SCIEX
The Power of Precision

LibraryView Software

Quick Start Guide

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Import 1

Import a LibraryView Package

The software can import LibraryView packages in the proprietary SCIEX (`lbp`) format or the structured data files (`sdf`) format.

Note: We recommend that library files be copied to and imported from a local drive.

1. Open the Library workspace.
2. Click **Import** ().
   The Library Importer dialog opens.
3. Do one of these steps:
   - To import an `lbp` file, click **LibraryView Package (*.lbp)**.
   - To import an `sdf` file, click **LibraryView Package (*.sdf)**.

   The Open dialog opens.
4. Browse to and select a file, and then click **Open**.
   The Library Importer dialog opens.
5. To add the compounds to a library, do one of these steps:
   - Select the applicable library from the **Add to Compound Library** list.
   - Type the name of the library in the **Add to Compound Library** field.
6. Do one of these steps:
   - To import all of the compounds, click **All** above the **Compound** column.
   - To import selected compounds, click each compound.

   Tip! To find compounds, use the **Search** field. As the search criteria is typed, the software searches the columns and filters the display to show only the entries that contain the typed text.
7. 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 been imported stay in the database. The software does not put the database back in the state from before the import.

8. If required, then resolve any conflicts. Refer to the section: Compound Conflicts.
9. Click **Finish**.

Import a Compound Database

Note: We recommend that library files be copied to and imported from a local drive.

1. Open the Library workspace.
2. Click **Import** ().
   The Library Importer dialog opens.
3. Do one of these steps:
   - Click **DiscoveryQuant Compound Database (*.mdb)**.
   - Click **Analyst Compound Database (*.mdb)**.

   The Open dialog opens.
4. Browse to and select a file, and then click **Open**.
   The Library Importer dialog opens.
5. Do one of these steps:
   - To import all of the compounds, click **All** above the **Compound** column.
   - To import selected compounds, click each compound.

   Tip! To find compounds, use the **Search** field. As the search criteria is typed, the software searches the columns and filters the display to show only the entries that contain the typed text.
6. To add the compounds to a library, do one of these steps:
   - Select the applicable library from the **Add to Compound Library** list.
   - Type the name of the library in the **Add to Compound Library** field.
7. 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 been imported stay in the database. The software does not put the database back in the state from before the import.
8. Resolve any conflicts, if required. Refer to the section: Compound Conflicts.
9. Click **Finish**.

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.

Add Compound Information 2

Add a Compound

Note: Compounds can also be added to a library using the **Edit Library** option.

1. In the Manage pane, expand the **Compounds** list.
2. Click **All Compounds**.
   A list of all of the available compounds is shown.
3. Click **Add** ().

   Note: The compound name is mandatory. All of the other information is optional.
4. Type the appropriate information in the fields on the Details tab.
5. Click **Save**.

Add a Mass Spectrum to a Compound

1. In the Manage pane, expand the **Compounds** list.
2. Click **All Compounds**.
   A list of all of the available compounds is shown.
3. Double-click a compound.

   Tip! To find compounds, use the **Search** field. As the search criteria is typed, the software searches the columns and filters the display to show only the entries that contain the typed text.

   The Details tab of the selected compound is shown.
4. Open the MS Spectra tab.
5. Click **Edit Mode** ().
6. Click **Add Spectra** ().
   The Add Mass Spectrum from *.wiff file to Compound dialog opens.
7. Click **Open *.wiff file**.
   The Open dialog opens.
8. Browse to and select a wiff or wiff2file, and then click **Open**.

9. To add the compounds to a library, do one of these steps:
   - For IDA data, expand the sample and then select the appropriate compound in the navigation pane on the left.
   - For EMS, MRM, and looped data, select the appropriate sample.
10. To add the mass spectra to a compound, do one of these steps:
   - For IDA data, click **Add Spectrum** in the Acquired Spectrum pane.
   - For EMS, MRM, and looped data, double-click the TIC and then click **Add Spectrum** in the Acquired Spectrum pane.
11. Repeat steps 9 through 18 for each spectrum to be added.
12. Click **Save**.
13. On the MS Spectra tab, click **Save** .

LibraryView Software Icons A

Icon	Name (Function)
	Add
	Add New Library
	Add Spectra
	Add to Favorites
	Close the window
	Delete
	Edit Library
	Edit Mode
	Empty Trash
	Export
	Import
	Maximize the window
	Quick Edit Mode
	Remove
	Remove from Favorites
	Report
	Restore

LibraryView Software Icons

Icon	Name (Function)
	**Restore the window to the original size**
	**Settings**
	**Update RT**
	**View items in Grid**
	**View items in List**
	**View items in Stack**

Glossary

fit	A measure of how well a library spectrum matches the unknown spectrum. It does not take into account those peaks present in the unknown spectrum but absent in the library spectrum. The software allows for the fact that the unknown spectrum might represent an impure mixture of components. A perfect fit gives a score of 1. The range of the score is 0 to 1. A fit score of 1 but a reverse fit score of less than 1 implies that all of the peaks in the library spectrum were found in the unknown spectrum, but additional peaks were found in the unknown spectrum that were not shown in the library spectrum. Determining an acceptable score is subjective and depends on the quality of the spectra. In general, an acceptable value is greater than 0.5.
intensity factor	A way to decrease the importance of spectral intensity differences between acquired and library spectra. Increasing the intensity factor increases the purity. Be careful when adjusting this setting. An incorrect setting can produce results with higher purities than the compound should have and thus increase the likelihood of false positive results.
intensity threshold	Used to remove small noise peaks from the spectrum and improve spectral purity scores. The default setting is 0.05, which means that all of the peaks with an intensity of 5% or less of the base peak (highest intensity peak) are not considered in the library search. Increasing this number eliminates more small peaks from consideration in the spectral searching. Be careful when adjusting this setting. Increasing the setting increases purity scores but it might cause the software to ignore other peaks that might be important in identifying a compound.
purity	A measure of how well the unknown spectrum matches the library spectrum. All of the peaks from both spectra are used. The purity ranges from 0 to 1. High values indicate a higher likelihood that the unknown spectrum has been correctly identified and that it does not contain peaks from additional compounds at a significant amount. Lower values indicate either that the match is less certain or that additional fragment ion peaks from another compound are present in the unknown spectrum. Refer to fit and reverse fit.
reverse fit	A measure of how well the unknown spectrum matches a library spectrum. It does not take into account those peaks present in the library spectrum but absent in the unknown spectrum. A perfect reverse fit gives a score of 1. The range for the score is 0 to 1. A reverse fit score of 1 but a fit score of less than 1 implies that all of the peaks in the unknown spectrum were found in the library spectrum but additional peaks were found in the library spectrum that were not shown in the unknown spectrum. This relatively rare situation occurs if the original library spectrum did not correspond to a pure compound. Determining an acceptable score is subjective. In general, an acceptable value is greater than 0.5.

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- sciex.com/contact-us
- sciex.com/request-support

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Documentation

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

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

To find hardware product documentation, refer to the documentation that comes with the system or component.

The latest versions of the documentation are available on the SCIEX website, at sciex.com/customer-documents.

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