

Natural Products HR-MS/MS Spectral Library 1.1



Introduction

Thank you for choosing SCIEX LC-MS/MS technology and the LibraryView™ software or the PeakView® software with the MasterView™ software. This guide provides instructions for installing and activating the Natural Products HR-MS/MS Spectral Library 1.1.

The Natural Products HR-MS/MS Spectral Library 1.1 is a searchable High Resolution-MS/MS (HR-MS/MS) library based on SCIEX standard spectra library architecture. The library enables customers to identify unknown natural product compounds. Along with the HR-MS information, which is available in the Natural Products Library - Traditional Chinese Medicine, this library product contains additional compound entries with structural information and MS/MS spectra for 800 selected compounds.

Requirements

To use this licensed HR-MS/MS library application, one of the following SCIEX software applications must be installed on the computer:

- LibraryView™ software, version 1.0 or higher
- PeakView® software, version 2.2 or higher with the MasterView™ software, version 1.1 or higher

Install and Activate the Natural Products HR-MS/MS Spectral Library 1.1

The Natural Products HR-MS/MS Spectral Library 1.1 can be installed from a DVD or from a package downloaded from the SCIEX Website.

1. To begin, log on to the computer as a Microsoft 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 Web site.

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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. Browse to the extracted files or to the DVD and then double-click the **LvPackageTCM_2.1_MSMS Library.exe** file.

Tip! If the User Account Control message dialog opens, then click **Yes**.

Tip! If the LibraryView Setup (Not Responding) window opens, then close the message dialog, right-click the .exe file, and select the **Run as administrator** option to start the installation again.

6. Click **Software Activation** on the LibraryViewPackages Feature Unavailable dialog.
7. Type the license key in the **Obtain the license key from the license certificate or packaging and enter here** field on the LibraryViewPackagesActivation dialog.

Note: If a valid license key is not available, then contact <http://sciex.com/request-support>.

8. Click **Generate Computer ID**.
9. Click **Copy ID to Clipboard**.
10. Click <https://licensing.sciex.com/activation/LibraryViewPackages>.

Note: Internet access is required to obtain a license for the library. If the computer where the library was installed has Internet access, then the Computer ID and the License Key fields are automatically populated with the information from the LibraryViewPackagesActivation dialog. If the computer where the library was installed does not have Internet access, then make a copy of the generated computer ID. On a computer with Internet access, go to <https://licensing.sciex.com/activation/LibraryViewPackages>, type the licence key and paste the copied Computer ID in the appropriate fields.

11. Complete the mandatory fields in the **LibraryView Packages License Activation** form and then click **Submit**.

Note: After the required information is submitted, a license file is e-mailed to all of the e-mail addresses provided.

12. Close the browser window.
13. When the license file is received, save the license (lic) file to the desktop.

14. Click **Install License File** on the LibraryViewPackages Activation dialog.

The Select the new license file to be installed dialog opens.

15. Browse to and select the license file and then click **Open**.

16. Do one of the following on the Library Importer dialog:

- Select all of the compounds to import.
- Select individual compounds to import.
- Select individual libraries to import a library and the associated compounds.

Note: Compounds saved in a selected library are automatically selected in the compound list.

17. Click **Next**.

18. Resolve any conflicts, if required.

Note:

- Merge—Adds new spectra, transitions, and retention times to the selected compounds.
 - Resolve—Deletes information from selected compounds and replaces with new information.
 - Keep Original—Makes no changes to the original compound and ignores the new compound information.
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19. Click **Finish** after all conflicts are resolved.

20. Double-click any of the other exe files to import the corresponding libraries or compounds.

21. Repeat steps 2 through 19 for each library executable to be installed and activated.

Workflow for Natural Products HR-MS/MS Spectral Library 1.1

The Natural Products HR-MS/MS Spectral Library 1.1 consists of entries with HR-MS/MS spectral information of natural product compounds collected using the SCIEX TripleTOF[®] mass spectrometers and collision settings such as the following:

Collision Settings	Positive Ionization	Negative Ionization
CE	40	-40

Note: The CES of 20 is used in positive and negative modes of acquisition.

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Note: To achieve the best results, it is recommended that the user acquire the query data using the same collision settings.

The following procedure explains how to match the library using the data (wiff files) acquired from a TripleTOF[®] mass spectrometer:



1. Open the wiff file of the acquired data in the PeakView[®] software to perform a search against the libraries.
2. Select MasterView[™] from the PeakView[®] software menu bar and then click **New Session**.
3. Set the peak finding criteria for the following types of peak finding:
 - For non-targeted peak finding:
 - Click  in the MasterView[™] software.
 - Select the **Non-Targeted Peak Finding** check box from the **Calculations** tab.
 - Adjust the sensitivity of the peak finding by using the **Peak Detection Sensitivity** slider.
 - For targeted peak finding:
 - Build an XIC table based on the compound of interest and type the names and molecular formulae of the compounds in the table within the MasterView[™] software window.
 - Make sure that the adduct column matches the XIC list as, +H or -H for compounds or adducts that ionize with the gain (for example, M -H⁺, M-NH₄⁺) or loss (for example, M - HCOO⁻) of a proton respectively.
 - Leave the adduct column blank if expecting ionic compounds or ionic adducts (for example, M-K/Na⁺, M-Cl⁻).
4. Set up the library search criteria as follows:
 - Click  in the MasterView[™] software.
 - Select the **Perform Library Search** check box in the **Library Searching** tab.
 - Select the **TCM MS/MS Library** check box from the **Libraries To Search**.
 - Enter the appropriate tolerance for **Collision Energy**, based on the acquired data.
 - Clear the **Use Collision Energy Spread** check box.

Figure 1-1 Library Searching Tab

The screenshot displays the 'Library Searching' tab in the MasterView software. The interface includes several sections:

- Perform Library Search:** A checked checkbox.
- Algorithm To Use During Library Search:** A dropdown menu set to 'Candidate Search'.
- Results Sorted By:** A dropdown menu set to 'Purity'.
- Libraries To Search:** A list of libraries with checkboxes. 'TCM MS/MS Library' is checked and highlighted with a red box. Other libraries include TCM Library - W, X, Y, and Z.
- Algorithm Parameters:** A section with two columns: 'Constraint' and 'Tolerance'.
 - Constraint:** Includes checkboxes for 'Precursor Mass' (checked), 'Collision Energy' (checked and highlighted with a red box), 'Retention Time' (unchecked), and 'Mass Tolerance' (unchecked).
 - Tolerance:** Includes input fields for values: 0.4 Da, 5 eV (highlighted with a red box), 0.5 min, and 0.4 Da.
- Additional Parameters:** Includes checkboxes for 'Use Polarity' (checked), 'Use Collision Energy Spread' (checked and highlighted with a red box), and 'Use Compound Specific Purity Threshold' (unchecked). It also features input fields for 'Maximal Number Of Hits' (5), 'Intensity Threshold' (0.05), 'Minimal Purity' (10 %), and 'Intensity Factor' (5).
- Buttons:** 'Reset Algorithm Values To Default', 'OK', and 'Cancel'.

Refer to the MasterView™ software *Help* to fine tune the library searches using the MasterView™ software.

5. Click **OK**.
6. Click **Process**.

Related Documentation

The following SCIEX technical application note publications are available:

- *Using Your QTRAP® LC/MS/MS System at Full Potential A Quick-Start Guide to Activate and Perform MS/MS Library Searching for Identification and Confirmation using MasterView™ and LibraryView™ Software*, Publication number: 10160414-01.
- *Using Your QTRAP® LC/MS/MS System at Full Potential A Quick-Start Guide to Import and Update MS/MS Libraries for Identification and Confirmation using MasterView™ and LibraryView™ Software*, Publication number: 10160614-01.

Technical Support

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 website at sciex.com.

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