



NIST Tandem (MS/MS) Library 1.0.1

High Resolution Accurate Mass Libraries

Release Notes

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Features

The NIST Standard Reference Database 1A version 17 is an extensive MS/MS library containing high resolution mass spectra (HRMS) and nominal mass spectra from 13 808 chemical compounds. These spectra have been thoroughly examined by experienced mass spectrometrists for correctness and consistency, using both human and computer methods. This library is packaged with the All-in-One HR-MS/MS Library to increase the potential hits for library searching.

Note: This version of the NIST Tandem (MS/MS) Library, version 1.0.1, resolves an issue where incorrect structures were assigned to some of the compounds. However, the spectra for all of the compounds were correct.

These libraries are compatible with:

- Data acquired using a combination of the MasterView™ 1.1 software and the PeakView® 2.2 software, on a TripleTOF® accurate mass system or a QTRAP® system.
- Data acquired using SCIEX OS 1.3 or higher on a SCIEX X500 QTOF accurate mass system.

Use these libraries in the MasterView™ software and in SCIEX OS to:

- Help accurately identify compounds and increase confidence in the reported results.
- Enable rapid compound searches for targeted and non-targeted screening.
- Leverage the accurate mass, retention time, and peak area reporting functionality in both the MasterView™ software and in SCIEX OS.
- Compare a sample against a control for qualitative review using the comparative profiling option available in both the MasterView™ software and in SCIEX OS.

Requirements

SCIEX OS	MasterView™ Software
An English (US) version of: <ul style="list-style-type: none"> Windows 7 (64-bit) operating system with SP1. Windows 10 (64-bit) operating system. 	An English (US) version of: <ul style="list-style-type: none"> Windows 7 (64-bit) operating system with SP1. Windows 10 (64-bit) operating system.
The user must be logged on to the computer as a user with Administrator privileges.	The user must be logged on to the computer as a user with Administrator privileges.
Internet access is required to obtain a license file for each installed High Resolution Accurate Mass (HRAM) library.	Internet access is required to obtain 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: <ul style="list-style-type: none"> A licensed version of SCIEX OS, version 1.3 or higher. A licensed version of the LibraryView™ software, version 1.2 or higher. 	At least one of the following software applications is required to install a library: <ul style="list-style-type: none"> A licensed version of the PeakView® software, version 2.2 or higher and a licensed version of the MasterView™ software, version 1.1 or higher. A licensed version of the LibraryView™ software, version 1.0.2 or higher
A licensed version of the LibraryView™ software, version 1.2 or higher, is required to edit the library.	A licensed version of the LibraryView™ software, version 1.0.2 or higher, is required to edit the library.

Supported Equipment

- A TripleTOF® accurate mass system
- A QTRAP® system
- A SCIEX 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, Known Issues, and Limitations

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NIST Standard Reference Database 1A v17 Data

Spectral data was not acquired or examined by SCIEX. However, spectra were acquired on multiple instruments from multiple vendors and then converted and condensed for use in SCIEX software. Spectra were preferentially taken from SCIEX X500 QTOF, TripleTOF[®] and Orbitrap instruments. If spectra were not available, then linear ion trap spectra (LIT) were included. MS³ and MSⁿ spectra were ignored. Spectra from the same instrument type were merged by Collision Energies into three groups: 0 to 60, > 60, and unknown.

Isobaric compounds with the same MS/MS pattern

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

The LibraryViewServiceHost stops responding intermittently

On the Windows 7 (64-bit) operating system, when the MasterView[™] software is opened from the PeakView[®] software menu bar, the LibraryViewServiceHost service occasionally stops responding. To resolve this issue, do the following:

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 starts the **LibraryViewServiceHost** service again.

The LibraryView[™] software occasionally stops responding when loading the library or results are not found when searching the library

To resolve these issues, do the following:

1. Make sure that the computer contains 32 GB RAM.
2. Start the computer again.
3. If the issue persists, contact SCIEX Technical Support at sciex.com/request-support and request that the SQL databases be cleared and that the libraries be installed again.

SCIEX OS and the MasterView[™] software occasionally stop responding when the Import compounds from LV database feature is used

The **Import compounds from LV database** feature is used to import compound names and formulas from the library into SCIEX OS and the MasterView[™] software.

As a workaround, for the NIST Library, perform non-target searches using the non-target peak finding algorithm in SCIEX OS and in the MasterView[™] software instead of importing the entire compound list into the components table or the XIC list.

Install a Licensed High Resolution Accurate Mass Library

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

Note: Internet access is required to obtain the license.

1. Log on to the computer as a Windows user with administrator privileges.
2. Do one of the following:
 - If the library is being installed from a DVD, then load the DVD in the DVD drive and continue with step 5.
 - If the library is being installed from a downloaded file, then continue with step 3.
3. 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.

4. After the download is complete, right-click the downloaded file and then click **Extract All**.
5. Go to <https://sciex.com/support/activate-software> and then log in using a SCIEX username and password.

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

The Activate Software page opens.

6. Select the appropriate instrument in the **Select Your Instrument** field.

Tip! If the instrument is not listed, then go to the [SCIEXNow](#) profile for the logged in user and add the instrument information.

Installation

7. In the Windows search field, type **ipconfig /all** to obtain 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.

8. Type all of the physical addresses in the **Computer ID** field.

Tip! A maximum of three physical addresses can be provided. 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.

9. Type the license key from the license card in the **License Key** field.

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

10. Click **Submit**.

After the required information is submitted, a license file is sent to the e-mail address registered to the SCIEX.com account.

11. Save the license file to the appropriate location:

- On a computer with version 1.0.2 or 1.0.3 of the LibraryView™ software installed, save the license file in the C:/Program Files/AB Sciex/LibraryView/LibraryViewFramework/Server folder.
- On a computer with version 1.2 or 1.3 of the LibraryView™ software installed, save the license file in the C:/Program Files/SCIEX/LibraryView/LibraryViewFramework/Server folder.

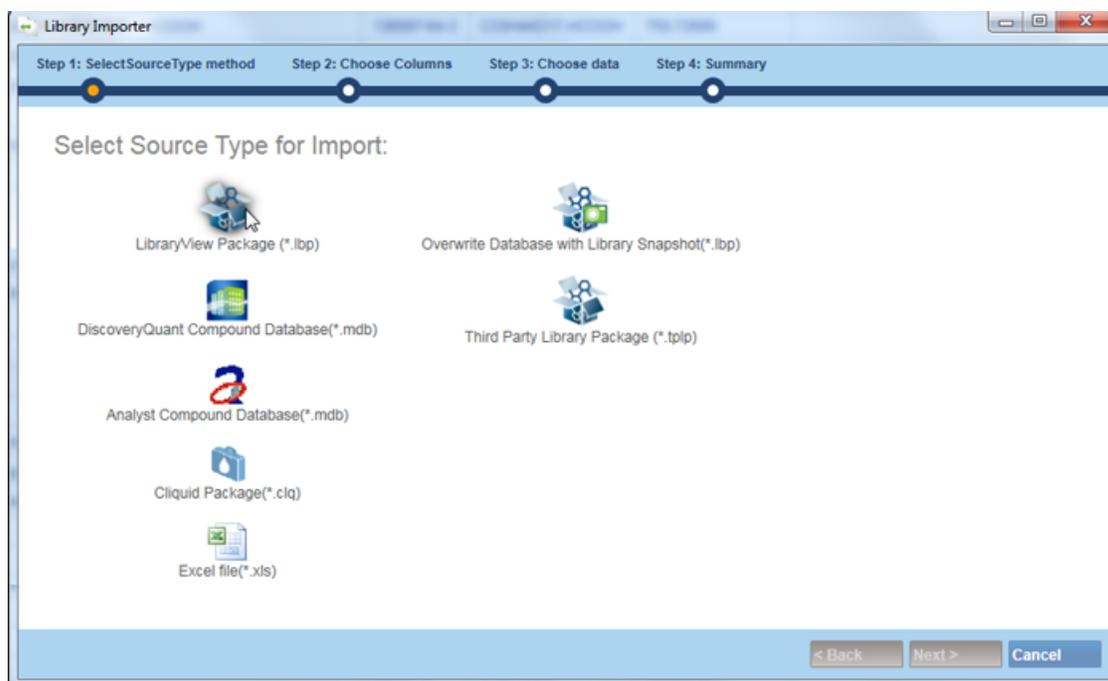
12. In the Windows search field, type **libraryviewpackager.exe** and then run the file.

Note: The **libraryviewpackager.exe** can also be accessed from one of the following locations, depending on the version of the LibraryView™ software that is installed.

- On a computer with version 1.0.2 or 1.0.3 of the LibraryView™ software installed, the **libraryviewpackager.exe** file is located in the C:/Program Files/AB Sciex/LibraryView/LibraryViewFramework/Packager folder.
 - On a computer with version 1.2 or 1.3 of the LibraryView™ software installed, the **libraryviewpackager.exe** file is located in the C:/Program Files/SCIEX/LibraryView/LibraryViewFramework/Packager folder.
-

The Library Importer dialog opens.

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

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

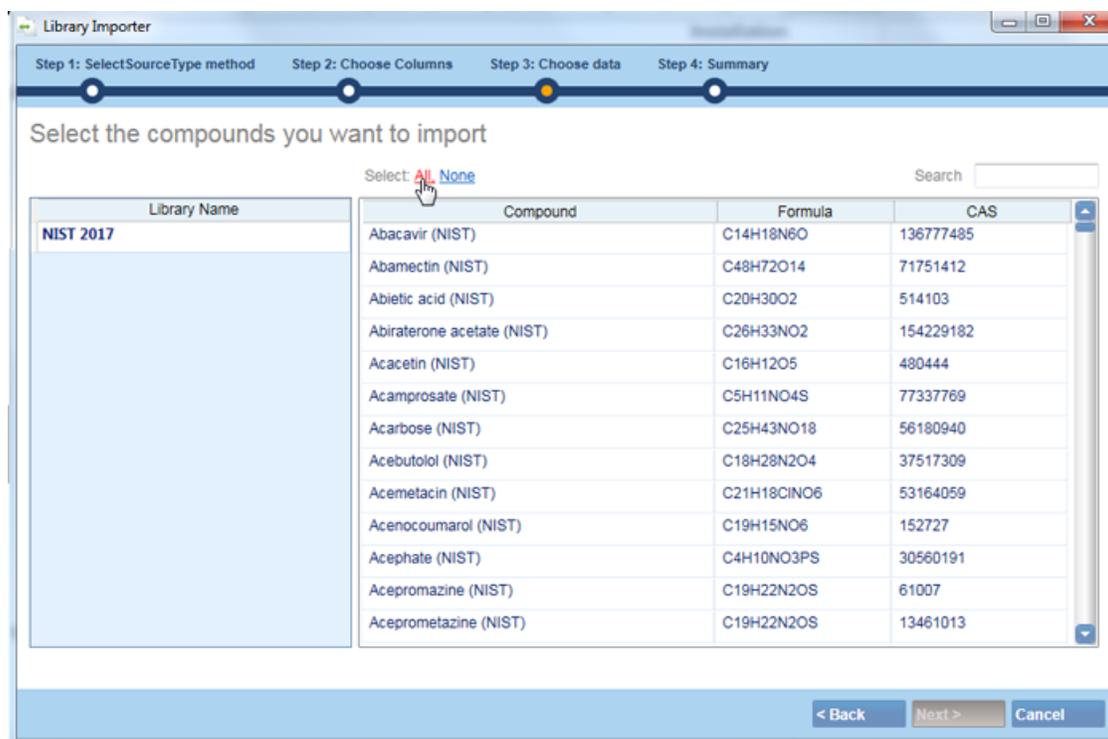
14. Browse to the files extracted in step 4 or to the DVD and then select the **NIST_1.0.1_Part_1.lbp** file.
15. Do one of the following:
 - Click **All** above the **Compound** column to import all of the compounds. Refer to [Figure 3-2](#).

Installation

- Click inside the appropriate row to import individual compounds.

Tip! To help locate 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 specified.

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



16. 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 remain in the database. The software will not revert the database to the pre-import state.

17. Resolve any conflicts, if required. Refer to [Compound Conflicts](#).

Note: If the original NIST Tandem (MS/MS) Library is already installed on the computer, then we recommend that the **Overwrite All** option is selected on the Library importer dialog to resolve the issue of incorrect structures being assigned to some of the compounds.

18. Click **Finish**.

Note: Due to the large size of the library, installation might take up to an hour for each part.

19. Browse to the files extracted in step 4 or to the DVD and then double-click **NIST_1.0.1_Part_2.lbp**.

20. Repeat step 15 to step 18.

21. Browse to the extracted files or to the DVD and then double-click **NIST_1.0.1_Part_3.lbp**.

22. Repeat step 15 to step 18.

After all of the parts of the library have been installed, the final library, containing all three parts, is shown as **NIST 2017**.

23. If the LibraryView™ software is installed, then create a backup of all of the libraries using the **Export > Library as snapshot (lbp)** feature after installation.

Note: If issues occur with any of the libraries, then the entire library can be imported as a snapshot more quickly than installing all of the libraries again using the exe packages.

Compound Conflicts

When installing a library containing a group of compounds or installing individual compounds, the software searches the database for compounds with the same name or formula as a compound in the package. If compounds are found, then the software flags the corresponding compounds in the package and waits for user input to continue.

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 stored in the database.
- Overwrite the compound information. Compound information from the package replaces the compound information stored in the database.
- Keep compound information. Compound information in the database is retained and the compound information from the package is discarded.

Conflict information is available to help the user make the correct choice.

View Compound Conflicts

1. Click **Resolve** beside the compound on the Library Importer dialog to view the details of the conflict.

Installation

2. Do one of the following:
 - Click **Keep Original** to keep the existing compound information and discard the new information.
 - Click **Use New** to replace the existing compound information with the new information.
3. Repeat steps 1 and 2 for each compound.
4. Click **Finish** after all of the conflicts are resolved.

Merge Compounds

1. Do one of the following on the Library Importer dialog:
 - Click **Merge** to merge new spectra, transitions, and retention times from individual compounds in the import package with the corresponding compound information stored in the database.
 - Click **Merge All** to merge new spectra, transitions, and retention times from all of the compounds in the import package with the corresponding compound information stored in the database.
2. Click **Finish** after all of the conflicts are resolved.

Overwrite Compounds

1. Do one of the following on the Library Importer dialog:
 - Click **Overwrite All** to overwrite all of the compound information stored in the database with the corresponding compound information from the import package.
 - Click **Resolve** beside the appropriate compound and then click **Use New** to overwrite the compound information stored in the database with the corresponding compound information from the import package.
2. Click **Finish** after all of the conflicts are resolved.

Keep Original Compounds

1. Do one of the following on the Library Importer dialog:
 - Click **Keep All Original** to keep all of the compound information stored in the database and discard the compound information from the import package.
 - Click **Keep Original** beside the appropriate compound to keep the individual compound information stored in the database and discard the compound information from the import package.
2. Click **Finish** after all of the conflicts are resolved.

Update Libraries that Contain Added Spectra

1. To prevent the loss of customer added spectra when libraries are updated, do the following:
 - a. Append "compound_lab name" to the compound name.
 - b. Click the X on the spectra entry in the LibraryView™ software to delete all of the data from the compound and keep only the customer appended spectra.
 - c. Import the new library.
2. Click **Finish** after all of the conflicts are resolved.

Note: A licensed version of LibraryView™ software is required to delete compound spectra.

Recommended Library Search Settings

The NIST library contains spectra from multiple instrument platforms and spectra that is merged from multiple spectra acquired at various Collision Energy (CE) settings. Therefore, the library search parameters must be carefully optimized to effectively search the library. [Figure 3-3](#) shows the recommended library search settings for the MasterView™ 1.1 software and SCIEX OS 1.3. Complete the following settings:

- Deactivate the Collision Energy filtering to prevent false negatives.
- Set the Precursor Mass Tolerance to 0.01 Da to accelerate the processing time.
- Increase the Intensity Factor to 10 to account for instrumental differences in relative intensity.

Installation

Figure 3-3 Recommended Search Settings for the NIST Library

Configure the library search parameters

Perform Library Search

Library Search Algorithm: Smart Confirmation Search

Results Sorted By: Purity

Library Spectra Type: Accurate Mass Only

Libraries To Search: Search All Libraries
 NIST 2017

Algorithm Parameters

Precursor Mass Tolerance +/- 0.01 Da

Collision Energy +/- 5 eV

Retention Time +/- 0.5 min

Fragment Mass Tolerance +/- 0.05 Da

Ignore Isotopes In Unknown Maximal Number Of Hits 5

Use Polarity Intensity Threshold 0.05

Use Collision Energy Spread Minimal Purity 10.0 %

Use Compound Specific Purity Threshold Intensity Factor 10

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- In Europe: Europe.CustomerTraining@sciex.com
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Online Learning Center

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SCIEX and its representatives maintain a staff of fully-trained service and technical specialists located throughout the world. They can answer questions about the system or any technical issues that might arise. For more information, visit the SCIEX website at sciex.com or contact us in one of the following ways:

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