Agilent MassHunter LC/SQ ChemStation Integration Software

Quick Start Guide

This guide describes how to use the Agilent MassHunter LC/SQ ChemStation Integration Software version B.04.00. This software has two main parts: an interactive translator and an automated translator that is run when you run a ChemStation method.

Interactive translator

You can use this program to manually translate one or more ChemStation LC/SQ data files to the MassHunter format. Data files are translated outside of the ChemStation program in a separate program, *LC/SQ ChemStation to MassHunter Translator*.

Agilent Technologies
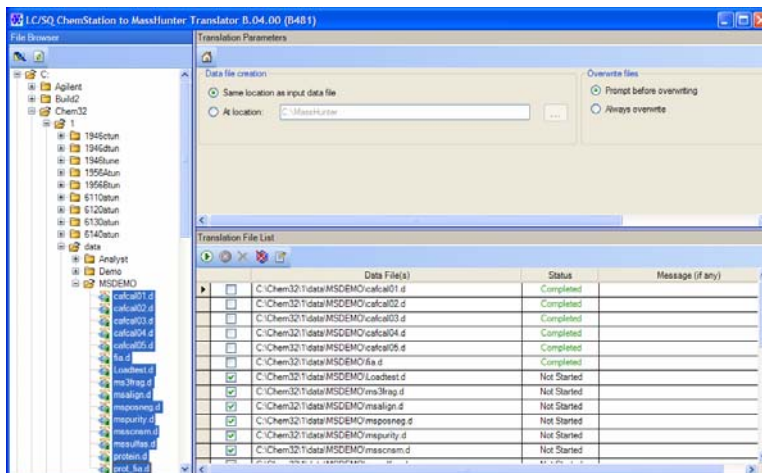
Automated translator

The automated translator is run as part of a ChemStation method. After the data is acquired, the data can be automatically translated to the MassHunter data format. In addition, you can automatically run a MassHunter Qualitative Analysis method when you run a ChemStation method.
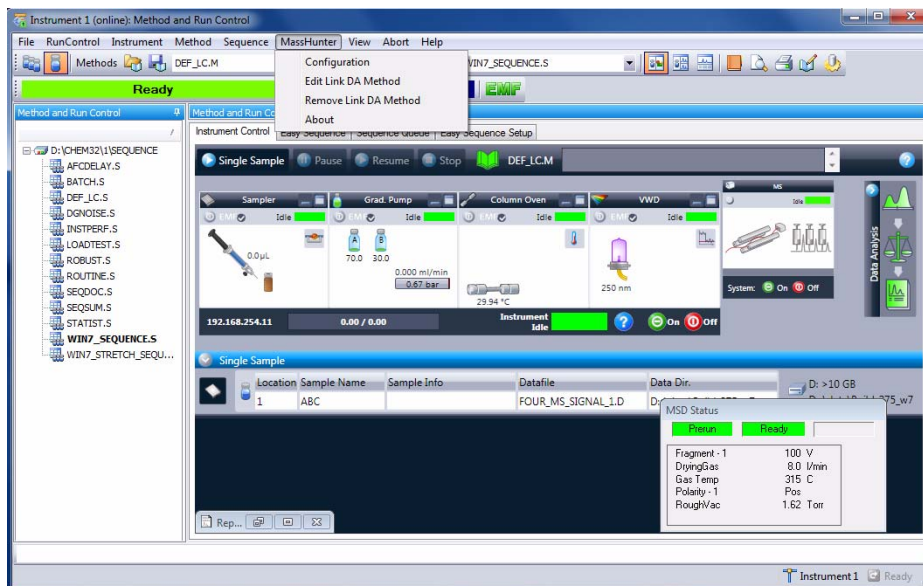
What is the Agilent MassHunter LC/SQ ChemStation Integration Software?

These programs let 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. You can either translate the data file after it is acquired automatically as part of running the method or interactively translate the data file later.

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 Table window to help you review and operate on an entire batch of data at once.

- Automatic detection and identification of outliers.

- Compounds-at-a-Glance.

- Rapid set up of Quantitative Analysis methods using information in the Acquisition method (compound names, SIM ions, ISTD designations, etc.).

- Easy export of the Batch Table to Excel spreadsheets or upload to a LIMS system.

Where to find more information

- Use the online Help for in-depth information not given in this *Quick Start Guide*. Two different online Help files are available for the ChemStation Integration program. Press **F1** in the interactive LC/SQ ChemStation to MassHunter Translator program to open the online Help for that program. Click the **Help** button in the dialog boxes in the ChemStation program to open the online Help for the automated ChemStation Integration program.

- 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, use the Windows Add or Remove Programs in the Control Panel to remove any previous versions.

3 If you have an installation disc:

   a Put the installation disc into the disc drive.

   b Browse to the folder **MassHunter LC & SQ ChemStation Integration Software**.

4 If you do not have an installation disc, copy the file **CSIntegrationSetup_xxx.exe** to your local hard drive.

5 For Windows 7 systems, right-click **CSIntegrationSetup_xxx.exe** and then click **Run as Administrator**. For Windows XP systems, double-click **CSIntegrationSetup_xxx.exe**.

6 In the Welcome page, click **Next**.

7 In the License Agreement page, 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.

8 In the **Choose Destination Location** page, click **Next** to accept the default destination location.

   The default is **C:\Program Files\Agilent\MassHunter\Workstation\ChemStationIntegration**.

9 In the **Choose location for customer data files** page, click **Next** to accept the default destination location.

   The default is **D:\MassHunter**.

10 In the **Start Copying Files** page, review the settings and then click **Next**.

11 When the InstallShield Wizard Complete message is displayed, click **Finish**.

12 Open the **readme.txt** file on the installation media.

Getting Started

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

These tasks are used in the interactive MassHunter Translator program:

- "To select one or more data files to translate" on page 6
- "To select the folder to use to place the translated data files" on page 7
- "To manually translate data files" on page 7

These tasks are used in the automated MassHunter Translator program:

- "To enable ChemStation Integration to MassHunter Qualitative Analysis" on page 8
- "To disable integration with MassHunter Qualitative Analysis" on page 9
- "To link Qualitative Analysis Method" on page 9
- "To remove link to Qualitative Analysis Method" on page 10

To select one or more data files to translate

This task is part of the interactive ChemStation Integration program.

1 Start the ChemStation Integration program. Do one of the following:

- Click **Start > All Programs > Agilent > MassHunter Workstation > LC-SQ ChemStation Translator**
- Click **Start > Programs > Agilent > MassHunter Workstation > LC-SQ ChemStation Translator**

2 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.

3 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.

This task is part of the interactive ChemStation Integration program.

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 manually translate data files

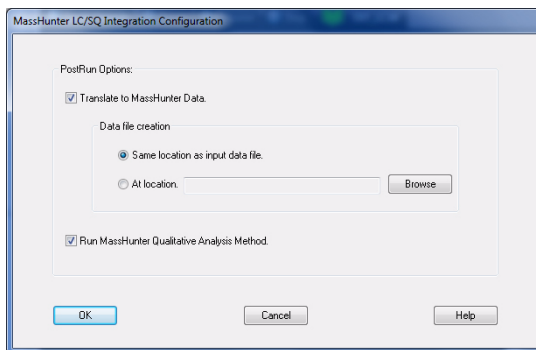This task is part of the interactive ChemStation Integration program.

1 Do the steps in "To select one or more data files to translate" on page 6.

2 Do the steps in "To select the folder to use to place the translated data files" on page 7.

3 Click in the Translation File List toolbar.

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

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

To enable ChemStation Integration to MassHunter Qualitative Analysis

This task is part of the automated ChemStation Integration that is part of the ChemStation program.

1 Click **MassHunter > Configuration** in the LC/MS ChemStation's **Method and Run Control** view. The **MassHunter LC/SQ Integration Configuration** dialog box is opened.

2 Mark the **Translate to MassHunter Data** check box. To use the ChemStation data file in the MassHunter Qualitative Analysis program, the ChemStation data file needs to be translated to the MassHunter format.

3 Click either the **Same location as input data file** button or the **At location** button.

4 If you click **At location**, then click the **Browse** button.   The **Select a destination folder** dialog box is opened. Then, select the folder where you want to place the translated data file and click **OK**.

5 Mark the **Run MassHunter Qualitative Analysis Method** check box. When this check box is marked, the MassHunter Qualitative Analysis Method is automatically run as part of the ChemStation method.

6 Click **OK**.

To disable integration with MassHunter Qualitative Analysis

This task is part of the automated ChemStation Integration that is part of the ChemStation program.

1 Click **MassHunter > Configuration** in the LC/MS ChemStation's **Method and Run Control** view. The **MassHunter LC/SQ Integration Configuration** dialog box is opened.

2 Clear the **Translate to MassHunter Data** check box. If this check box is cleared, then the ChemStation data file is not automatically translated.

3 Clear the **Run MassHunter Qualitative Analysis Method** check box. When this check box is cleared, the MassHunter Qualitative Analysis Method is not run as part of the ChemStation method.

4 Click **OK**.

To link Qualitative Analysis Method

This task is part of the automated ChemStation Integration that is part of the ChemStation program.

1 Click **MassHunter > Edit Link DA Method** in the main menu.

2 Select the correct folder in the **Folders** list box. The name of the selected folder is shown directly above the list box. If necessary, select a different drive in the Drives box.

3 In the list box under the **Name** field, select the MassHunter Qualitative Analysis method name.

4 Click the **OK** button. You can also double click the name of the method in the list box to close this dialog box.
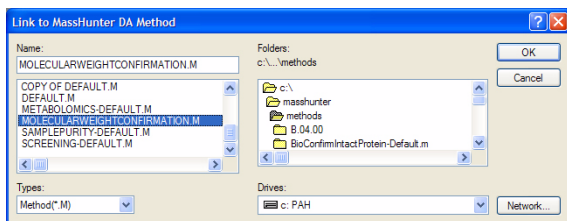
5 In ChemStation, click the **Method > Run Time Checklist** command. In the **Run Time Checklist** dialog box, mark the **Standard Data Analysis** check box.

To remove link to Qualitative Analysis Method

This task is part of the automated ChemStation Integration that is part of the ChemStation program.

1 Click the **MassHunter > Remove linked DA Method** command.

2 Verify that you want to remove the link to the MassHunter Qualitative Analysis method that is shown in the box.

3 Click the **OK** button.

Interactive 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:

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.

Automated LC/SQ Chemstation To MassHunter Translator Menu

This section contains information on the user interface for the Automated LC/SQ Chemstation to MassHunter Translator program. This user interface is part of the LC/MSD ChemStation user interface.

- "MassHunter Menu" on page 15
- "Translation Parameters Pane" on page 12
- "Translation File List Pane" on page 12
- "Translation Status Details Pane" on page 14

MassHunter Menu

Configuration   Opens the "MassHunter LC/SQ Integration Configuration Dialog Box" on page 15.

Edit Link DA Method   Opens the "Link to Masshunter DA Method Dialog Box" on page 16.

Remove Link DA Method   Opens the "Remove linked DA Method Dialog Box" on page 17.

About   Opens the **About** dialog box.

MassHunter LC/SQ Integration Configuration Dialog Box

You select whether or not to translate the ChemStation data file automatically here, and you also select whether or not to run the MassHunter Qualitative Analysis method as part of running a method in ChemStation.

PostRun Options

Translate to MassHunter Data   Whether or not to automatically translate the ChemStation data format to the MassHunter data format.

If this check box is marked, then any ChemStation method that is run needs to have a MassHunter Qualitative Analysis method linked to it. When you save a ChemStation method, the software checks if a MassHunter Qualitative

Analysis method is linked to the current ChemStation method. If no
Qualitative Analysis method is linked, you are automatically asked to select a
MassHunter Qualitative Analysis method to link to the ChemStation method
that you are saving.

Data file creation

Same location as input data file   The MassHunter data file that is created is
placed in the same folder as the ChemStation data file.

At location   The Masshunter data file that is created is placed in the specified
folder. You can directly type the folder name in the text box.

Browse button   Opens the **Select a destination folder** dialog box. After
selecting the location to place the data file, you click **OK** to close the dialog
box.

Run MassHunter Qualitative Analysis Method   Whether or not to automatically
run the Qualitative Analysis method when the ChemStation method is run. If
this check box is marked but the data file was not translated, the MassHunter
Qualitative Analysis method is not run.

Link to Masshunter DA Method Dialog Box

You select the method to run in the MassHunter Qualitative Analysis program
in this dialog box. This method is linked to the current ChemStation method.

Name   The name of the MassHunter Qualitative Analysis method to link to.
This MassHunter method is run when you mark the option to run the
MassHunter Method in the **MassHunter LC/SQ Integration Configuration**
dialog box.

Type   Either Method(*.M) or All Types (*.*). This value limits the type of files
and folders that are shown in the list box below the Name box. You select the
MassHunter method in the list box below the Name box. The value
Method(*.M) is the proper value in this dialog box.

Folders   The folder that is currently shown in the list box below the Name box.
This is the path to the MassHunter method. You can change this path by
selecting a different folder in the list box below this.

Drives   The currently selected drive. You can switch to a different drive if the MassHunter method is stored on a different drive.

Remove linked DA Method Dialog Box

You can remove the link to a MassHunter Qualitative Analysis method by using this dialog box. You are only removing the link. The MassHunter Qualitative Analysis method is not removed or changed.

DA Method to be removed   The name of the MassHunter Qualitative Analysis method that is currently linked to this ChemStation method. If you click OK, the link to this MassHunter method is removed.

NOTE	The MassHunter Qualitative Analysis Method is not removed.

Familiarization Exercises for Automated Workflows

This section shows you the different workflows that you can do when you combine the LC/MSD ChemStation Data Acquisition software with the MassHunter Qualitative Analysis program and the MassHunter Quantitative Analysis program.

Exercise 1. Synthetic compound confirmation and purity assessment

The MassHunter Qualitative Analysis program can confirm the molecular weight that you enter in the Sequence table.

The following three tasks will lead you through this workflow.

Task 1. Set up Molecular Weight Confirmation method in MassHunter Qualitative Analysis

In this task, you use the Qualitative Analysis program to update the worklist parameters to run a Molecular Weight Confirmation algorithm. The worklist actions are run when the Qualitative Analysis method is run.

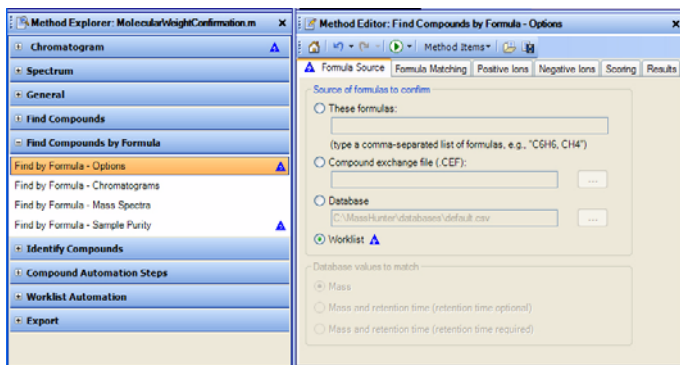| Steps	Detailed Instructions	Comments
1 In MassHunter Qualitative Analysis, open your most up-to-date method for this analysis.	**a** Double-click the Qualitative Analysis icon. **b** Open the method default.m. **c** Save the method to a new name (for example, *iii_MolecularWeight Confirmation.m*, where *iii* are your initials.	• Make sure that you are opening a MassHunter Qualitative Analysis method.
2 Set up the parameters for the Find Compounds by Formula algorithm.	**a** Click **Find by Formula** - **Options** in the Find Compounds by Formula section in the Method Explorer. **b** Click the **Formula Source** tab. **c** Click the **Worklist** button. **d** Review the other parameters in this section.	• You can use any of the demo files that are supplied with the software to test the worklist actions. • You can get help on any tab in the Method Editor window by pressing the **F1** key.

Figure 1   Find Compounds by Formula - Options section in the Method Editor in Qualitative Analysis

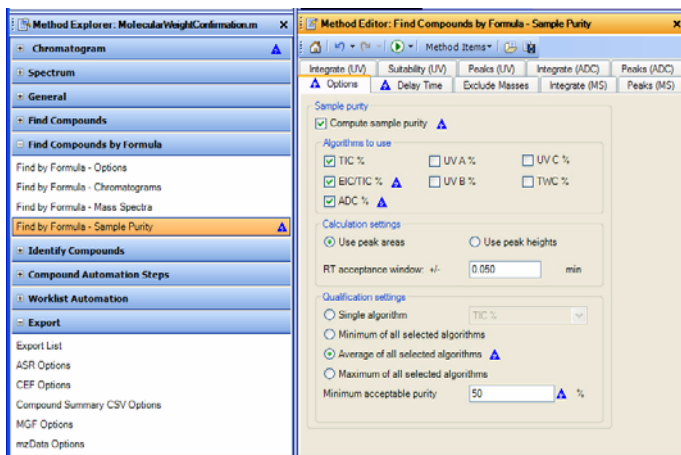| Steps	Detailed Instructions	Comments
3 (optional) Set up the parameters for the Sample Purity options of the Find Compounds by Formula algorithm.	**a** Click **Find by Formula - Sample Purity** in the Find Compounds by Formula section in the Method Explorer. **b** Click the **Options** tab. **c** Mark the **Compute sample purity** check box. **d** Review the other parameters in this section.	

Figure 2 Find Compounds by Formula - Sample Purity section in the Method Editor in Qualitative Analysis

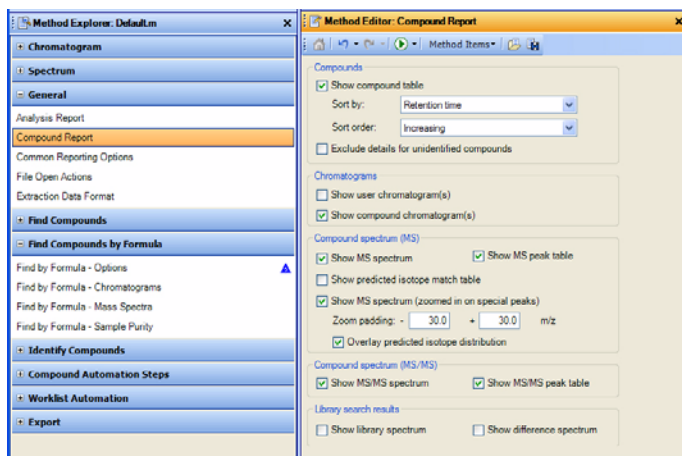| Steps	Detailed Instructions	Comments
4 Set up the parameters for generating a compound report	**a** Click **Compound Report** in the General section in the Method Explorer. **b** Mark the sections that you want to include in the report in this tab. **c** Click **Common Reporting Options** in the General section in the Method Explorer. **d** (optional) Change the template for the Compound report template. **e** Click the **Options** tab. **f** Review the parameters.	• If you want to customize a report, you can learn how by using the *Agilent MassHunter Workstation Software Reporting Familiarization Guide*.

Steps	Detailed Instructions	Comments

Figure 3 Compound Report section in the Method Editor in the Qualitative Analysis program

Steps	Detailed Instructions	Comments
5 Set up the parameters for the destination for the report.	**a** Click **Reporting Options** in the Worklist Automation section in the Method Explorer. **b** Mark whether or not to print the report. **c** (optional) Select the printer to use. **d** (optional) Mark whether or not to save the report as an Excel file and/or as a PDF file.	• The settings in this tab are used when the method is run automatically.

Steps	Detailed Instructions	Comments
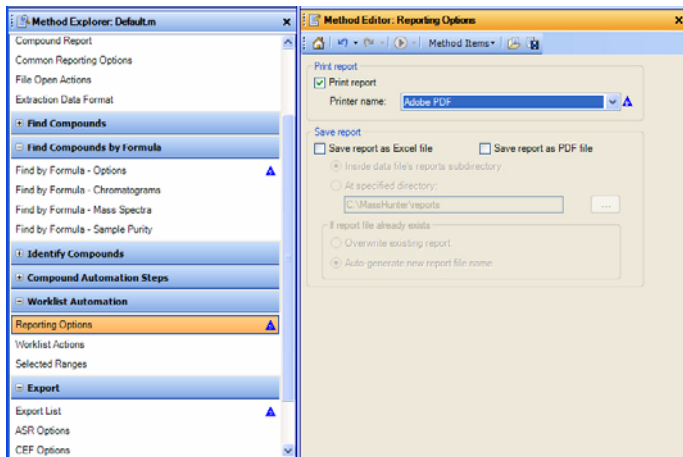
Figure 4   Reporting Options Section in Qualitative Analysis

6 Set up the parameters for the Worklist Actions.	**a** Click **Worklist Actions** in the Worklist Automation section on the Method Explorer. **b** Click the ⊠ button to clear the items in the Actions to be run list. **c** Double-click the **Find Compounds by Formula** action in the Available actions list. **d** Click the **Generate Compound Report** action in the **Available actions** list and then click the ⏷ button to copy the action to the **Actions to be run** list. **e** (optional) Click the **Export** action in the Available actions list and then click the ⏷ button to copy the action to the **Actions to be run** list.	• The actions in the Actions to be run list are executed in order. Make sure the actions are in the order shown in "Worklist Actions in Qualitative Analysis" on page 24. • If you want to use the Analytical Studio Reviewer program, you need to export an ASR file.

Steps	Detailed Instructions	Comments
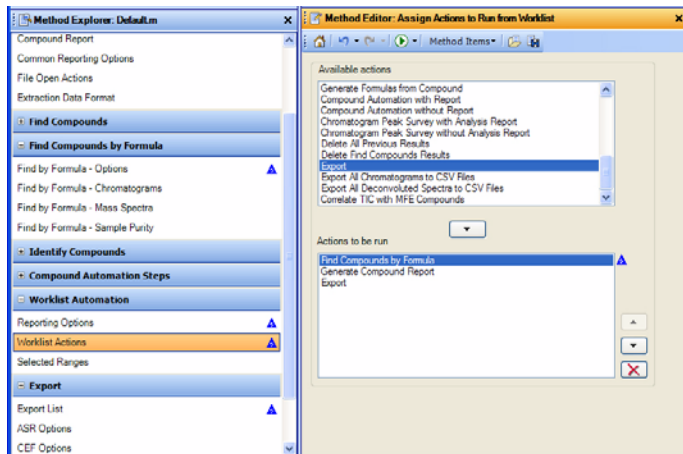
Figure 5   Worklist Actions in Qualitative Analysis

7 Save the method.	• Click **Method > Save** to save the method to the current method. • Or click **Method > Save As** to give the method a new name.	

Task 2. Set up ChemStation Method and ChemStation

This task gives you the basic steps to set up an LC/MS method with the ChemStation Data Acquisition software.

Before you start

• Read the *Agilent 6100 Series Quadrupole LC/MS Systems Quick Start Guide* that came with your system.

For more information on setting up methods in the LC/MS ChemStation software, see the *Agilent 6100 Series Single Quad LC/MS System Familiarization Guide* that came with your system.

Steps	Detailed Instructions	Comments
1 Edit the entire method.	**a** Display the Method and Run Control view. **b** Open the method **DEF_LC.M**. **c** Save the method under a new name. **d** Edit all LC parts of the method. **e** Select Data Acquisition and Data Analysis in the Run Time checklist. **f** Save the method again.	• If you need help, see Task 1 in the "Set up a full-scan acquisition method" section of the *Agilent 6100 Series Quadrupole LC/MS System Familiarization Guide*.
2 Enter MS acquisition parameters.	**a** Enter parameters for the quadrupole mass spectrometer (MS). **b** Enter parameters for the spray chamber of the ion source. **c** Save the method.	• You can use the **Method > Edit Entire Method** command to review and edit every section of the method, including the Data Analysis portion.
3 Configure ChemStation to translate the ChemStation data file to the MassHunter data file format and to run a MassHunter Qualitative Analysis method.	**a** Click **MassHunter > Configuration**. **b** Mark the **Translate to MassHunter Data** check box. **c** Click the **Save location as input data file** button. **d** Mark the **Run MassHunter Qualitative Analysis Method** check box. **e** Click **OK**.	• These parameters are not part of a method. You only need to do this step once, and then these parameters are set until you change them.

Steps	Detailed Instructions	Comments
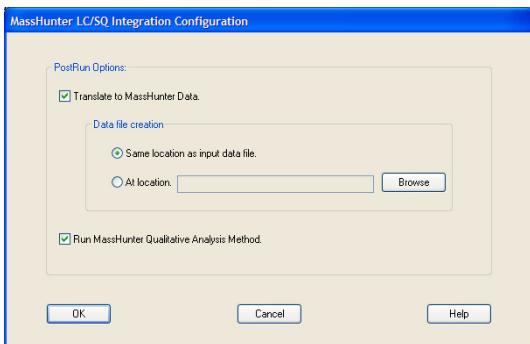
Figure 6   **MassHunter LC/SQ Integration Configuration** dialog box in LC/MSD ChemStation

Steps	Detailed Instructions	Comments
4 Link the current ChemStation method to the MassHunter method.	**a** Click **MassHunter > Edit Link DA Method.** **b** Select the method to link to. **c** Click **OK**.	• You need to do this step for any method that you are going to run. Each ChemStation method contains a link to a MassHunter Qualitative Analysis method. Multiple ChemStation methods can link to the same Qualitative Analysis method.

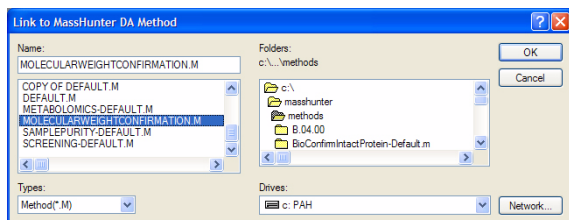**Figure 7**   Link to MassHunter DA Method in ChemStation

Steps	Detailed Instructions	Comments
5 Save the ChemStation method.	**a** Click **Method > Save Method As**. **b** Give the method a name and click **OK**.	

Task 3. Run a sequence in ChemStation

After you set up the ChemStation method to automatically link to the MassHunter Qualitative Analysis method, you run a sequence to do molecular weight confirmation.

Steps	Detailed Instructions	Comments
1 Review parameters in the **Sequence Parameters** dialog box.	**a** Click the **Sequence > Sequence Parameters** command. **b** Review the parameters and make any necessary changes. **c** Click OK.	

| Steps	Detailed Instructions	Comments
2 Add a sample to the Sequence Table. Add the target mass to the table in the Targeted Mass column.	**a** Click the **Sequence > Sequence Table** command. **b** Enter the parameters for the sample. **c** Enter the target masses in the Target Masses column. **d** Click **Run Sequence**.	• You enter the ChemStation method in this table. You also enter the **Target Masses** in this table.
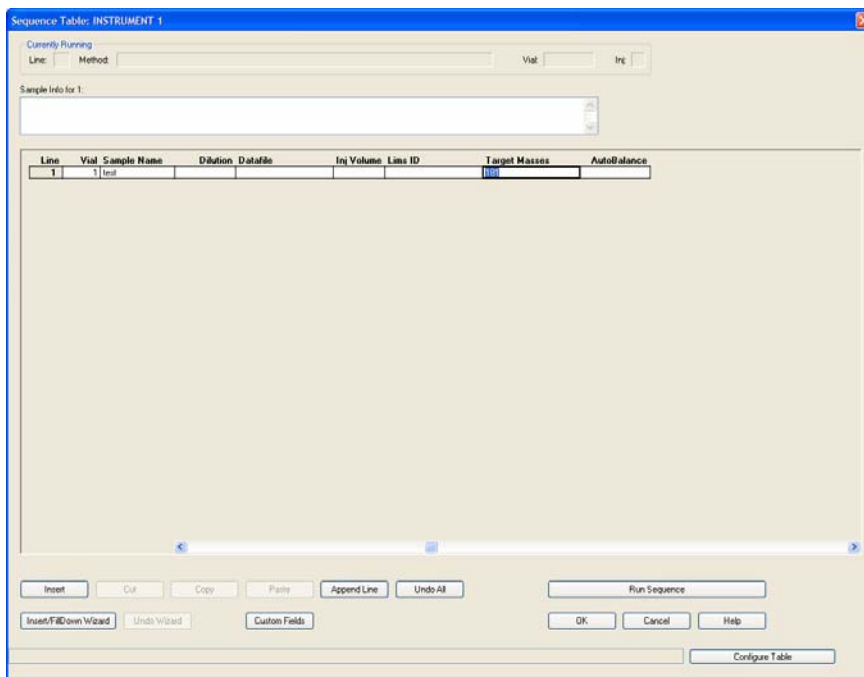
Figure 8   **Sequence Table** dialog box in ChemStation

Exercise 2. Protein Confirmation

The MassHunter Qualitative Analysis program can do Protein Confirmation when you use the additional product Agilent MassHunter BioConfirm software.

Task 1. Set up the Qualitative Analysis method to do Protein Confirmation

The *Agilent MassHunter BioPharma Workflow Guide* describes the process for setting up a method to automate Sequence matching.

Task 2. Set up ChemStation method to run the MassHunter Protein Confirmation method

Follow the steps in "Task 2. Set up ChemStation Method and ChemStation" on page 25 to set up the ChemStation method to link to the method created in the previous task.

Task 3. Run a sequence in ChemStation to do Protein Confirmation

Follow the steps in "Task 3. Run a sequence in ChemStation" on page 27 to run the ChemStation method developed in the previous task. When this ChemStation method is run, the MassHunter Qualitative Analysis method that is linked to the ChemStation method is also run.

Exercise 3. High Throughput Screening

The MassHunter Quantitative Analysis program can screen for compounds.

The following three tasks will lead you through this workflow.

Task 1. Set up ChemStation method to translate the ChemStation data files to the MassHunter Data File Format

This task gives you the basic steps to set up an LC/MS method with the ChemStation Data Acquisition software.

Steps	Detailed Instructions	Comments
1 Edit the entire method.	**a** Display the Method and Run Control view. **b** Open the method **DEF_LC.M**. **c** Save the method under a new name. **d** Edit all LC parts of the method. **e** Select Data Acquisition and Data Analysis in the Run Time checklist. **f** Save the method again.	• If you need help, see Task 1 in the "Set up a full-scan acquisition method" section of the *Agilent 6100 Series Quadrupole LC/MS System Familiarization Guide*.
2 Enter MS acquisition parameters.	**a** Enter parameters for the quadrupole mass spectrometer (MS). **b** Enter parameters for the spray chamber of the ion source. **c** Save the method.	• You can use the **Method > Edit Entire Method** command to review and edit every section of the method, including the Data Analysis portion which is described in the next task.

| Steps	Detailed Instructions	Comments
3 Configure ChemStation to translate the ChemStation data file to the MassHunter data file format but do not run a MassHunter Qualitative Analysis method.	**a** Click **MassHunter > Configuration**. **b** Mark the **Translate to MassHunter Data** check box. **c** Click the **Save location as input data file** button. **d** Clear the **Run MassHunter Qualitative Analysis Method** check box. **e** Click **OK**.	• You clear the **Run MassHunter Qualitative Analysis Method** check box because this workflow uses the MassHunter Quantitative Analysis program, so you do not want to run the MassHunter Qualitative Analysis program.
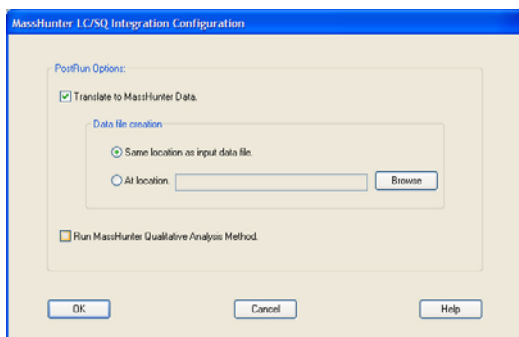
Figure 9   **MassHunter LC/SQ Integration Configuration** dialog box in LC/MSD ChemStation

4 Save the method.	**a** Click **Method > Save Method As**. **b** Give the method a name and click **OK**.	

**Task 2. Run a sequence in ChemStation to get the data files to do
High-Throughput Screening**

Follow the steps in "Task 3. Run a sequence in ChemStation" on page 27 to run
the ChemStation method developed in the previous task. This method does
translate the ChemStation data file into the MassHunter data format, but it
does not run a MassHunter Qualitative Analysis method.

Task 3. Run a batch in the MassHunter Quantitative Analysis Program

Follow the directions in the *Agilent MassHunter Workstation Software
Quantitative Analysis Familiarization Guide*, except use the data files you
generated in "Task 2. Run a sequence in ChemStation to get the data files to do
High-Throughput Screening" on page 32.

Exercise 4. Quantification (Target Compound Analysis)

Task 1. Set up ChemStation method to translate the ChemStation data files to the MassHunter Data File Format for Target Compound Analysis

Follow the steps in "Task 1. Set up ChemStation method to translate the ChemStation data files to the MassHunter Data File Format" on page 30 to run the ChemStation method developed in the previous task. This method does translate the ChemStation data file into the MassHunter data format, but it does not run a MassHunter Qualitative Analysis method.

Task 2. Modify a method in ChemStation to set up Compound Names and ISTDs

In the **Set Up MSD Signals** dialog box, you enter the Compound Names and the ISTDs. To use this feature, you need to install the patch on B.04.03 or install C.01.xx or greater. This patch is available on the Agilent MassHunter LC/SQ ChemStation Integration Software media.
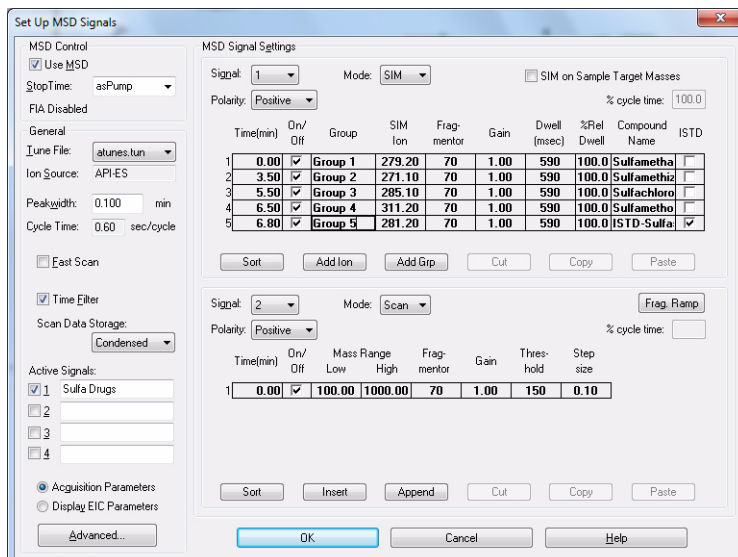

Figure 10 **Set Up MSD Signals** dialog box

Task 3. Run a sequence in ChemStation to get the data files to do Target Compound Analysis

Follow the steps in "Task 3. Run a sequence in ChemStation" on page 27 to run the ChemStation method developed in the previous task. This method does translate the ChemStation data file into the MassHunter data format, but it does not run a MassHunter Qualitative Analysis method.

Task 4. Run a batch in the MassHunter Quantitative Analysis Program

Follow the directions in the Agilent MassHunter Workstation Software *Quantitative Analysis Familiarization Guide*, except use the data files you generated in "Task 2. Run a sequence in ChemStation to get the data files to do High-Throughput Screening" on page 32.

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In this book

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

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