

# Agilent MassHunter StreamSelect Software

# **Quick Start Guide**

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### 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.

A silves Merel Jones Ocean Coles Councils					
File View Batch Queue Tools Help					
Layout Defaultlyt - 🔲 - 🍙 Start - 🧰 Stop - 🌧 Submit Batch	W Checktune				
Instrument Status - LC1		×	Status Monitor		×
			Analytical	1: Pressure (bar)	Loading 1: Pressure (bar)
	No. 1 Street 3				
0.00 / 0.00	Instrument Not Ready	🧿 💿 on 🧿 off		000	
Instrument Status - LC 2		×	Analytical	2: Pressure (bar)	Loading 2: Pressure (bar)
			0	000	0000
0.00 / 0.00	Instrument Not Ready	🪺 🗐 On 🔞 Off	System Counters	LC Status	
Chromatogram Plot - LC 1		×	Chromatogram Pl	ot - MS: QQQ	×
Loading 1: Pressure	Analytical 1: Pressure			TIC	
6an			9000000		
0			2000000		
1210 1220 1230 1240	1250	1280 min	0000000		
Chromatogram Plot - LC 2		×	5000000		
Analytical 2: Pressure	Loading 2: Pressure		4000000		
50 26			2000000 - 1000000 -		
1340 1350 1380 1380	1370	1380 min	1181	1182 118	13 1184 1185 min
Batch Queue					×
Profile: NewProfile.p System State: Initialized System Message: Sleep timeout occurred.		Stream (Stream Stream (Stream	1) 2)		
Name Submitter	Batch Status	Batch Size		PlateMapFile	Sampler Plate Positions
Long Batch 10 Edmond	Pending	1			PI
Batch Quoue Completed Batches					

**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.



**Instrument Status Window** 

# **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.

Instru	ment Status - LC 1								×
ент <u>к</u> 00	Analytical 1 9	Loading 1 9 = =	Column Comp 1 9 = =	QQQ 9 = •	😧 Valve 9 🔤				
204	P).A1 CSR1-02	81.0 20.0 0.000 mL/min 0.000 ber	Part 1 → 6	07 01 11 11	Position 3 (Channel 3)				
	0.00 / 0.00					Instrument Not Ready	1	🗐 0n 🧿	Off
instru	ment Status - LC 2								×
instru	ment Status - LC 2	Loading 2 9	🗸 Column Comp 2 🤉 🖃 🚺	© QQQ 9 = ■ ⊃ O Standby					×
	ment Status - LC 2	Looding 2 9 3 Standby 200 200 0.000 mL/min 0.00 ber	Column Comp 2 2	Stendby Of Control of					×

## **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

Status Monitor	×	Status Monitor	×
Analytical 1: Pressure (bar)	Loading 1: Pressure (bar)	Sampler #Inj.	2838
0000	0000	Valve V3 Switch	5205
Analytical 2: Pressure (bar)	Loading 2: Pressure (bar)		0200
0000	0000	MSQQQ: MS #Inj.	2804
System Counters LC Status		System Counters LC Status	

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.





### MassHunter StreamSelect Console

**Batch Queue Window** 

### **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.

Bat Pro Sy Sy	ofi st	Queue ile: 1 em State: h em Message: S	11.p nitialized Sleep timeout occi	urs in 00:54:50.	Stream (LC 1)	ldle	×
		Name	Submitter	Batch Status	Batch Size	PlateMapFile	Sampler Plate Positi
1	•	11 Batch	Rome	Pending	1		P1
2		11 Batch csv	Rome	Pending	1		P2
3		11 Batch txt	Rome	Pending	1		P3
Bat	ch (	Queue Completed Bat	iches				

### **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.

Pro Sys Sys	ofile: stem State: stem Messa	111.p Initialized age: Sleep time	eout occurs in 00:53:5	55.	Stream (LC 1) Idle			
	Name	Submitter	Batch Status	Profile	Data File Location	Batch Si	Actual End Time	-
1	11 Batch	Rome	CompletedWithE	8989_1.p	D:\MassHunter\Data\2013-07-1	1	07/17/2013 19:26:00	Ξ
2	7 Batch	Rome	Completed	113.p	D:\MassHunter\Data\2013-07-1	1	07/16/2013 16:24:26	
3	8 Batch	Rome	Completed	113.p	D:\MassHunter\Data\2013-07-1	1	07/16/2013 16:23:52	
4	10 Batch	Rome	Completed	113.p	D:\MassHunter\Data\2013-07-1	1	07/16/2013 16:23:18	
5	9 Batch	Rome	Completed	113.p	D:\MassHunter\Data\2013-07-1	1	07/16/2013 14:37:07	
		-			D 114 11 1 10 1 10010 07 1		07/15/0010 17 01 05	

### 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** 

# **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 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.

t Batch Wizard			
2	Batch Submissior	n	
Batch Name:	Batch 01	Submitter:	
Calibrator Map:	Do not use calibrator map		-
Import File:	ExampleImportFile02.xl	\$	-
Plate Assignment	Details:		
Batch Plate	Assigned	Sampler Plate	Barcode
P1	P3:CStk1	03 👻	

- **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

### 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.

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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:



- **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				-		+ Timeta	able (empty)		
۰	Use current valve	e position 🔫			ľ	Time 🗠	Function		Parameter
0	Use valve positio	n							
	Position 1 (Chan	nel 1)	•						
Position	switch at end of ru	in		Ε					
۰	Do not switch	-	-						
0	Switch to position	n at beginning of run							
0	Increase valve po	osition							
0	Decrease valve p	position							
0	Use valve positio	n							
	Position 1 (Chan	nel 1)	<b>T</b>						
Position	Names								
Valve	Position	Description				Add	Remo	ove	Clear all
<mark>Positio</mark>	on 1	Channel 1	•	Ŧ		Cut	Сор	y][	Paste

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

To set up methods for Data Acquisition

- 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.

HTS/HTC: Edit Cycle Parameters	
Actual Syringe: 100 μl	Injection Volume:
- Available Cycles	Cycle Arguments
LC-Ini_DLW_Fast_Rev03_StreamSelect	Parameter
	Airgap Volume (µl)
Syringe	Front Volume (µl)
100ulDLW	Rear Volume (µl)
- Description	Filling Speed (µl/s)
	Pullup Delay (ms)
	Injection Speed (µl/s
	Pre Inject Delay (ms
	Post Inject Delay (m
	Needle Gap Valve (

- 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.

### 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

### 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.

🖞 Checktune

- **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.

- 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.

nstrument i	name:	Instru	ument 1		
🖉 Mass Sp	pectromete	er			
💿 Agi	lent 6400	Series Trip	le Quadrupole	192	2.168.254.12
🔿 Agi	lent 6500	Series Qua	drupole Time of Flight		
🖸 Aqi	lent 6200	Series Time	e of Flight		
Agilant I C	lent 6200	Series Time	e of Flight		
C Agi Agilent LC Stream No.	lent 6200 System Default	Series Time	of Flight Stream IP	Valve Position	
Agilent LC Stream No.	System Default	Series Time Name LC 1	of Flight Stream IP 192.168.254.11	Valve Position	Device Config
C Agilent LC Stream No.	System	Name	Stream IP	Valve Position	Douise Confin

### **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.

### www.agilent.com

# In this Book

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

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