



Agilent MassHunter LC/SQ ChemStation Integration Software

Quick Start Guide

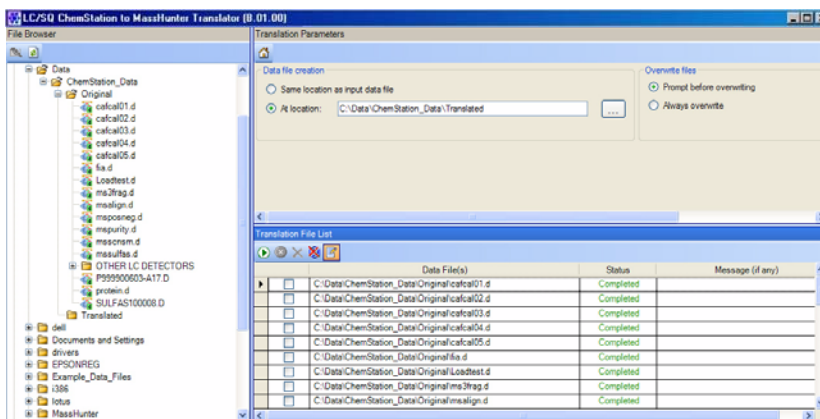
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This guide describes how to use the Agilent MassHunter LC/SQ ChemStation Integration Software version B.01.00.



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What is the Agilent MassHunter LC/SQ ChemStation Integration Software?

This program lets you translate LC/MS ChemStation data files to the MassHunter format so that they can be analyzed with the Agilent MassHunter Workstation Software - Qualitative Analysis and Quantitative Analysis programs.

LC/MS ChemStation Data and the Qualitative Analysis Program

With the Qualitative Analysis program, you can do Find Compounds by Formula on your translated LC/MS ChemStation data.

The Qualitative Analysis program can also present large amounts of data for review in one central location. You can do these tasks for any type of LC/MS data that you open:

- Extract and display chromatograms.
- View and extract peak spectra.
- Subtract background.
- Integrate the chromatogram.
- Create basic reports from preconfigured templates.
- Customize report templates using the Report Designer Add-in that is run in Microsoft Excel.

You can also set up methods to automatically do the tasks in the list, as well as others, when you open the data files.

LC/MS ChemStation Data and the Quantitative Analysis Program

You can also quantitate your translated LC/MS ChemStation data with the Quantitative Analysis program.

You can quantitate very low amounts of material with the following unique features:

- Curve-fit assistant to test all fits and statistics on curve quality.
- Automated, parameter-free integrator that uses a novel algorithm, which has been optimized for triple quad data, but can work well for single quad data also.
- Batch-at-a-Glance results window to help you review and operate on an entire batch of data at once.
- Automatic detection and identification of outliers.

Where to find more information

- Use the online Help for in-depth information not given in this *Quick Start Guide*. Press **F1** in the LC/SQ Chemstation to MassHunter Translator program to open the online Help.
- Use the online Help for the Qualitative Analysis program and the Quantitative Analysis program to learn how to use these programs. Click the **Help > Contents** command or press **F1** in either program to open the online Help for that program.
- Refer to these guides to learn how to use the Agilent MassHunter Workstation Software data analysis programs. They are included with the MassHunter Workstation software:
 - *Qualitative Analysis Familiarization Guide*
 - *Quantitative Analysis Familiarization Guide*

Installation

- 1 Check that no other program is running on your system, including Windows Update.
- 2 If a previous version of the Agilent MassHunter LC/SQ ChemStation Integration Software is present, it must be uninstalled before loading the latest version. Please use the Windows Add/Remove Programs in the Control Panel to remove any previous versions.
- 3 Put the CD labeled **MassHunter LC/SQ ChemStation Integration Software** into the CD drive.
- 4 From the CD, double-click **Setup.exe**.
- 5 In the Welcome screen, click **Next**.
- 6 In the License Agreement screen, click **I accept the terms of the license agreement**, then click **Next**. If you want to print the License Agreement, click **Print** and the License Agreement is printed to the default printer.
- 7 In the Choose Destination Location screen, click **Next** to accept the default destination location.

The default is C:\Program Files\Agilent\MassHunter\Workstation\ChemStationIntegration.
- 8 In the Choose location for customer data files screen, click **Next** to accept the default destination location.

The default is D:\MassHunter.
- 9 In the Start Copying Files screen, review the settings and then click **Next**.
- 10 When the InstallShield Wizard Complete message is displayed, click **Finish**.
- 11 Open the readme.txt file on the installation CD.

Getting Started

This section contains the tasks you need to know to operate the LC/SQ Chemstation to MassHunter Translator program.

- “To select one or more data files to translate” on page 5
- “To select the folder to use to place the translated data files” on page 5
- “To translate data files” on page 6

To select one or more data files to translate

- 1 Select the LC/MS ChemStation data file (s) that you wish to translate from the File Browser list.

To choose multiple files that are listed next to each other, press the **Shift** key while selecting the data files with the left mouse button.

To choose multiple files that are not listed next to each other, press the **Ctrl** key while selecting the data files with the left mouse button.

- 2 Click  in the File Browser toolbar.

You can also right-click the File Browser pane and then click **Add File(s)** from the shortcut menu.


To select the folder to use to place the translated data files

You can either place the translated data files into the same folder as the input data file or you can select a new folder.

Same folder as data files

- 1 Click **Same location as input data file** under **Data file creation**.


Selected folder

- 1 Click **At location** under **Data file creation**.
- 2 Click  under **Data file creation**. The Browse For Folder dialog box is opened.
- 3 Select the folder where you want to place the translated files. You click **Make New Folder** to create a new folder.

If the MassHunter Workstation Software - Qualitative Analysis program or Quantitative Analysis program is installed on the same computer, you may select the default MassHunter data folder that is usually **D:\MassHunter\Data**. If the folder that you specify does not exist when you start the translation, the translation fails.

- 4 Click **OK**.

To translate data files

- 1 Do the steps in [“To select one or more data files to translate”](#) on page 5.
- 2 Do the steps in [“To select the folder to use to place the translated data files”](#) on page 5.
- 3 Click  in the Translation File List toolbar.

You can also right-click the Translation File List pane and click **Translate** in the shortcut menu to start translating the selected data files.

- 4 Check the **Status** column to verify that each translation completed successfully.

LC/SQ Chemstation To MassHunter Translator Panes

Main Window

This section contains information on the user interface for the LC/SQ Chemstation to MassHunter Translator program. The user interface contains four different panes:

- “File Browser Pane” on page 7
- “Translation Parameters Pane” on page 8
- “Translation File List Pane” on page 8
- “Translation Status Details Pane” on page 10

This program is started from the Agilent MassHunter Workstation group. You click the **LC/SQ Chemstation Translator** command.

File Browser Pane

You can browse through the files on the system and select LC/MS ChemStation data files that you wish to translate. If you double-click on the name of an LC/MS ChemStation data file, that data file name is added to the Translation File List table. You can also right-click this pane and click **Add File(s)** from the shortcut menu to add one or more files to the Translation File List table.

Toolbar



Adds the currently selected Chemstation data file to the Translation File List table



Refreshes the File Browser list

Shortcut Menu


Add File(s) Adds the currently selected files to the Translation File List table.

Translate Adds the currently selected files to the Translation File List table and starts the translation process for the files marked for translation.

Translation Parameters Pane

Data file creation

Same location as input data file The translated data files are placed in the same folder as the LC/MS ChemStation data files. If you click this option, then the MassHunter version of the data will be added to the ChemStation .D folder, and the same data file can be processed in ChemStation and MassHunter.

At location The translated LC/MS ChemStation data files are placed in the folder specified. You click  to select a different folder. If the specified folder does not exist when you translate the data files, the translation fails.

Overwrite files

Prompt before overwriting When the translation program is running, a message box is displayed if a data file would be overwritten. This message box asks whether or not you want to overwrite the existing data file.

Always overwrite When the translation program is running, data files are overwritten if the same name as an existing data file is used. No message box is displayed.

Translation Parameters Toolbar



Restores the default parameters in the Translation Parameters pane

Translation File List Pane

Translation File List Table

Check Box Allows you to select which files to translate. When a data file is first added to the **Translation File List** table, the check box in that row is marked. When the data file is translated, the check box is cleared. When new data files are added to this table, they are appended to the end of the table and the check boxes are marked automatically.

Data File(s) The name of the data file to translate.

Status The status of the translation process. When you first add a data file to the Translation File List table, the **Status** column is set to **Not Started**. When a file has been translated, the **Status** column is set to **Completed**. If an error occurs during the translation, the **Status** column is set to **Failed**.

An icon is placed next to the **Status** if a problem occurred.



An error occurred while the file was being translated. The problem is described in the **Message (if any)** column.



A warning occurred while the file was being translated. The warning is described in the **Message (if any)** column.

Message (if any) If an error or warning occurred while translating the ChemStation data file, the error or warning message is listed in this column.

Toolbar



Starts translating the files that are listed in the Translation File List table.



Stops translating the files. This button is only available when you are translating files.



Deletes the currently selected rows from the Translation File List table.



Clears all lines in the Translation File List table.



Toggles whether or not to show the Translation Status Details pane.

Shortcut Menu

Translate Starts translating the files listed in the Translation File List table.

Stop Stops translating the files listed in the Translation File List table.

Delete Rows Deletes the currently selected row or rows from the Translation File List table.

Clear Table Deletes all rows in the Translation File List table.

Set check mark on highlighted files Marks the check box in the Check Box column for each row that is highlighted.

Remove check mark on highlighted files Clears the check box in the Check Box column for each row that is highlighted.

Translation Status Details Pane

File The name of the file that is selected in the Translation File List table.

Translation Status The status of the translation process. Possible values include:

- Not Started
- Completed
- Completed with warning
- Failed

Translation Time The length of time it took to translate the ChemStation file.

Message (if any) If an error or warning occurred during translation, it will be displayed here.

Error Details (if any) If an error or warning occurred during translation, details from the program are shown here. This information is for internal use only.

Shortcut menu

Copy Copies the information in this pane to the Clipboard.

Select All Selects all information in this pane.

www.agilent.com

In this book

This guide has instructions for installing and using the Agilent MassHunter LC/SQ ChemStation Integration Software.

Please send any comments on this guide to feedback_lcms@agilent.com.

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