Wiley HR-MS/MS Mass Spectral Libraries

Release Notes

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Introduction

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Features

The Wiley High Resolution Mass Spectrometry Mass Spectral (HR-MS/MS) Libraries are extensive HR-MS/MS libraries that include the following:

- Maurer/Meyer/Helfer/Weber (MMHW) LC-HR-MS/MS library of drugs and poisons, and their metabolites
- Wiley registry of tandem mass spectral data—MS for ID

The MMHW LC-HR-MS/MS library of drugs and poisons, and their metabolites, contains HR-MS/MS and nominal mass spectra of 5,006 chemical compounds. These spectra have been carefully examined by recognized spectrometrists for correctness and consistency, using both human and computer methods.

The Wiley HR-MS/MS Mass Spectral Libraries are compatible with:

- Data acquired on a TripleTOF® system or a QTRAP® system, using a combination of the MasterView™ 1.1 Software and the PeakView® 2.2 Software.
- Data acquired on a SCIEX X500 QTOF system, using SCIEX OS 1.4 or higher.

Use these libraries in the MasterView™ Software and PeakView® Software included in SCIEX OS to:

- Accurately identify compounds and increase confidence in the reported results.
- Enable rapid compound searches for targeted and non-targeted screening.
- Leverage the accurate mass and peak area reporting functionality.
- Compare a sample against a control for qualitative review, using the comparative profiling functionality.

Requirements

- An English version of:
  - Windows 7, 64-bit, operating system, with SP1.
  - Windows 10, 64-bit, operating system.

- Internet access is required to obtain a license file for each installed HR Accurate Mass Library.
- The user must be logged on the computer as a user with administrator privileges.
- One of the following applications must be installed on the computer to install the library:
    - A licensed version of the PeakView® Software, version 2.2 or higher, combined with a licensed version of the MasterView™ Software, version 1.1 or higher.
    - A licensed version of SCIEX OS, version 1.4 or higher.
    - A licensed version of the LibraryView™ Software, version 1.0.2 or higher.

Note: A licensed version of the LibraryView™ Software, version 1.2 or higher, is required to edit the library.

Supported Equipment

- TripleTOF® system
- QTRAP® system
- SCIEX X500 QTOF system
- Dell Precision T3600 computer, or later model with 32 GB of RAM, provided by SCIEX

Notes on Use and Known Issues 2

Notes on Use

Wiley HR-MS/MS Mass Spectral Libraries

The spectral data was not acquired by SCIEX OS or examined using SCIEX OS. However, the spectral data was converted and condensed for use in SCIEX OS. Spectra were acquired on multiple instruments, however the spectra acquired using the SCIEX X500 QTOF System or SCIEX Triple Quad™ System is preferred. If an instrument was not available, then ion trap spectra were included. MS^3 and MS^n spectra were disregarded.

Isobaric compounds with the same HR-MS/MS pattern

Because the isobaric compounds have similar product ion spectra, they are differentiated by retention time.

Known Issues

The LibraryViewServiceHost software occasionally stops responding

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 File 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

To resolve this issue, do the following:

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

The LibraryView^{TM} Software occasionally stops responding when results are not found when searching the library

To resolve this issue, do the following:

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

SCIEX OS and the MasterView^{TM} Software occasionally stop responding when the Import compounds from LV database feature is used after compound names and formulas were imported to the MasterView^{TM} Software and SCIEX OS

For the Wiley HR-MS/MS Mass Spectral Libraries, perform non-target searches using the non-target peak finding algorithm in the MasterView^{TM} Software and SCIEX OS rather than importing the entire compound list in the components table or XIC list.

Installation 3

Install a Licensed High Resolution Accurate Mass Library

A licensed library can be installed from a DVD or from a zip file downloaded from the SCIEX website. For each library compound, the application file can include the compound name, CAS number, precursor *m/z*, a mol file, collision energy, collision energy spread, and positive and negative HR-MS/MS 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 (https://sciex.com/software-support/software-downloads).

   Tip! To prevent potential installation issues, save the file to a location other than the computer desktop and disconnect any external USB storage devices.
4. After the download is complete, right-click the downloaded file and then click **Extract All**.
5. Obtain the license key from the product packaging.
6. Go to https://sciex.com/support/activate-software.
7. Click **login**.
8. Do one of the following:
   - Type the **Email Address** and **Password** of an existing account and then click **Log in**.
   - Click **Create An Account** and then follow the instructions provided.

After the log on or account creation is completed, the Activate Software web page opens. The first name, last name, and e-mail address of the user are shown in the first three fields in the form.

9. Select the appropriate 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.

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10. In the Windows search field, type "cmd" to open the command prompt and then 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.

11. Type 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.

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12. Type the license key from the license package 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.

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13. Click **Submit**.

    A message is shown indicating that an e-mail with the license file will be sent.

14. When the e-mail containing the license file is received, save the license file to the appropriate location:
    - On a computer with the MasterView™ Software installed, save the license file in the C:/Program Files/AB Sciex/LibraryView/LibraryViewFramework/Server folder.
    - On a computer with SCIEX OS installed, save the license file in the C:/Program Files/SCIEX/LibraryView/LibraryViewFramework/Server folder.
15. In the Windows search field, type **libraryviewpackager.exe** and then run the file.

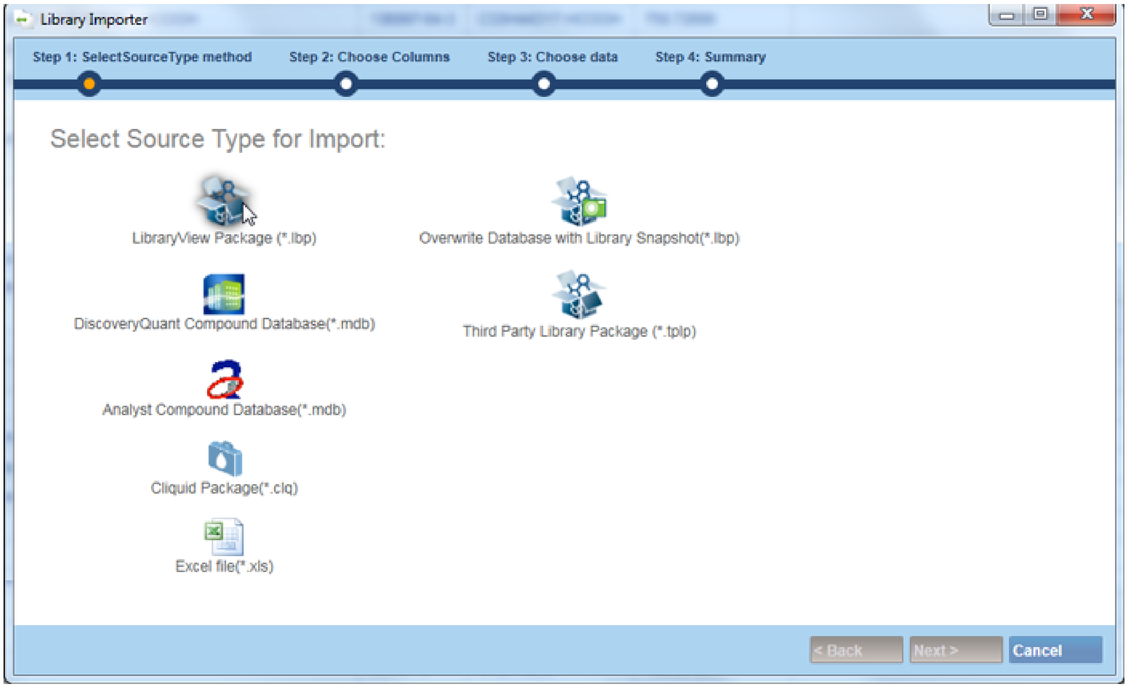
Note: The **libraryviewpackager.exe** can also be accessed from one of the following locations, depending on the version of the LibraryView™ Software that is installed:

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

The Library Importer dialog opens.

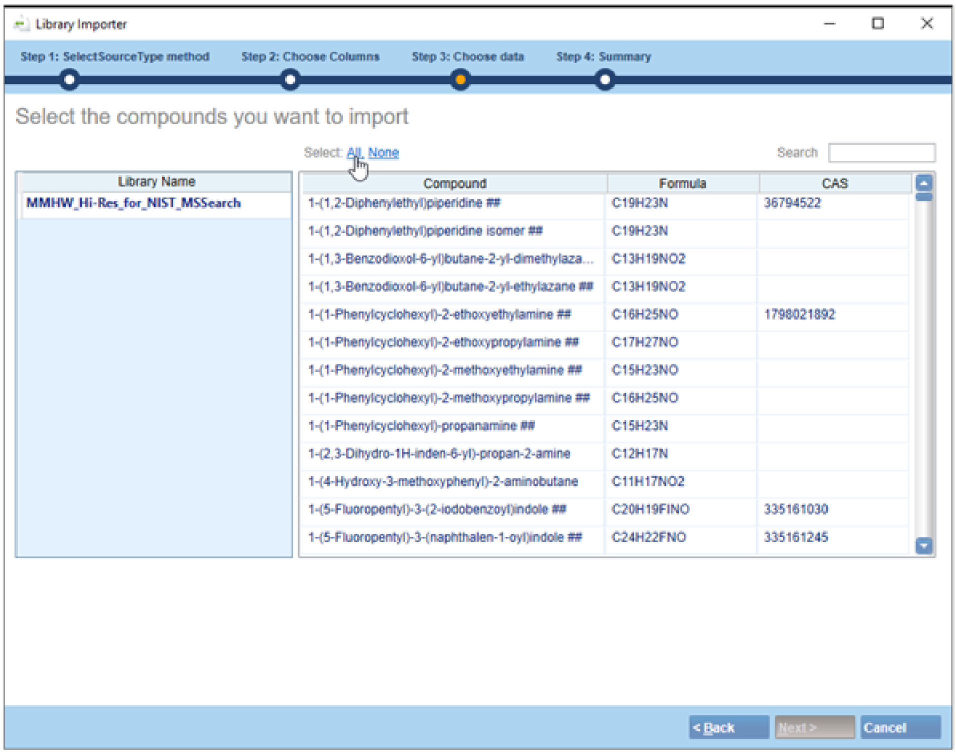
16. Click **LibraryView Package (*.lbp)**.

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



17. Do one of the following:
    - Browse to the files extracted in step 4 or to the DVD and then select the Wiley HR-MS/MS Mass Spectral Libraries file.
    - Click **All** above the **Compound** column to import all of the compounds. Refer to Figure 3-2.

Figure 3-2 Library Importer Dialog—Select the compounds you want to Import



Select the compounds you want to import

Library Name
MMHW_Hi-Res_for_NIST_MSSearch

Compound	Formula	CAS
1-(1,2-Diphenylethyl)piperidine ##	C19H23N	36794522
1-(1,2-Diphenylethyl)piperidine isomer ##	C19H23N	
1-(1,3-Benzodioxol-6-yl)butane-2-yl-dimethylaza…	C13H19NO2	
1-(1,3-Benzodioxol-6-yl)butane-2-yl-ethylazane ##	C13H19NO2	
1-(1-Phenylcyclohexyl)-2-ethoxyethylamine ##	C16H25NO	1798021892
1-(1-Phenylcyclohexyl)-2-ethoxypropylamine ##	C17H27NO	
1-(1-Phenylcyclohexyl)-2-methoxyethylamine ##	C15H23NO	
1-(1-Phenylcyclohexyl)-2-methoxypropylamine ##	C16H25NO	
1-(1-Phenylcyclohexyl)-propanamine ##	C15H23N	
1-(2,3-Dihydro-1H-inden-6-yl)-propan-2-amine	C12H17N	
1-(4-Hydroxy-3-methoxyphenyl)-2-aminobutane	C11H17NO2	
1-(5-Fluoropentyl)-3-(2-iodobenzoyl)indole ##	C20H19FINO	335161030
1-(5-Fluoropentyl)-3-(naphthalen-1-oyl)indole ##	C24H22FNO	335161245

18. Click inside the appropriate row on the Library Importer dialog 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.

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19. 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.

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20. Resolve any conflicts, if required. Refer to Compound Conflicts.
21. Click **Finish** and then restart the computer.

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

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22. Extract the other library files from the .zip folder and repeat step 5 to step 21.

Tip! If the LibraryView^{TM} Software is installed, then create a backup of all of the libraries using the **Export > Library as snapshot (*.lbp)** feature after the libraries are properly installed. If problems persist with the libraries, import the entire library as a snapshot rather than installing it 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.
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. On the Library Importer dialog, do one of the following :
    - 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. On the Library Importer dialog, do one of the following:
    - 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.

Maintain Added Spectra Not Included the Original Library Package

1. To prevent losing customer-added spectra when updating libraries:
    - Append the "compound_lab name" to the compound name.

  - Click X on the spectra entry in the LibraryView™ Software and keep only the spectra appended by the customer.

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

  - Import the new library following the standard instructions for update.

2. Click **Finish** after all of the conflicts are resolved.

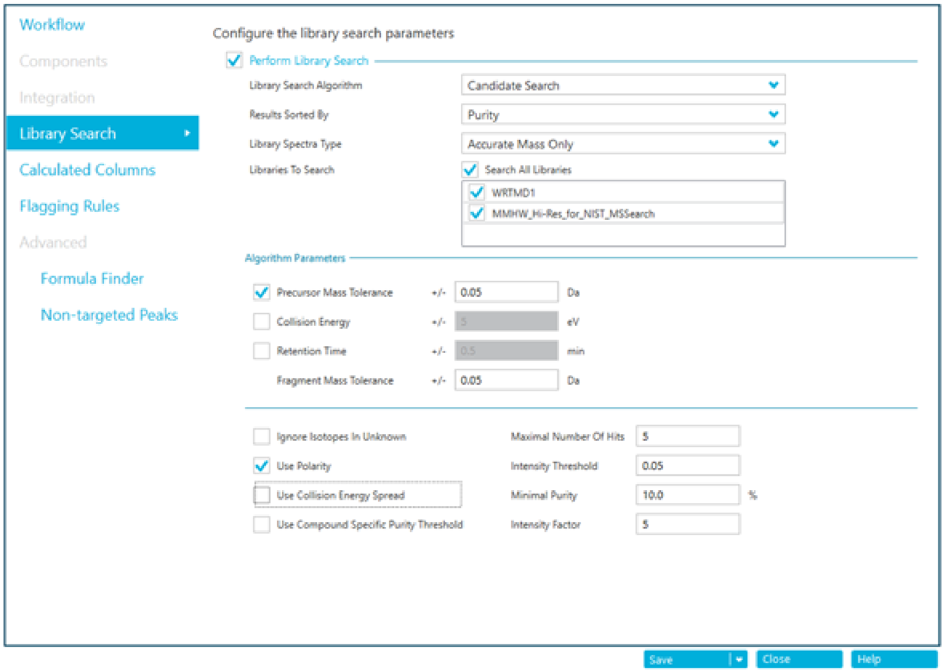
Recommended Library Search Settings

The Wiley HR-MS/MS Mass Spectral Libraries contain spectra acquired using multiple instruments 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™ Software, version 1.1, PeakView® Software, version 2.2, and SCIEX OS, version 1.4.

The following alternate settings may be helpful:

- To prevent false negatives, clear the **Collision Energy** check box.
- To accelerate the processing time, select the **Precursor Mass Tolerance** check box and then type 0.1 in the field provided.
- To account for differences in relative intensity caused by the use of different instruments, increase the **Intensity Threshold** to 10.

Figure 3-3 Recommended Search Settings for the Wiley HR-MS/MS Mass Spectral Libraries



Configure the library search parameters

☑ Perform Library Search

Library Search Algorithm: Candidate Search
Results Sorted By: Purity
Library Spectra Type: Accurate Mass Only
Libraries To Search: ☑ Search All Libraries
☑ WRTMD1
☑ MMHW_Hi-Res_for_NIST_MSSearch

Algorithm Parameters

☑ Precursor Mass Tolerance +/- 0.05 Da
☐ Collision Energy +/- 5 eV
☐ Retention Time +/- 0.5 min
Fragment Mass Tolerance +/- 0.05 Da

☐ Ignore Isotopes In Unknown
☑ Use Polarity
☐ Use Collision Energy Spread
☐ Use Compound Specific Purity Threshold

Maximal Number Of Hits: 5
Intensity Threshold: 0.05
Minimal Purity: 10.0 %
Intensity Factor: 5

For information about the library search parameters settings in the MasterView^{TM} Software, refer to the *High Resolution Accurate Mass Libraries Release Notes* available at https://download.sciex.com/HRAM-Libraries-Release-Notes-secured.pdf.

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