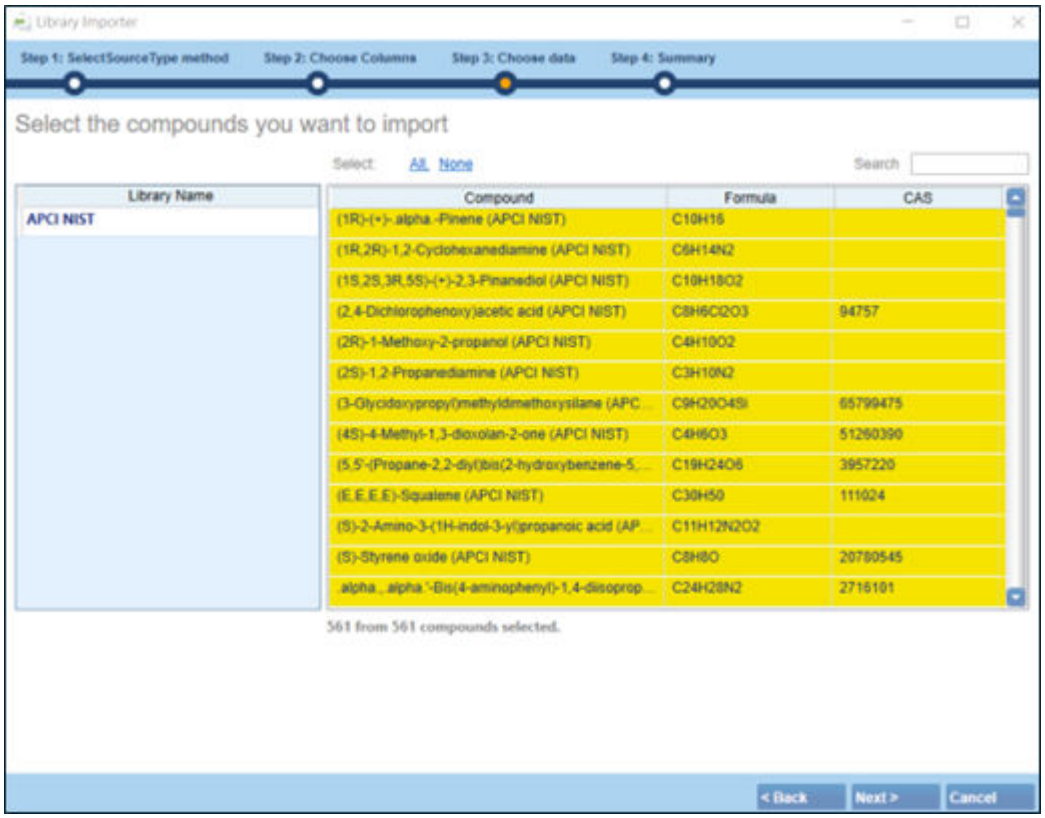
20. Click **Merge All**.

Figure 6-5 Library Importer Dialog: Merge All of the Compounds Conflicts



21. Browse to the files extracted in step 3 and then double-click `APCI NIST`.
22. Do step 14 to step 16.

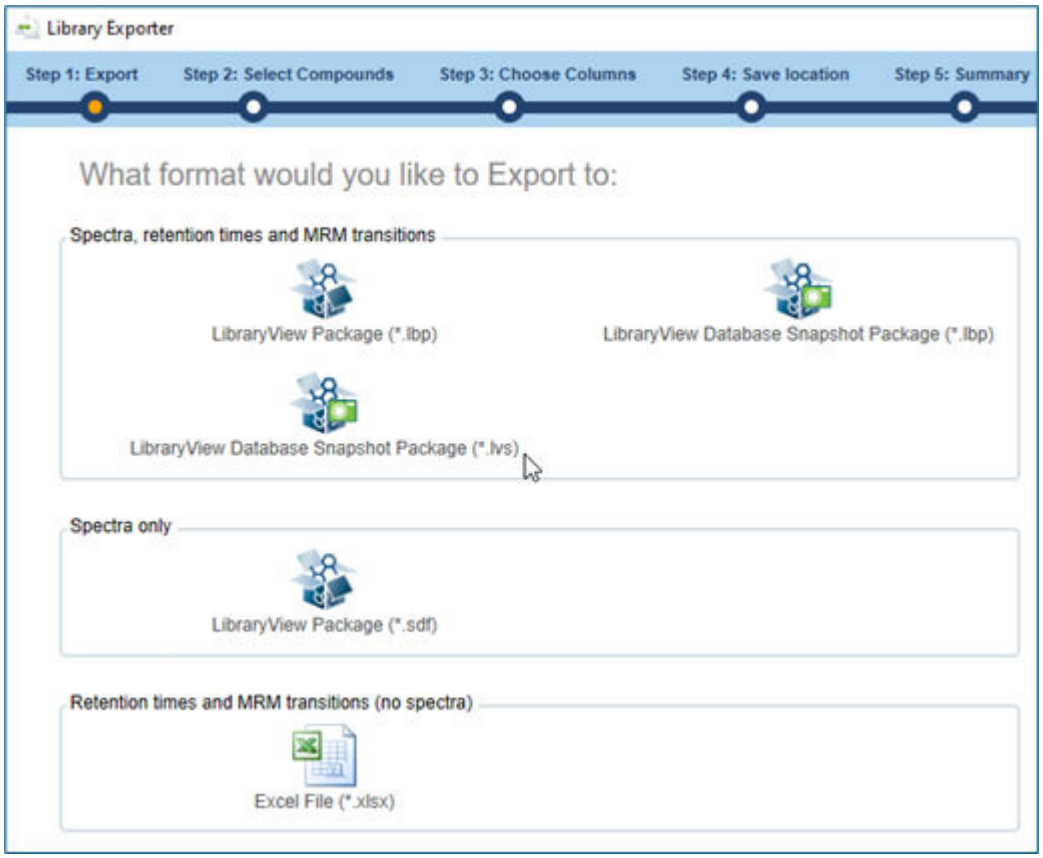
Figure 6-6 Library Importer Dialog: APCI NIST



23. After the installation is completed, make a backup copy of all of the libraries with the **Export > LibraryView Database Snapshot Package (*.lvs)** feature after installation.

Note: If issues occur with any of the libraries, then it is faster to import the full library as a snapshot than to use the sdf packages to install all of the libraries again.

Figure 6-7 Library Exporter



Recommended Library Search Settings 7

The NIST23 library includes spectra from different instrument platforms and spectra merged from multiple spectra acquired at different collision energy (CE) settings. Thus, the library search parameters must be carefully optimized for effective searches. Use the recommended values in the library search settings for the SCIEX OS software 3.4.5. Refer to the figure: Figure 7-1 and Figure 7-2.

Suggestions for Library Search settings:

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

Figure 7-1 Recommended Search Settings for NIST23 MSMS Library

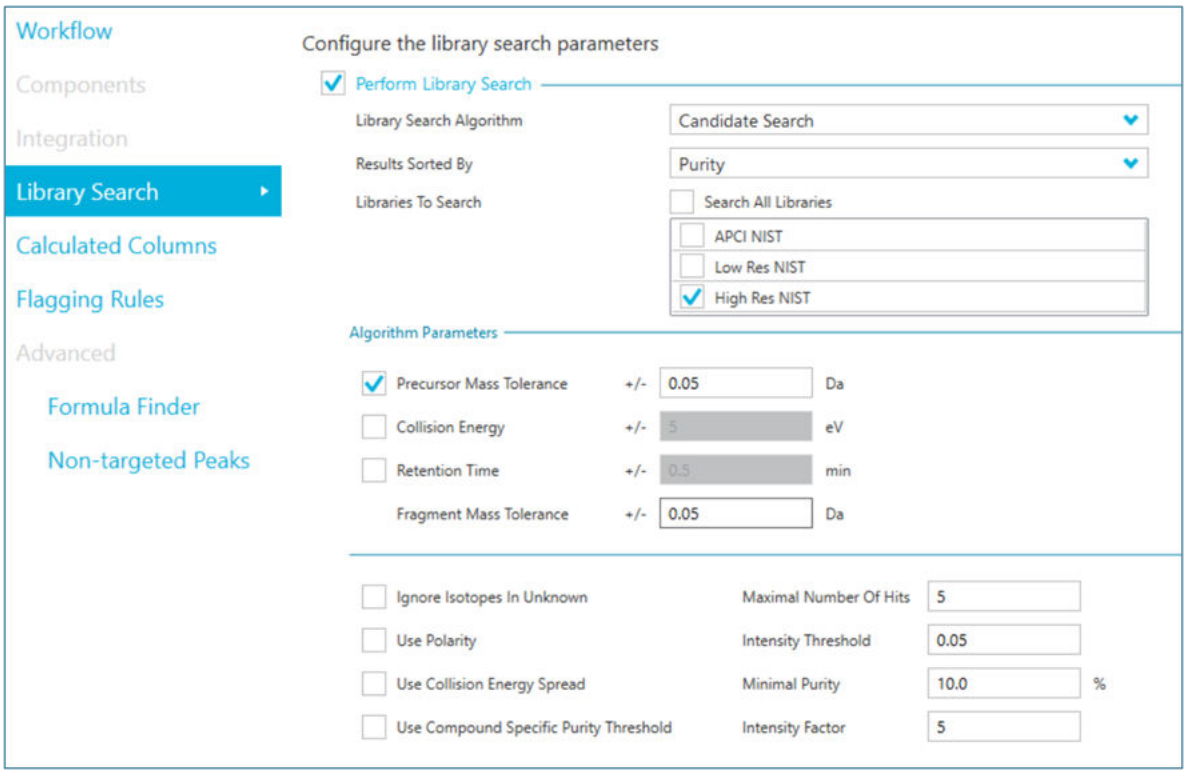
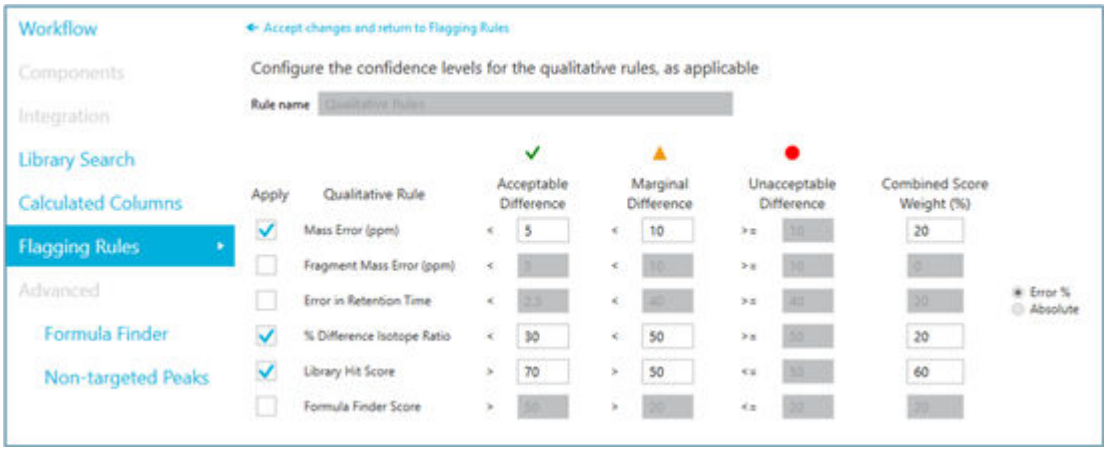


Figure 7-2 Recommended Flagging Rules for NIST23 MSMS Library



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