Agilent MassHunter StreamSelect Software

Quick Start Guide

What is Agilent MassHunter StreamSelect Software? 2
What's New in B.07.00 2
MassHunter StreamSelect Console 4
  Six Contexts 5
  Instrument Status Window 7
  Status Monitor Window 7
  Chromatogram Plot Window 8
  Batch Queue Window 9
  Actuals Window 11
  RTP Overlay Window 12
  Profile Editor Window 13
  System Level Settings Window 14
  Method Editor Window 15
  Sample Run Window 16
  Worklist Window 17
  Tune Window 18
Batch Sample Submission and Data Acquisition Method Setup 19
  To submit batches 20
  To start, stop, and resume batches 21
  To set up methods for Data Acquisition 22
  To verify an acquisition method using a worklist 25
  To do a checktune on the instrument 26
Reference 28
  MassHunter StreamSelect Instrument Configuration 29

For Research Use Only. Not to be used for diagnostic procedures.

Agilent Technologies

What is Agilent MassHunter StreamSelect Software?

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

What’s New in B.07.00

- You can have up to four streams in your system, so your system can run up to four times faster.
- You can select one of six contexts to use to perform different tasks.
- You can develop a unified method (for devices on all of the streams) when you use the **Method Development** context.
- You can run a sample or a worklist when you use the **Method Development** context.
- You can select one or more streams to use for a single sample run or a worklist.
- You can run an autotune or a manual tune in this program when you use the **Tune** context.
- You can select either to share all of the streams or to directly specify a stream when you run a batch (**Private Stream** or **Shared Stream** mode).
- You can specify a different profile to use with each batch. You can specify a different Data Acquisition method to use in each profile.
- You can run a different batch on each of the four streams.
- You can specify pre-batch and post-batch scripts in the profile.
- You can submit one script or a group of scripts to the Batch Queue.
- You can visualize the instrument better in the updated Instrument Status window.
- You can examine chromatograms from multiple data files in the Overlay Plot window.
- You can see the estimated batch completion time in the **Batch Acquisition** context.
- You can monitor Actuals for each stream in the Actuals window.
- You can overlap injections.

Where to Find More Information

For more information about the MassHunter StreamSelect Software, see the *Agilent MassHunter StreamSelect Setup Guide (G2709-90005)*

MassHunter StreamSelect Online Help

Refer to the online Help and tooltips available in these components of the MassHunter StreamSelect System:

- MassHunter StreamSelect Console
- MassHunter StreamSelect Instrument Configuration

MassHunter Data Acquisition Online Help

Refer to the MassHunter Data Acquisition for Triple Quadrupole LC/MS online Help for help on the Tune Window. This online Help can be opened from the Tune Window. The Data Acquisition online Help also contains additional information for the Method Editor, Sample Run, and Worklist windows.

MassHunter Data Acquisition Quick Start Guide

Refer to the *Agilent 6400 Series Triple Quadrupole LC/MS System Quick Start Guide* for more information about the MassHunter Data Acquisition program. You can open the *Quick Start Guide* from the MassHunter Data Acquisition online Help, or find the guide on the MassHunter Data Acquisition installation media.

Agilent Web Site

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

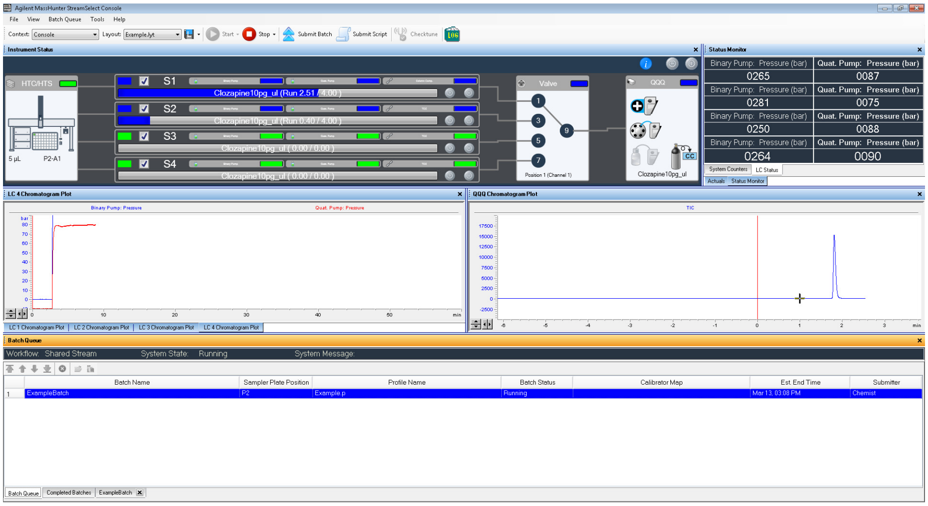
http://www.chem.agilent.com

MassHunter StreamSelect Console

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

To open the MassHunter StreamSelect Console

- Click **Start > Agilent > MassHunter Workstation > StreamSelect**.
- From the desktop folder **Agilent MassHunter Workstation**, click **StreamSelect**.



Context: Console
Layout: Example.lyt

5 µL P2-A1

Clozapine10pg_ul (Run 2.51 / 4.00)
Clozapine10pg_ul (Run 0.40 / 4.00)
Clozapine10pg_ul (0.00 / 0.00)
Clozapine10pg_ul (0.00 / 0.00)

Position 1 (Channel 1)

Clozapine10pg_ul

Binary Pump: Pressure (bar)	Quat. Pump: Pressure (bar)
0265	0087
0281	0075
0250	0088
0264	0090

Workflow: Shared Stream System State: Running System Message:

	Batch Name	Sampler Plate Position	Profile Name	Batch Status	Calibrator Map	Est. End Time	Submitter
1	ExampleBatch	P2	Example.p	Running		Mar 13, 03:08 PM	Chemist

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 or the menus. You can save a different layout for each **Context**.


Layout: Example.lyt

Six Contexts

You select one of six contexts when you use StreamSelect. Each context has a different purpose, and each context has a different set of windows that are available. The toolbar and the menus also change depending on which context is selected. You select the **Context** in the toolbar.

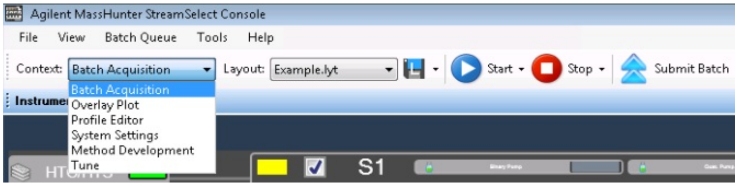


Figure 1 Six available Contexts in the toolbar

Batch Acquisition Context

The **Batch Acquisition** context is used to submit batches and scripts to the Batch Queue. You can also run a Checktune from this context. These windows are available in this context:

- "Instrument Status Window" on page 7
- "Status Monitor Window" on page 7
- "Chromatogram Plot Window" on page 8
- "Batch Queue Window" on page 9
- "Actuals Window" on page 11

Overlay Plot Context

The **Overlay Plot** context is used to examine the real-time plot. You can overlay the LC and MS plots for up to the last 25 runs. This window is available in this context:

- "RTP Overlay Window" on page 12

Profile Editor Context

The **Profile Editor** context is used to edit a Profile. A Profile is a set of parameters that set how you want to do acquisitions. It includes the name of the acquisition method to use, warning and stopping limits for the pumps, data file naming rules, scripts to run before and after a batch, and the Batch Import Map File which determines the format that must be used when submitting a batch file. The Profile Editor Window has three different views. The following window is available in this context:

- "Profile Editor Window" on page 13

System Settings Context

The **System Settings** context is used to set system parameters. You choose whether the system is executed as a **Shared Stream** or as a **Private Stream**. You also specify a script to execute when the Batch Queue starts running, plus you can specify an error script and a sleep script. The following window is available in this context:

- "System Level Settings Window" on page 14

Method Development Context

The **Method Development** context is used to develop a data acquisition method. In this context, you can edit a method, run a sample, and run a worklist. You cannot switch to this context if the Batch Queue is running. The following windows are available in this context:

- "Chromatogram Plot Window" on page 8
- "Instrument Status Window" on page 7
- "Actuals Window" on page 11
- "Method Editor Window" on page 15
- "Sample Run Window" on page 16
- "Worklist Window" on page 17

Tune Context

The **Tune** context is used to tune the instrument. You can run CheckTune and Autotune. You can also manually tune the instrument. The following windows are available in this context:

- "Tune Window" on page 18
- "Actuals Window" on page 11
- "Instrument Status Window" on page 7

Instrument Status Window

The Instrument Status window is visible in the **Batch Acquisition** context, the **Method Development** context, and the **Tune** context.

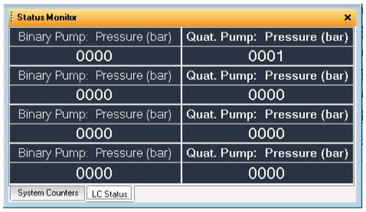
This window in the MassHunter StreamSelect Console shows the status of the instrument components of all streams, such as autosampler, pump, column compartment, mass spectrometer, and valve. The progress of the current sample run is also shown for each stream.

Status Monitor Window

The Status Monitor window is only visible in the **Batch Acquisition** context.

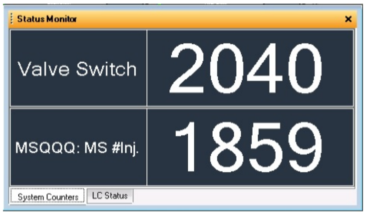
This window shows the following information:

- actual values of key instrument parameters on the **LC Status** tab
- current counter values on the **System Counters** tab



Status Monitor

Binary Pump: Pressure (bar)	Quat. Pump: Pressure (bar)
0000	0001
Binary Pump: Pressure (bar)	Quat. Pump: Pressure (bar)
0000	0000
Binary Pump: Pressure (bar)	Quat. Pump: Pressure (bar)
0000	0000
Binary Pump: Pressure (bar)	Quat. Pump: Pressure (bar)
0000	0000



Status Monitor

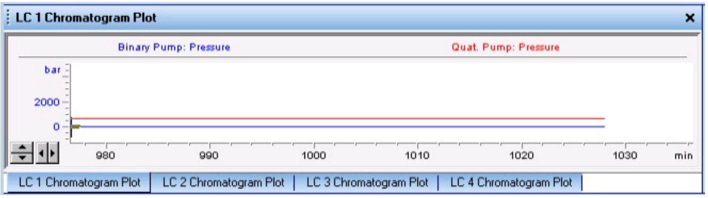
Valve Switch	2040
MSQQQ: MS #Inj.	1859

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

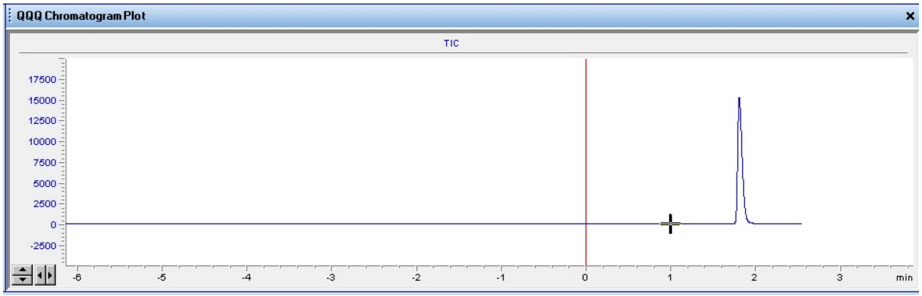
Chromatogram Plot Window

The Chromatogram Plot window is visible in the **Batch Acquisition** context and the **Method Development** context.

These windows in the MassHunter StreamSelect Console can be configured to plot data being acquired. The LC Chromatogram Plot windows are tabbed together by default. Each stream is shown in a different window. The initial plots are the Binary Pump pressure and Quat. Pump pressure. You can add or change the displayed plots in the **Edit Signal Plot** dialog box.



By default, the QQQ Chromatogram Plot contains the TIC for the mass spectrometer. You can add or change the displayed plots in the **Edit Signal Plot** dialog box which starts when you right-click the plot and click **Change**.



Batch Queue Window

The Batch Queue window is only visible in the **Batch Acquisition** context.

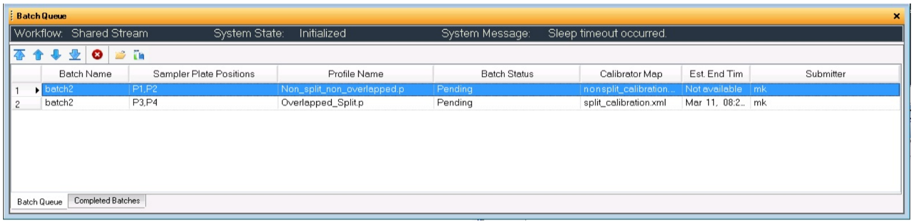
This window at the bottom of the MassHunter StreamSelect Console shows the following information:

Batch Status Pane

The pane at the top of the Batch Queue window shows status information for the Batch Queue, including the Workflow (Shared or Private stream), System state, the currently running sample, the System Message, 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. Batches are run in the order in the table. You can change the order of the batches in the Batch Queue using the buttons in the toolbar.



Workflow: Shared Stream System State: Initialized System Message: Sleep timeout occurred.

	Batch Name	Sampler Plate Positions	Profile Name	Batch Status	Calibrator Map	Est. End Tim	Submitter
1	batch2	P1,P2	Non_split_non_overlapped.p	Pending	nonsplit_calibration....	Not available	mk
2	batch2	P3,P4	Overlapped_Split.p	Pending	split_calibration.xml	Mar 11, 08:2...	mk

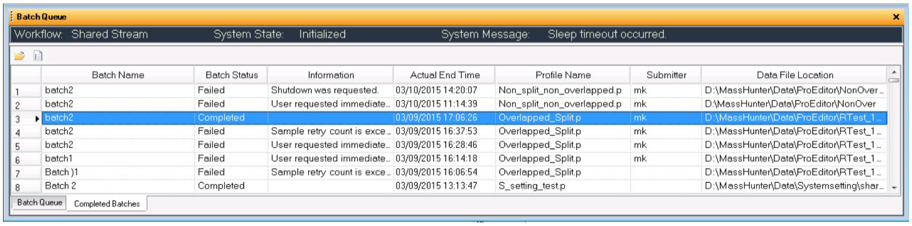
Batch Queue Tab Toolbar

Toolbar Button	Action
⤒	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 bottom of the queue

Toolbar Button	Action
✖	Delete the selected batch or batches
📂	Open the data folder for the selected batch
📋	View a list of samples in the selected batch. See "Completed Batches Tab Toolbar" on page 10.

Completed Batches Tab

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



Workflow: Shared Stream System State: Initialized System Message: Sleep timeout occurred.

	Batch Name	Batch Status	Information	Actual End Time	Profile Name	Submitter	Data File Location
1	batch2	Failed	Shutdown was requested.	03/10/2015 14:20:07	Non_split_non_overlapped.p	mk	D:\MassHunter\Data\ProEditor\NonOver…
2	batch2	Failed	User requested immediate…	03/10/2015 11:14:39	Non_split_non_overlapped.p	mk	D:\MassHunter\Data\ProEditor\NonOver
3	batch2	Completed		03/09/2015 17:06:26	Overlapped_Split.p	mk	D:\MassHunter\Data\ProEditor\RTest_1…
4	batch2	Failed	Sample retry count is exce…	03/09/2015 16:37:53	Overlapped_Split.p	mk	D:\MassHunter\Data\ProEditor\RTest_1…
5	batch2	Failed	User requested immediate…	03/09/2015 16:28:46	Overlapped_Split.p	mk	D:\MassHunter\Data\ProEditor\RTest_1…
6	batch1	Failed	User requested immediate…	03/09/2015 16:14:18	Overlapped_Split.p	mk	D:\MassHunter\Data\ProEditor\RTest_1…
7	Batch)1	Failed	Sample retry count is exce…	03/09/2015 16:06:54	Overlapped_Split.p		D:\MassHunter\Data\ProEditor\RTest_1…
8	Batch 2	Completed		03/09/2015 13:13:47	S_setting_test.p		D:\MassHunter\Data\Systemsetting\shar…

Completed Batches Tab Toolbar

Toolbar Button	Action
📂	Open the folder for the selected batch in File Explorer.
📄	Opens the **Batch Log** dialog box which shows information on events for the selected, completed batch.

Sample List Tab

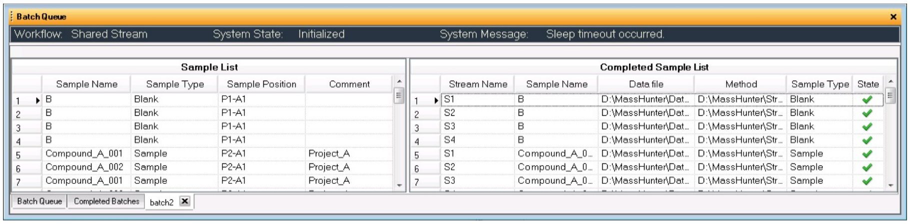
To view information about the samples in a batch, highlight the batch of interest in the Batch Queue tab, and then click the **View Sample List** (📋) button. The Sample List tab opens and is labeled with the name of the selected batch. The Sample List tab has the following two panes of information:

- 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 only view 4 batches at a time in Sample List tabs. If you try to open a fifth batch, the first batch you opened is automatically closed.

You can close the Sample List tab by clicking the X in the tab.



Workflow: Shared Stream System State: Initialized System Message: Sleep timeout occurred.

Sample List

	Sample Name	Sample Type	Sample Position	Comment
1	B	Blank	P1-A1	
2	B	Blank	P1-A1	
3	B	Blank	P1-A1	
4	B	Blank	P1-A1	
5	Compound_A_001	Sample	P2-A1	Project_A
6	Compound_A_002	Sample	P2-A1	Project_A
7	Compound_A_001	Sample	P2-A1	Project_A

Completed Sample List

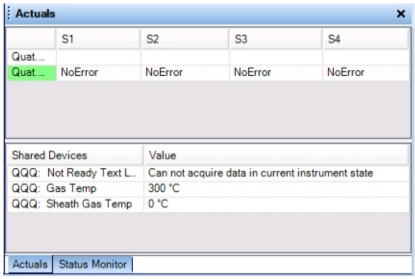
	Stream Name	Sample Name	Data file	Method	Sample Type	State
1	S1	B	D:\MassHunter\Dat...	D:\MassHunter\Str...	Blank	✓
2	S2	B	D:\MassHunter\Dat...	D:\MassHunter\Str...	Blank	✓
3	S3	B	D:\MassHunter\Dat...	D:\MassHunter\Str...	Blank	✓
4	S4	B	D:\MassHunter\Dat...	D:\MassHunter\Str...	Blank	✓
5	S1	Compound_A_0...	D:\MassHunter\Dat...	D:\MassHunter\Str...	Sample	✓
6	S2	Compound_A_0...	D:\MassHunter\Dat...	D:\MassHunter\Str...	Sample	✓
7	S3	Compound_A_0...	D:\MassHunter\Dat...	D:\MassHunter\Str...	Sample	✓

Actuals Window

The Actuals window is visible in the **Batch Acquisition** context, the **Method Development** context, and the **Tune** context.

The Actuals window contains two tables showing the current values of selected instrument parameters. The upper pane shows the values for different instrument parameters for different streams. The lower pane shows the values for instrument parameters that are the same for all streams.

You can customize the parameters that are displayed. You right-click in the window and click Actual Settings. The **Actuals Selection** dialog box is opened.



	S1	S2	S3	S4
Quat....				
Quat....	NoError	NoError	NoError	NoError

Shared Devices	Value
QQQ: Not Ready Text L...	Can not acquire data in current instrument state
QQQ: Gas Temp	300 °C
QQQ: Sheath Gas Temp	0 °C

RTP Overlay Window

The RTP Overlay window is only visible in the **Overlay Plot** context.

You can see real-time plots in this window along with the previous data files. You can either see all streams combined into one plot (**Combined View** tab) or streams separated into different tabs (**Stream View** tab). The plots that you can see include an MS trace (a total ion chromatogram or TIC) and LC traces (Binary Pump trace and Quat. Pump trace). In this window you have options to change which traces are displayed, which streams are displayed, and which data files are displayed.

On the right side of this window, you can place two additional panes. By default these panes are hidden at the edge of the window. When you click the label for the pane, the pane is visible. When you move the cursor away from this pane, the pane is hidden again. You can make these panes be visible continuously when you click on the pin in the title of the pane.

These panes allow you to customize which data files are displayed. You mark the data files in the **Data file** pane. You select how many data files to show in the **Settings** pane. You can also remove the data files from the list when you click **Clear Data Files** on the **Settings** pane.

Trace Display
☑ ■ S1
☑ ■ S2
☑ ■ S3
☑ ■ S4
☑ Resize plot according to data file

Options
MS Trace Display
☑ TIC
Pumps Displays
☑ Binary Pump
☑ Quat. Pump

Data file
☑ S1-Clozapinestd-001.d
☑ S2-Clozapinestd-002.d
☑ S3-Clozapinestd-003.d
☑ S4-Clozapinestd-004.d

Profile Editor Window

The Profile Editor window is only visible in the **Profile Editor** context.

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

Profile Editor Views

You 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 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. You select the method to use in this view.

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 dialog box

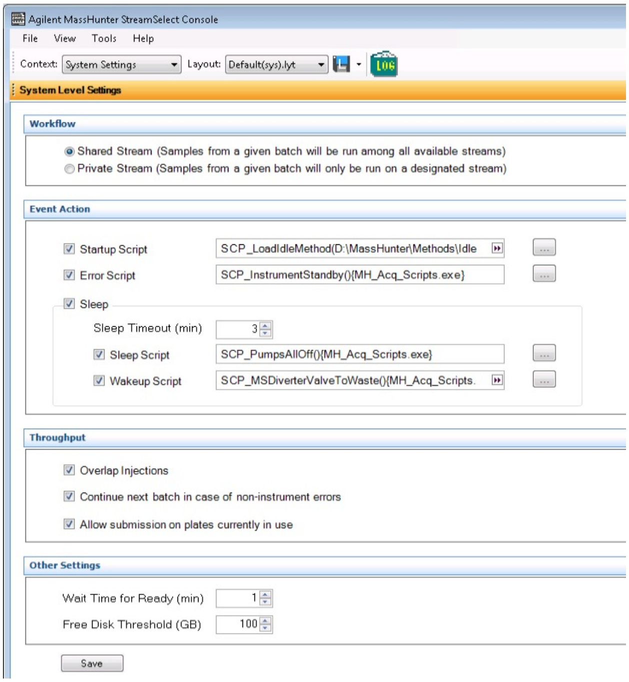
You click the + button in the **Calibrator Map** section of the System View to open the **Calibrator Map dialog** box.

This dialog box lets you create or edit calibrator maps. Calibrator maps are listed in the Calibrator Map section of the **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; changes that are made to a calibrator map affect all profiles that reference that calibrator map.

System Level Settings Window

The System Level Settings window is only visible in the **System Settings** context.

You set parameters that affect every user in this window. See the online Help for more information on this window. If you click **Shared Stream**, then samples from your batch are run on any available stream. If you click **Private Stream**, then all samples in your batch are run on the stream which you select when you submit the batch.



Context: System Settings

Layout: Default(sys).lyt

Workflow

● Shared Stream (Samples from a given batch will be run among all available streams)

○ Private Stream (Samples from a given batch will only be run on a designated stream)

Event Action

☑ Startup Script SCP_LoadIdleMethod(D:\MassHunter\Methods\Idle

☑ Error Script SCP_InstrumentStandby(){MH_Acq_Scripts.exe}

☑ Sleep

Sleep Timeout (min) 3

☑ Sleep Script SCP_PumpsAllOff(){MH_Acq_Scripts.exe}

☑ Wakeup Script SCP_MSDiverterValveToWaste(){MH_Acq_Scripts.

Throughput

☑ Overlap Injections

☑ Continue next batch in case of non-instrument errors

☑ Allow submission on plates currently in use

Other Settings

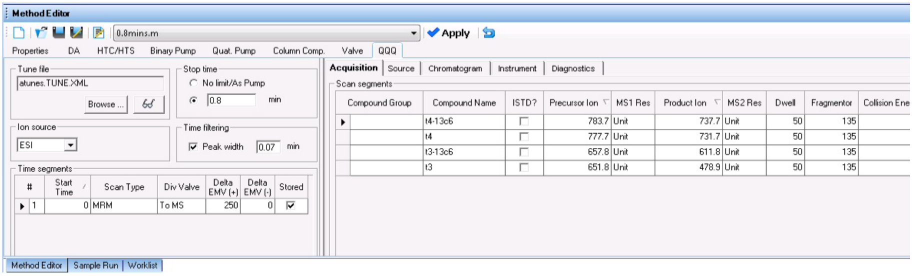
Wait Time for Ready (min) 1

Free Disk Threshold (GB) 100

Method Editor Window

The Method Editor window is only visible in the **Method Development** context.

This window allows you to create a method that consists of setpoints for the instrument. The tabs that appear in the window are only for devices that are currently configured on the system. The Method Editor window is dynamic. It allows you to both view and modify the current setpoints of the instrument. In addition, it has the **Apply** and **Reset** buttons. If a worklist is running, the setpoints change depending on which method is currently loaded on the instrument. You can get help on any tab in the Method Editor by pressing **F1**.



0.8mins.m

Tune file: atunes.TUNE.XML

Stop time: ○ No limit/As Pump ● 0.8 min

Ion source: ESI

Time filtering: ☑ Peak width 0.07 min

Time segments

#	Start Time	Scan Type	Div Valve	Delta EMV (+)	Delta EMV (-)	Stored
1	0	MRM	To MS	250	0	☑

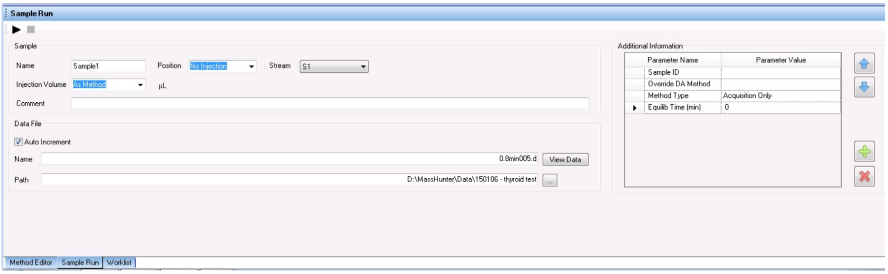
Scan segments

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Dwell	Fragmentor	Collision Ene
	t4-13c6	☐	783.7	Unit	737.7	Unit	50	135	
	t4	☐	777.7	Unit	731.7	Unit	50	135	
	t3-13c6	☐	657.8	Unit	611.8	Unit	50	135	
	t3	☐	651.8	Unit	478.9	Unit	50	135	

Sample Run Window

The Sample Run window is only visible in the **Method Development** context.

You can submit a single sample when you use this window. You specify the data file name and path, the position of the sample, the stream, the injection volume, and the name. You can also modify some of the **Additional Information**.



Sample

Name: Sample1
Position: No Injection
Stream: S1
Injection Volume: As Method µL
Comment:

Data File

☑ Auto Increment
Name: 0.8min005.d
Path: D:\MassHunter\Data\150106 - thyroid test

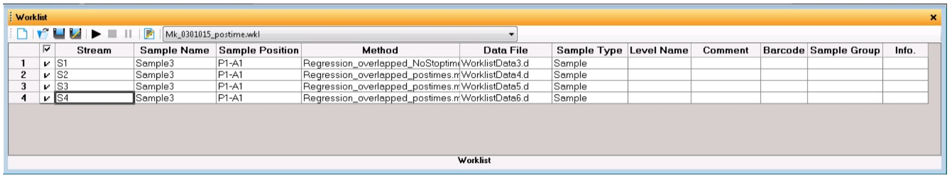
Additional Information

Parameter Name	Parameter Value
Sample ID	
Override DA Method	
Method Type	Acquisition Only
Equilib Time (min)	0

Worklist Window

The Worklist window is only visible in the **Method Development** context.

The Worklist window allows you to create a list of samples to run. When you are developing a new method, you can create a worklist to run the method multiple times with different samples. You can use the menus to modify the worklist. You can also use the shortcut menus in the Worklist window. The shortcut menu changes depending on where you clicked on the table: a cell, a row, a column, or the upper left empty box.

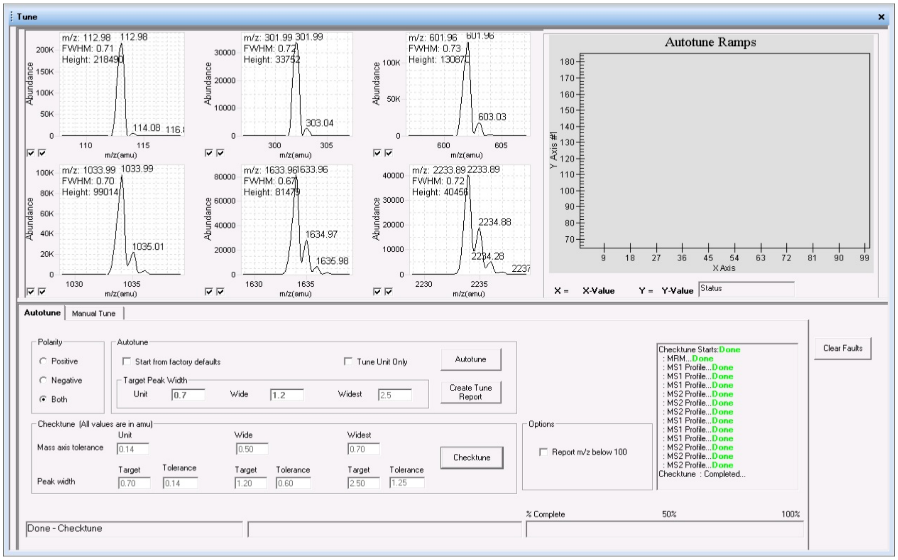


	☑	Stream	Sample Name	Sample Position	Method	Data File	Sample Type	Level Name	Comment	Barcode	Sample Group	Info.
1	✓	S1	Sample3	P1-A1	Regression_overlapped_NoStoptime	WorklistData3.d	Sample					
2	✓	S2	Sample3	P1-A1	Regression_overlapped_postimes.m	WorklistData4.d	Sample					
3	✓	S3	Sample3	P1-A1	Regression_overlapped_postimes.m	WorklistData5.d	Sample					
4	✓	S4	Sample3	P1-A1	Regression_overlapped_postimes.m	WorklistData6.d	Sample					

Tune Window

The Tune window is only visible in the **Tune** context.

You can run an Initial Autotune, an Autotune, or a Checktune from the Tune window. You can also manually tune the instrument from this window.



m/z: 112.98 FWHM: 0.71 Height: 218490
m/z: 301.99 FWHM: 0.72 Height: 33752
m/z: 601.96 FWHM: 0.73 Height: 130870
m/z: 1033.99 FWHM: 0.70 Height: 99014
m/z: 1633.96 FWHM: 0.67 Height: 81479
m/z: 2233.89 FWHM: 0.72 Height: 40456

Status

Polarity
○ Positive
○ Negative
● Both

Autotune
☐ Start from factory defaults
☐ Tune Unit Only

Target Peak Width
Unit 0.7
Wide 1.2
Widest 2.5

Checktune (All values are in amu)

	Unit		Wide		Widest	
Mass axis tolerance	0.14		0.50		0.70	
	Target	Tolerance	Target	Tolerance	Target	Tolerance
Peak width	0.70	0.14	1.20	0.60	2.50	1.25

Options
☐ Report m/z below 100

Checktune Starts:Done
: MRM...Done
: MS1 Profile...Done
: MS1 Profile...Done
: MS1 Profile...Done
: MS2 Profile...Done
: MS2 Profile...Done
: MS2 Profile...Done
: MS1 Profile...Done
: MS1 Profile...Done
: MS1 Profile...Done
: MS2 Profile...Done
: MS2 Profile...Done
: MS2 Profile...Done
Checktune : Completed...

Done - Checktune

Batch Sample Submission and Data Acquisition Method Setup

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 22.
- Create or modify a profile for your analysis in the **Profile** context. 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. See “Profile Editor Window” on page 13 for a description of the Profile Editor window.

NOTE You specify the profile when you submit a batch.

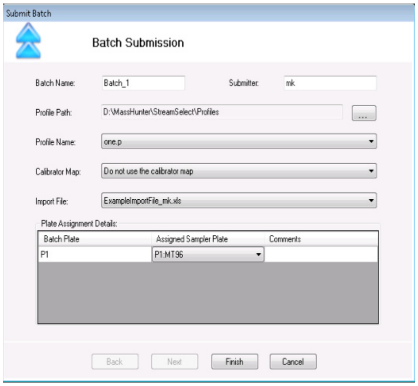
- Do a checktune on the instrument to verify performance as necessary. See “To do a checktune on the instrument” on page 26.

To submit batches

1 Open the MassHunter StreamSelect Console. See “To open the MassHunter StreamSelect Console” on page 4.

2 If necessary, select **Batch Acquisition** as the **Context** in the toolbar.

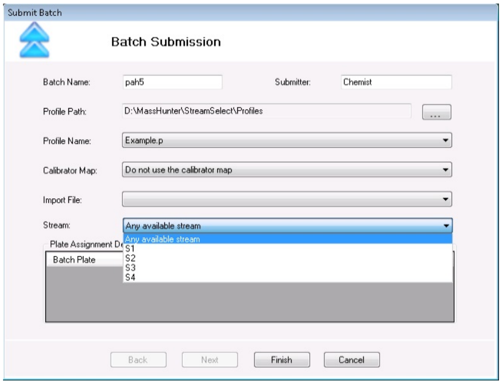
3 Click **Submit Batch** on the toolbar of the MassHunter StreamSelect Console. If you select **Shared Stream** in the System Settings context, then the **Stream** parameter is not included in this dialog box.



Batch Name: Batch_1
Submitter: mk
Profile Path: D:\MassHunter\StreamSelect\Profiles
Profile Name: one.p
Calibrator Map: Do not use the calibrator map
Import File: ExampleImportFile_mk.xls

Plate Assignment Details:

Batch Plate	Assigned Sampler Plate	Comments
P1	P1:MT96	



Batch Name: pah5
Submitter: Chemist
Profile Path: D:\MassHunter\StreamSelect\Profiles
Profile Name: Example.p
Calibrator Map: Do not use the calibrator map
Import File:
Stream: Any available stream

Any available stream
S1
S2
S3
S4

4 On the Submit Batch dialog box, 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.
- **Profile Path** and **Profile Name**: Select a profile for the type of analysis that you are doing.
- **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 13 for more information. If you select **Do not use Calibrator Map**, then the samples in the Import File are either run on the stream which you selected (if you clicked **Private Stream** in the System Level Settings window) or run on alternating streams in the order they appear in the list (if you click **Shared Stream** in the System Level Settings window). For example on a **Shared Stream** system, sample line 1 runs on Stream 1, sample line 2 runs on Stream 2, and so on. If one stream shuts down during the run, then the remaining samples for that stream run or will run on a different stream.

- **Import File**: Select the file that contains the list of samples for the batch.
- **Stream**: If you select **Private Stream**, then you also need to select which Stream to use.

5 In the **Plate Assignments Details** table, assign a position in the autosampler to the plates in the **Import File** and **Calibrator Map**. By default, only plates that are not currently in use by any other batches can be assigned. See "System Level Settings Window" on page 14 to learn how to be allowed to use plates that are currently in use by other batches.

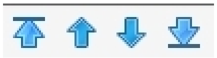
6 Click **Finish**.
The batch appears in the Batch Queue window.

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**.

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.

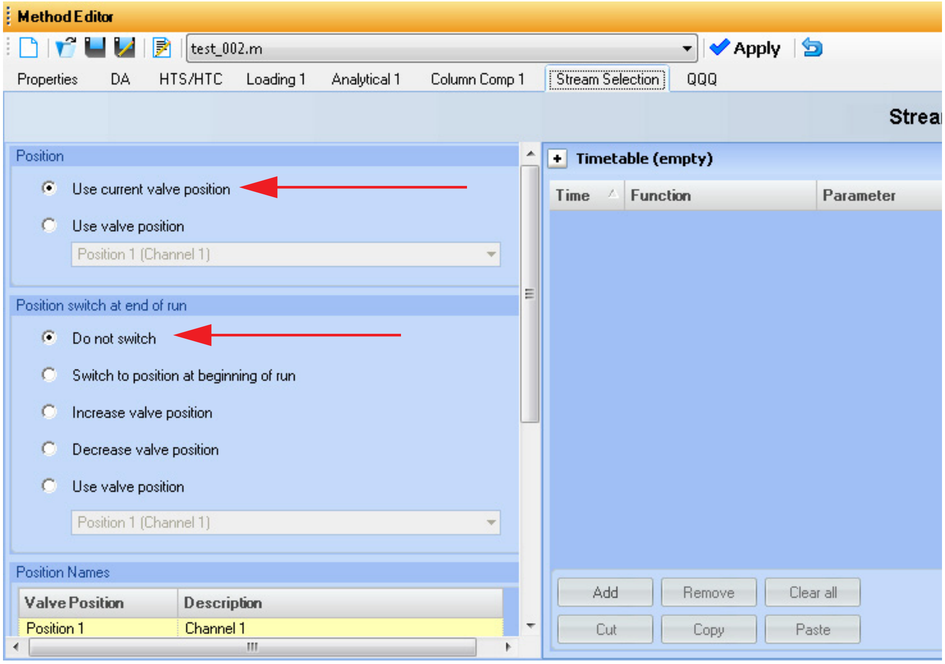
5 To view information about the samples in a batch, highlight the batch of interest, and then click the **View Sample List** button.

The sample information is shown in the Sample List tab of the Batch Queue window.

To set up methods for Data Acquisition

You use the **Method Development** context to set acquisition method parameters. If the Batch Queue is running, you cannot select the **Method Development** context.

1. Select **Method Development** for the **Context**.
2. Click the **Method Editor** window.
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**.



Position
● Use current valve position
○ Use valve position
Position 1 (Channel 1)

Position switch at end of run
● Do not switch
○ Switch to position at beginning of run
○ Increase valve position
○ Decrease valve position
○ Use valve position
Position 1 (Channel 1)

Position Names

Valve Position	Description
Position 1	Channel 1

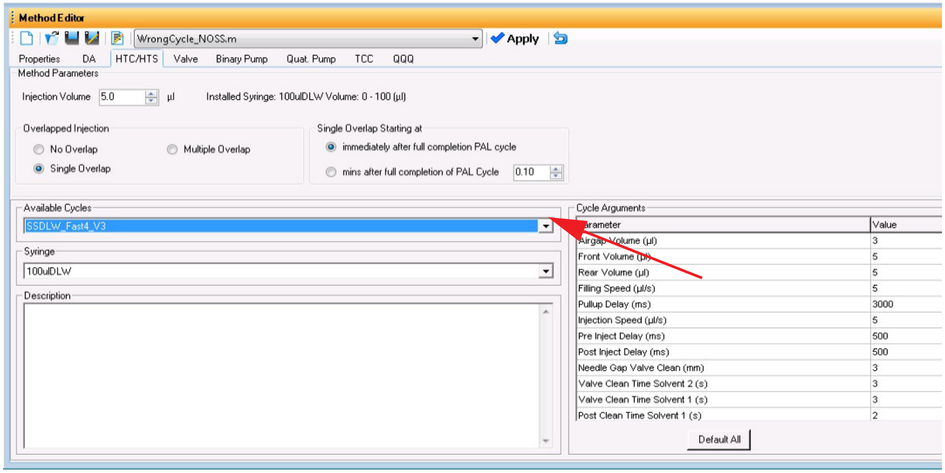
Note that tab names can be customized; your system may have different labels.

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, select a cycle from the **Available Cycles** list.

   b Review the other parameters on this tab.



WrongCycle_NOSS.m

Method Parameters

Injection Volume 5.0 µl   Installed Syringe: 100ulDLW Volume: 0 - 100 (µl)

Overlapped Injection
○ No Overlap   ○ Multiple Overlap
● Single Overlap

Single Overlap Starting at
● immediately after full completion PAL cycle
○ mins after full completion of PAL Cycle 0.10

Available Cycles: SSDLW_Fast4_V3

Syringe: 100ulDLW

Description

Cycle Arguments

Parameter	Value
Airgap Volume (µl)	3
Front Volume (µl)	5
Rear Volume (µl)	5
Filling Speed (µl/s)	5
Pullup Delay (ms)	3000
Injection Speed (µl/s)	5
Pre Inject Delay (ms)	500
Post Inject Delay (ms)	500
Needle Gap Valve Clean (mm)	3
Valve Clean Time Solvent 2 (s)	3
Valve Clean Time Solvent 1 (s)	3
Post Clean Time Solvent 1 (s)	2

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 Set other LC parameters.

8 Set the parameters on the **QQQ** tab.

9 Set the parameters on the **DA** tab.

10 Set the parameters on the **Properties** tab.

11 Save the method.

12 Set up a worklist to verify the method for your analysis as explained in the next section.

To verify an acquisition method using a single sample

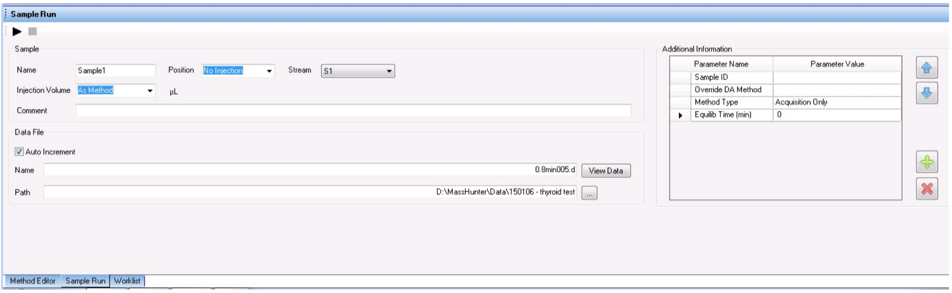
You use the **Method Development** context to run a single sample as follows.

This task helps you test the new method you created in “To set up methods for Data Acquisition” on page 22.

For more information on running samples, see the *online Help* for MassHunter Workstation Data Acquisition software.

1 Select **Method Development** as the **Context** from the toolbar.

2 Click the **Sample Run** tab. If this tab is not visible, click **View > Sample Run**.



Sample

Name: Sample1 Position: No Injection Stream: S1

Injection Volume: As Method µL

Comment:

Data File

☑ Auto Increment

Name: 0.8min005.d

Path: D:\MassHunter\Data\150106 - thyroid test

Additional Information

	Parameter Name	Parameter Value
	Sample ID	
	Override DA Method	
	Method Type	Acquisition Only
▶	Equilib Time (min)	0

3 Enter the following information:

- **Name** (Sample)
- **Position**
- **Stream**
- **Injection volume**
- **Name** (Data File)

4 If necessary, modify other parameters under **Additional Information**.

5 Click **Sample > Run** or press **F5**.

6 (optional) Examine the real-time plots in the Chromatogram Plots window or switch to the **Overlay Plot** context and view the real-time plots in that context.

To verify an acquisition method using a worklist

You use the **Method Development** context to set up a worklist as follows.

You can test the new method you created in "To set up methods for Data Acquisition" on page 22 by creating a worklist. For more information on setting up worklists, see the *online Help* for MassHunter Workstation Data Acquisition software.

1 If necessary, select **Method Development** for the **Context**.

2 Set up a worklist as follows. The worklist runs your sample of interest on two LC streams.

   a 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 a **Stream** to use for this sample in the Worklist. You select the **Stream** in the **Stream** column in the worklist table.
   - Fill out the information for this sample, using the **Method** you developed in the previous steps of this procedure.

   b Add additional sample rows to the Worklist table:

   - Click **Add Sample** from the Worklist menu. A new sample row is added to the Worklist table.
   - Select a **Stream** to use for this row in the Worklist
   - Fill out the information for this second sample, using the same **Sample Position** and **Method** as used for the first sample.

   c Click **Worklist Run Parameters** from the Worklist menu to set parameters on the Worklist Run Parameters dialog box.

   d (*optional*) Save the worklist.

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

4 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 all LC streams.

   c Modify the method parameters if necessary.

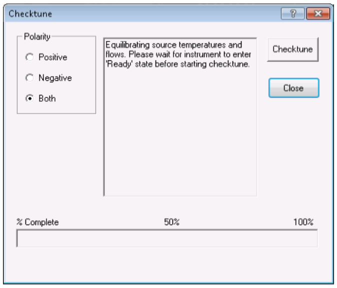
   d Save the method if you make any changes.

You are now ready to use the Batch Queue. See “To submit batches” on page 20.

To do a checktune on the instrument

Run the Checktune procedure as needed to verify the performance of the Triple Quadrupole. Checktune checks the mass axis tolerance and the peak width for three different peak widths and displays the result. You can also run a Checktune from the Tune context. See “Tune Window” on page 18.

1. Open the MassHunter StreamSelect Console. See “To open the MassHunter StreamSelect Console” on page 4.
2. If the mass spectrometer is in standby, right-click the **QQQ** device pane in the Instrument Status window and click **On** to turn it on.
3. Click the **Checktune** icon on the toolbar.



Polarity
○ Positive
○ Negative
● Both

Equilibrating source temperatures and flows. Please wait for instrument to enter 'Ready' state before starting checktune.

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, select the **Tune** context, and run an Autotune on the QQQ.

Reference

In addition to the MassHunter StreamSelect Acquisition Console, the MassHunter StreamSelect software includes:

- "MassHunter StreamSelect Instrument Configuration" on page 29, which lets you configure instruments for MassHunter StreamSelect. For more information, see the *MassHunter StreamSelect Setup Guide*.

Agilent MassHunter Workstation Data Acquisition software

Several of the windows in the Method Development context are very similar to windows in the MassHunter Data Acquisition program. The Tune window in the Tune context is very similar to the Tune window in MassHunter Data Acquisition. You can also refer to the documentation for the MassHunter Data Acquisition program for additional help.

Agilent MassHunter Workstation Qualitative Analysis software

You do the following in the MassHunter Qualitative Analysis program if you want to identify which stream was used to acquire a data file:

1. Open the MassHunter Qualitative Analysis program.
2. Open the data file.
3. Open the Sample Information window.

The stream is shown in the **Stream Name** information.

Agilent MassHunter Workstation Quantitative Analysis software

You do the following in the MassHunter Quantitative Analysis program if you want to identify which stream was used to acquire a data file:

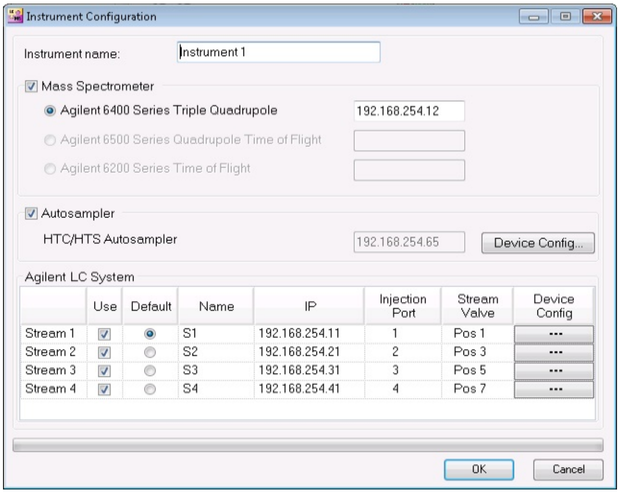
1. Open the MassHunter Quantitative Analysis program.
2. Create a batch. Select the data file to be part of the batch.
3. Add the **Sample Group** column, which is part of the **Sample** columns.
4. Click **View > Toolbars > Filtering** to display the filtering toolbar.
5. Filter which streams are displayed in the table.

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, do one of the following:

- Click **Start > Agilent > MassHunter Workstation> Acq Tools > Instrument Configuration**.
- From the desktop folder **Agilent MassHunter Workstation**, open the **Acq Tools** folder and click **Instrument Configuration**.



Instrument name: Instrument 1

☑ Mass Spectrometer

● Agilent 6400 Series Triple Quadrupole 192.168.254.12

○ Agilent 6500 Series Quadrupole Time of Flight

○ Agilent 6200 Series Time of Flight

☑ Autosampler

HTC/HTS Autosampler 192.168.254.65

Agilent LC System

	Use	Default	Name	IP	Injection Port	Stream Valve	Device Config
Stream 1	☑	●	S1	192.168.254.11	1	Pos 1	...
Stream 2	☑	○	S2	192.168.254.21	2	Pos 3	...
Stream 3	☑	○	S3	192.168.254.31	3	Pos 5	...
Stream 4	☑	○	S4	192.168.254.41	4	Pos 7	...

www.agilent.com

In this Book

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

Microsoft®, Windows®, and Excel® are either registered trademarks or trademarks of Microsoft Corporation in the United States and/or other countries.

Printed in USA
Revision A, April 2015

G2709-90006

Agilent Technologies