Agilent MassHunter StreamSelect Software

Quick Start Guide

MassHunter StreamSelect Console  3
  Instrument Status Window  4
Status Monitor Window  4
Chromatogram Plot Windows  5
Batch Queue Window  6
Batch Sample Submission and Data Acquisition Method Setup  8
  To submit batches  9
  To start, stop, and resume batches  10
  To set up methods for Data Acquisition  11
  To verify an acquisition method using a worklist  13
  To do a checktune on the instrument  14

Other User Interface Elements for MassHunter StreamSelect Software  15

MassHunter StreamSelect Profile Editor  16
MassHunter StreamSelect Instrument Configuration  17
What is Agilent MassHunter StreamSelect Software?

Agilent MassHunter StreamSelect Software provides the coordination and valve switching that is necessary for the robust and efficient handling of LC/MS analyses utilizing a Triple Quadrupole Mass Spectrometer and two Liquid Chromatography systems. MassHunter StreamSelect LC Analysis offers higher productivity by maximizing the efficiency of LC/MS analysis with staggered, parallel, multi-LC channel flows into a single mass spectrometer.

Where to Find More Information

You can access more information about the MassHunter StreamSelect Software program as follows.

*Agilent MassHunter StreamSelect Setup Guide (G2709-90000)*

MassHunter StreamSelect Online Help

Consult the online Help and tooltips available in the following components of the MassHunter StreamSelect Software System.

- MassHunter StreamSelect Console
- MassHunter StreamSelect Profile Editor
- MassHunter StreamSelect Instrument Configuration

Triple Quadrupole Data Acquisition Online Help

Consult the MassHunter Triple Quadrupole Data Acquisition online Help when setting up acquisition methods.

Agilent Web Site

To view support information for MassHunter StreamSelect and other Agilent products, see:

http://www.chem.agilent.com
MassHunter StreamSelect Console

This program lets you submit, run, and monitor batches of samples for analysis.

To open the MassHunter StreamSelect Console, click **StreamSelect Console** on the Windows Start menu or desktop.

**Tip** The windows on the MassHunter StreamSelect Console can be resized, moved, or hidden to display only the information of interest. The layout can be saved; different layouts can be selected using the **Layout** controls on the toolbar.
Function of the Instrument Status Window

This window in the MassHunter StreamSelect Console shows the status of the instrument components of both streams, such as autosampler, pump, column compartment, mass spectrometer, and valve. The progress of the current sample run is also shown for each stream. The Valve device pane is shown only for Stream 1, since it is physically connected to Stream 1 via a CAN cable.

The Status Monitor Window

This window shows the following information:

- Actual values of key instrument parameters on the LC Status tab
- Current counter values on the System Counters tab

Counters can be reset by right-clicking and selecting Reset from the shortcut menu.
**Chromatogram Plot Windows**

These windows in the MassHunter StreamSelect Console can be configured to plot data being acquired. By default, the windows show plots for the MS QQQ TIC chromatogram and Pump pressures for Streams 1 & 2, as shown in the examples below.
**Batch Queue Window**

This window at the bottom of the MassHunter StreamSelect Console shows the following information:

**Batch Status Pane**

The pane at the top of the Batch Queue window shows status information for the batch queue, including the System state/Profile name, the currently running sample, and any approaching event like sleep timeout or the command requested by the user.

**Batch Queue Tab**

The Batch Queue tab shows the batches that have been submitted.

**Batch Queue Tab Toolbar**

In order from left to right, the Toolbar buttons let you:

- Move the selected batch to the top of the queue.
- Move the selected batch up one position in the queue.
- Move the selected batch down one position in the queue.
- Move the selected batch to the end of the queue.
- Delete the selected batch or batches.
- Open the folder for the selected batch.
- View a list of samples in the selected batch. See “Sample List Tab” on page 7.
Completed Batches Tab

The Completed Batches tab shows the batches that have been completed.

Sample List Tab

To view information about the samples in a batch, click to highlight the batch of interest, then click the View Batch Sample List button. The Sample List tab opens and is labeled with the name of the selected batch. The Sample List tab has the following two panes of information:

- The Sample List pane shows the list of samples in the batch.
- The Completed Samples List pane shows the samples that have been run and tells which stream they ran on, the methods used, and the data file names.

You can select a different batch to display in the Sample List tab.

You can close the Sample List tab by clicking the X in the tab.
Batch Sample Submission and Data Acquisition Method Setup

Before you start

This section describes how to submit batches of samples in Agilent MassHunter StreamSelect Software, set up data acquisition methods for your analyses, and do a checktune on the instrument.

Before you start

- If methods have not yet been set up for your analysis, see “To set up methods for Data Acquisition” on page 11.
- Create or open a profile for your analysis in MassHunter StreamSelect Profile Editor. MassHunter StreamSelect profiles can be developed for each type of analysis done in your lab to simplify daily operation. MassHunter StreamSelect profiles are based on representative data collected with Agilent MassHunter Data Acquisition Software. See “MassHunter StreamSelect Profile Editor” on page 16 for a description of the MassHunter StreamSelect Profile Editor and refer to MassHunter StreamSelect Profile Editor online Help for information on creating MassHunter StreamSelect profiles.

**NOTE**

The profile that was most recently open in MassHunter StreamSelect Profile Editor is used to acquire data for all batches in the queue in StreamSelect Console.

- Do a checktune on the instrument to verify performance as necessary. See “To do a checktune on the instrument” on page 14.
To submit batches

1. Click **Submit Batch** on the toolbar of the MassHunter StreamSelect Console.

![Submit Batch screenshot]

2. On the Import Batch screen, enter the following information:
   - **Batch Name**: Enter a name for the batch, which is used to determine where the batch folder is created based on Batch Naming settings.
   - **Submitter**: The field is optional, but may be used in batch folder naming.
   - **Calibrator Map**: Select a Calibrator map from the list. Calibrator maps are created and assigned to a profile in the MassHunter StreamSelect Profile Editor; see page 16 for more information. If you select **Do not use Calibrator Map**, then the samples in the Import File are run on alternating streams in the order they appear in the list. That is, sample line 1 runs on Stream 1, sample line 2 runs on Stream 2, sample line 3 runs on Stream 1, and so on. If one stream shuts down during the run, then the remaining samples for that stream run on the other stream.
   - **Import File**: Select the file that contains the list of samples for the batch.

3. In the **Plate Assignments Details** table, assign a position in the autosampler to the plates in the Import File and Calibrator Map. Only plates that are not currently in use by any other batches can be assigned.

4. Click **Finish**.
   The batch appears in the Batch Queue window of the StreamSelect Console.
To start, stop, and resume batches

Use this procedure to manage the Batch Queue.

1. If the queue has stopped, restart it with one of the following options:
   - Click Batch Queue > Start > Start Batch.
   - Click Batch Queue > Start > Resume Batch.
   - Click Batch Queue > Start > Start at Next Batch.

2. If you need to reorder the batches in the queue, use the arrow buttons on the Batch Queue tab.

3. If you need to stop the batch before completion:
   - Click Batch Queue > Stop > Stop Batch.
   - Click Batch Queue > Stop > Stop after Current Sample.
   - Click Batch Queue > Stop > Stop after Current Batch.

4. Monitor baseline and adjust plot in the Chromatogram Plot windows, as described in MassHunter StreamSelect Console online Help.

5. To view information about the samples in a batch, click to highlight the batch of interest, then click the View Batch Sample List button.

The sample information is shown in the Sample List tab of the Batch Queue window.
To set up methods for Data Acquisition

Use Agilent MassHunter Workstation Data Acquisition Software, which has been modified for use with MassHunter StreamSelect, to set acquisition method parameters as follows.

1. Click **Data Acquisition** on the Windows Start menu or desktop.
2. Select **Stream 1** in the toolbar as shown in the example below:

   ![Data Acquisition Toolbar Example](image)

3. On the **Valve** tab in the **Method Editor** window:
   - For **Position**, click **Use current valve position**.
   - For **Position switch at end of run**, click **Do not switch**.

   ![Valve Tab Example](image)

Note that tab names can be customized; your system may have different labels.
4 Set the **Stoptime** for devices in the **Method Editor** window:
- On the **Pump** and **QQQ** tabs, set the **Stoptime** to the same values.
- For all other devices, such as TCC, set the **Stoptime** to the default value of **As Injector/No Limit**.

5 Set cycle parameters:
   a On the **HTS/HTC** tab in the **Method Editor** window, click **Edit Cycle Parameters**.
   b On the Cycle Parameters dialog box, select a cycle from the **Available Cycles** list that ends in “*StreamSelect*”, as shown in the example below.
   c When you are done setting Cycle Parameters, click **OK**.

6 Set additional method parameters on the **Column Comp.** tab in the **Method Editor** window.

   For information on setting Acquisition method parameters, see the *online Help* for MassHunter Workstation Data Acquisition software.

7 Save the method.

8 Set up a worklist to verify the method for your analysis as explained in the next section.
Batch Sample Submission and Data Acquisition Method Setup
To verify an acquisition method using a worklist

To verify an acquisition method using a worklist

Use Agilent MassHunter Workstation Data Acquisition Software, which has been modified for use with MassHunter StreamSelect, to set up a worklist as follows. For more information on setting up worklists, see the online Help for MassHunter Workstation Data Acquisition software.

1  To test the new method you created in “To set up methods for Data Acquisition” on page 11, set up a worklist as follows. The worklist will run your sample of interest on both LC streams.
   a  Select the Worklist Execution context from the toolbar in the Data Acquisition program.
   b  Add the first sample to the worklist:
      •  Click Add Sample from the Worklist menu. A new sample row is added to the Worklist table.
      •  Select Stream Index 1 for this sample.
      •  Fill out the information for this sample, using the Method you developed in the previous steps of this procedure.
   c  Add a second sample row to the Worklist table:
      •  Click Add Sample from the Worklist menu. A new sample row is added to the Worklist table.
      •  Select Stream Index 2 for this sample.
      •  Fill out the information for this second sample, using the same Sample Position and Method as used for the first sample.
   d  Click Worklist Run Parameters from the Worklist menu to set parameters on the Worklist Run Parameters dialog box.
   e  (optional) Save the worklist.

2  Place the sample in the proper location if it is not already there.

3  Run the worklist and evaluate the results.
   a  Click Worklist > Run.
   b  When the analyses are completed, compare the results in MassHunter Qualitative Analysis to make sure the method gives the expected results for both LC streams.
   c  Modify the method parameters if necessary.
   d  Save the method if you make any changes.

4  Close Data Acquisition.
You are now ready to run samples. See “To submit batches” on page 9.
To do a checktune on the instrument

Run the Checktune procedure as needed to verify the performance of the mass spectrometer. Checktune checks the mass axis tolerance and the peak width for three different peak widths and displays the result.

1. To open the MassHunter StreamSelect Console, click **StreamSelect Console** on the Windows Start menu or desktop.
2. If the mass spectrometer is in standby, right-click on the **QQQ** device pane in the Instrument Status window and select **On** to turn it on.
3. Click the **Checktune** icon on the toolbar.
4. On the Checktune dialog box:
   a. Set the **Polarity** to use during Checktune:
      - **Positive**
      - **Negative**
      - **Both** (positive and negative polarities)
   b. Click **Checktune**.

When you start Checktune, the triple quadrupole may go to a “Not Ready” state. Checktune parameters take time to stabilize. Checktune begins automatically when the triple quadrupole is ready and can take up to 15 minutes to run.

**NOTE**
- The system automatically runs the correct checktune, depending on whether a standard tune file or a fast scan tune file is loaded.
- The Checktune for a Fast Scan autotune file only checks the MS2 operation and reports only the MS2 operation.

When Checktune is finished:
- If the Checktune passes, a message is displayed stating that it passed.
- If the Checktune does *not* pass, a message is displayed that says that Autotune is recommended.
  - A Checktune Report appears in the Print Preview dialog box.
5. If the Checktune does *not* pass, open MassHunter Workstation Data Acquisition software and Autotune the instrument.
Other User Interface Elements for MassHunter StreamSelect Software

In addition to the MassHunter StreamSelect Acquisition Console described in the previous section, MassHunter StreamSelect software consists of the following user interface elements:

- **“MassHunter StreamSelect Profile Editor”** on page 16, which lets you create MassHunter StreamSelect profiles for each type of analysis done in your lab to simplify daily MassHunter StreamSelect operation.

- **“MassHunter StreamSelect Instrument Configuration”** on page 17, which lets you configure instruments for MassHunter StreamSelect. For more information, see the *MassHunter StreamSelect Setup Guide*.

- Data acquisition methods are set up using Agilent MassHunter Workstation Data Acquisition program, see “To set up methods for Data Acquisition” on page 11 for more information.
MassHunter StreamSelect Profile Editor

MassHunter StreamSelect Profile Editor lets you create MassHunter StreamSelect profiles for each type of analysis done in your lab to simplify daily MassHunter StreamSelect operation. MassHunter StreamSelect profiles are based on representative data collected with MassHunter Data Acquisition.

To display the MassHunter StreamSelect Profile Editor window, click Profile Editor on the Windows Start menu or desktop.

Profile Editor Views

Click the appropriate icon in the left pane to display the view of interest for the parameters you want to set. For more information, see MassHunter StreamSelect Profile Editor online Help.

Acquisition View   This view lets you view and edit method information, such as selecting reference data files, setting the LC run time and MS start and stop times for the TIC, and setting pressure warning and stopping limits.

Data File Naming View   This view lets you specify options for naming the data files for MassHunter StreamSelect. You can specify a location for the root data file directory, select names for data subdirectories, and components to make up the data file names.

System View   This view lets you specify batch import settings, calibration settings, event actions, plate settings, and other parameters, such as Wait Time for Ready and free disk threshold values.

Calibrator Map Window

You click the + button in the Calibrator Map section of the System View of the MassHunter StreamSelect Profile Editor to open the Calibrator Map window. This window lets you create or edit calibrator maps. Calibrator maps are listed in the Calibrator Map section of the MassHunter StreamSelect Profile Editor System view. A subset of the calibrator maps that have been defined for the system can be selected for use in a particular MassHunter StreamSelect profile. Calibrator Maps are global, that is, changes that are made to a calibrator map affect all profiles that reference that calibrator map.
MassHunter StreamSelect Instrument Configuration

This dialog box lets you configure instruments for MassHunter StreamSelect. For more information, see the MassHunter StreamSelect Setup Guide.

To display the MassHunter StreamSelect Instrument Configuration window, click Instrument Configuration on the Windows Start menu or desktop.

Device Configuration UI

To open the Device Configuration UI dialog box, click the Device Config button on the Instrument Configuration dialog box.

This dialog box lets you configure device settings on tabs for different devices, such as Quat. Pump, Column Comp., and Valve. Press F1 in this dialog box to get help for setting the parameters.

You can rename LC devices, set options, and reorder the devices if there are multiple devices of the same type in the stack. For example, on Stream #1, you could rename “Binary Pump_1” as “Loading Pump 1” and “Binary Pump_2” as “Analytical Pump 1” to make identification of devices easier in MassHunter StreamSelect Console.
In this Book

The *Quick Start Guide* helps you get started using the Agilent MassHunter StreamSelect Software.

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