

# MassHunter Study Manager for K6460 and K6420 Quick Start Guide

### For In Vitro Diagnostic Use

The K6460 and K6420 mass spectrometers are intended to be used to identify inorganic or organic compounds in human specimens by ionizing the compounds and separating the resulting ions by means of electrical field according to their mass.

What is MassHunter Study Manager? 2

Help 2

User Interface 3 Home Tab in the Ribbon 4

Settings Tab in the Ribbon 5 Current/Stopped Study Pane 7 Pending Studies Tab 7 Completed Studies Tab 8 Select Study Creator Dialog Box 9 Study Worklist-Only Study Wizard 13 Bioanalysis Study Wizard 15 Optimizer Automation Study Wizard 17 Getting Started 19 Basic Tasks 20 Submitting a Study 24 Starting and Stopping the Study Queue 32 Modifying the Pending Studies Table 34 Other actions 36 What is MassHunter Study Manager?

Familiarization Exercise 39Task 1. Submit and run a Worklist Import Study 39Task 2. Submit and run multiple worklist-only studies 44Bioanalysis Study and Compliance 50

What is MassHunter Study Manager?

#### Overview

MassHunter Study Manager provides a way to create and run one or more studies. A study is a collection of samples and operations that are grouped together; four of the study types create a worklist that is run to analyze the samples. The fifth study uses the Optimizer program. The data files, worklist and methods can be placed into the same Study folder. You can add multiple studies to the Pending Studies table, and these studies will be executed sequentially when you start running the studies in the Study Queue. The Study Queue is the current study and the studies in the Pending Studies table.

#### Creating Studies

With Mass Hunter Study Manager, these studies can be created:

- Worklist-Only
- Worklist Import
- Bioanalysis
- Optimizer Automation

### Help

2

**Press F1** To get more information about a pane, window, dialog box or page of a wizard, click the cursor on the pane, window, dialog box or page of the wizard of interest and press **F1**.

Help menu From the Help icon, access "How-to" help and reference help.

User Interface Help

# User Interface

The MassHunter Study Manager has the following UI elements that let you enter parameters, set options, and perform functions:

- "Home Tab in the Ribbon" on page 4
- "Settings Tab in the Ribbon" on page 5
- "Current/Stopped Study Pane" on page 7
- "Pending Studies Tab" on page 7
- "Completed Studies Tab" on page 8

### Other Dialog Boxes and Wizards

- "Select Study Creator Dialog Box" on page 9
- "Study Worklist-Only Study Wizard" on page 13
- "Bioanalysis Study Wizard" on page 15
- "Optimizer Automation Study Wizard" on page 17

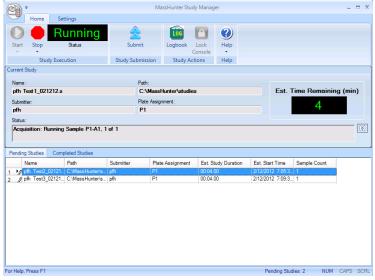


Figure 1. MassHunter Study Manager main window

# Home Tab in the Ribbon

The following toolbar buttons are available in the MassHunter Study Manager toolbar:



**Start** Lets you start the Study Queue. You select whether to start/resume the current study, restart the current stopped study or skip over the stopped study in the Study Queue. Once the Study Queue is running, it continues to run until you stop it using one of the commands in the Stop Menu. See "To run a study" on page 32. It continues running studies from the Study Queue even if you close the user interface.



**Stop** Lets you stop the Study Queue. You select whether to stop the current run immediately, the current study after the current run completes or the Study Queue. If you choose to stop the Study Queue, then the next study is not started. See "To exit the Study Manager program" on page 21.



**Status** Shows the state of the Study Queue. It can be **Stopped**, **Stopping**, **Running** or **Idle**. The state is **Stopped** if a user directly stopped the queue or the study encountered an error (and the **Stop Study Queue on error** check box is marked.) The state is **Stopping** if a user clicks one of the commands in the **Stop** menu, but the Study Queue is not stopped yet. The state is **Running** when a study is in progress. The state is **Idle** when there are no pending or current studies, but the Study Queue is not stopped. If the Study Queue is Idle and you submit a study, the status automatically changes to **Running**.



**Submit** Lets you create a new study for use in MassHunter Study Manager. You can submit the following studies:

- "To submit a Worklist Import study" on page 24
- "To submit a Worklist-Only study" on page 26
- "To submit a Bioanalysis study" on page 28
- "To submit an Optimizer Automation study" on page 30



**Logbook** Opens the Logbook program. The logbook contains a list of errors and messages from the Data Acquisition software and the Study Manager software. See "To check the Logbook" on page 36.



**Lock Console** Lets you lock the Data Acquisition program (also known as the console). When the Data Acquisition program is locked, you cannot modify the method in the method pane or the worklist in the worklist pane in the Data Acquisition program. Also, you cannot overwrite a data file which was acquired when the Data Acquisition program is locked. The worklist pane in the Data Acquisition program automatically shows the worklist that is being run as a part

User Interface Settings Tab in the Ribbon

of the current study. See "To lock the console" on page 37.



**Help** Opens the online Help program or shows the **About** dialog box for the Study Manager program. The online Help contains additional information on the Study Manager program and the Data Acquisition program. You can also see the current version of the program.

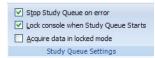
# Settings Tab in the Ribbon

The following toolbar buttons are available in the Settings tab in the Ribbon in the MassHunter Study Manager:

Home Settings			
<ul> <li>Stop Study Queue on error</li> <li>Lock console when Study Queue Starts</li> </ul>	Enable stand	dby script execut	
✓ Lock console when Study Queue Starts Acquire data in locked mode	Wait for	10	min
Study Queue Settings	S	cript Configurati	ion

Figure 2. Settings Tab in the Ribbon

### **Study Queue Settings**



**Stop Study Queue on error** Whether or not to stop the Study Queue when an error occurs. If this check box is cleared, then the study moves to the Completed Studies table with an error indicated. You can resubmit this study to the queue.

If the check box is marked, then the Study Queue is stopped, and you have to start the Study Queue again. The study is kept in the Current Study pane and the label of the pane is changed to **Stopped Study**. You can resume the study, restart the study from the beginning or start the next study in the Pending Studies table.

**Lock Console when Study Queue Starts** Toggles whether or not to automatically lock the console when you start the queue. If you lock the console, then no one can modify the method or the worklist in the Data Acquisition program while the study is running. The system automatically unlocks the console when the queue is stopped. It is recommended that you mark this check box.

If you manually lock the console, then this check box has no effect. You manually lock/unlock the console when you click the **Lock Console** icon () in the Home tab. You should only unlock the console to make any required charges and then quickly lock the console again. If you need to make extensive changes, then you should stop the Study Queue first.

Acquire data in locked mode Toggles whether or not to lock the data file so that it cannot be overwritten. If this check box is marked, then any data file that is acquired in locked mode is marked so that the worklist will not try to overwrite the file. In a worklist if you have a data file that already exists, it will ask you if you wish to overwrite the data file. If the data file is locked, then clicking **Yes** will still not allow the worklist to run. In addition, the door of the sampler is locked.

### Script Configuration

This section is only available to modify if the **Lock Console on Queue Start** check box is marked or if the Console is locked. If you enter values in this section, they are only active if the Console is locked. A script only runs if the Console is locked.

Standby Script SCP_InstrumentStandby()	Enable stand	by script execution on idle	
	Standby Script	SCP_InstrumentStandby()	
Wait for 10 min	Wait for	10	min
Script Configuration	So	ript Configuration	

**Enable standby script execution on idle** Whether or not to allow a script to run when the Study Manager is idle. Any of the scripts that are available in the acquisition program can be used. This feature is useful to turn off the pumps or to load a method in the acquisition program.

**Standby Script** The name and parameters of the script to run when the Study Manager is idle. When you click the Browse button, the **Select Script** dialog box opens. For a list of possible scripts, see the online Help.

**Wait for** The number of minutes to wait after the last study completes before executing the **Standby Script**.

User Interface Current/Stopped Study Pane

# **Current/Stopped Study Pane**

In this pane, you can see some of the information about the Current Study. This information is updated when you start running the Study Queue. See **"To run a study"** on page 32. The **Est. Time Remaining** section shows an estimate of the time until the current study is complete. If the study takes longer, then the display will show 1 to 3 dots in a repeating cycle. The estimated time of the study depends on many factors including the run time of the method. An estimated run time is computed when the method is saved. For older methods, you need to open and then save the method in order to have an estimated run time calculated; otherwise, the estimated run time is 0.

Stopped Study			
Name: PFH Test.s		Path: C:\MassHunter\Studies	Est. Time Remaining (min)
Submitter: PFH		Plate Assignment:	0.0
Status:			
			×
·	0		

Figure 3. Current/Stopped Study Pane

# **Pending Studies Tab**

In this tab, you can examine and rearrange the studies in the Pending Studies table. See **"To run a study"** on page 32 and **"To rearrange the pending studies in the Study Queue"** on page 35.

Per	ding Studies Completed Stu	dies					
	Name	Path	Submitter	Plate Assignment	Est. Study Duration	Est. Start Time	Sample Count
1	Ø 091310_Bioanalysis.s	C:\MassHunter\studi	Your Name	P2	00:03.00	9/23/2010 1:56:5	12
2	Ø 091410_Bioanalysis.s	C:\MassHunter\studi	Your Name	P2	00:03.00	9/23/2010 1:59:5	12
3	🖉 092010.s	C:\MassHunter\studi		P1	00:03.00	9/23/2010 2:02:5	33

Figure 4. Pending Studies tab

# **Completed Studies Tab**

You can see the studies that have already completed. The Completion and the Status columns show how the study completed. You can also resubmit a study to the Pending Studies table which is useful if the study completed with an error or if you want to run a new set of samples using the same study. See **"To resubmit a study from the Completed Studies tab"** on page 31.

Pendi	ng Studies	Comp	leted Studies						
	Name		Path	Submitter	Plate Assignment	Completion	Status	Start Time	End Time
1 🕨	WkTestSP.s		D:\MassHunter\	Eric	None	×	Stopped by User	1/4/2010 10:36:5	1/4/2010 10:37:3
2	WkTest1.s		D:\MassHunter\	YH	None	<b>V</b>	Completed	1/4/2010 10:34:2	1/4/2010 10:36:5

Figure 5. Completed Studies tab

8

# Select Study Creator Dialog Box

This dialog box appears when you click the **Submit** icon (<sup>somt</sup>) in the Home tab in the Ribbon if you have enabled more than one study type. For more information on submitting a study, see:

- "To submit a Worklist Import study" on page 24
- "To submit a Worklist-Only study" on page 26

The following study types are only available for a Triple Quadrupole Data Acquisition system.

- "To submit a Bioanalysis study" on page 28
- "To submit an Optimizer Automation study" on page 30

Study types are only available if they are enabled. See **"To enable a study using the Study Creator Enabler program"** on page 22. If you only have one Study type enabled, then this dialog box is not shown.

Bioanalysis			
Drug Disco Optimizer A	ery Screening		
Vorklist Imp			
Vorklist-On	y		
lelp			
	udy that automatical (Lab Information Ma		
	presponding worklist	The worklist cont	ains 🗉
creates a c nformation	presponding worklist pertaining to target co	ompounds and inte	mal 🗌
eates a c formation	presponding worklist	ompounds and inte	mal

Figure 6.

"Select Study Creator" Dialog Box for Triple Quadrupole Data Acquisition

# Study Worklist Import Study Wizard

The Worklist Import Study Wizard box allows you to submit a **Worklist Import** study. This wizard has three different pages. See **"To submit a Worklist-Only study"** on page 26.

	klist Import
Import File	
Import File:	SystemData.txt 💌
Import File Path:	C:\MassHunter\worklist_import\
	Generate data files in study
Study File	
Study Name:	Date (MMDDYY)
	✓ Use separator between name items Separator:
Study File Path:	C:\MassHunter\studies
Map File	
Map File:	SystemDataMap.xml 💌
Map File Path:	C:\MassHunter\worklist_import\
Submitter:	pfh 🔹

Figure 7. Worklist Import Study Wizard - Worklist Import page

On the Acquisition page for the Worklist Import Study, you can reassign the plates in the worklist.

### CAUTION

When you click Next after you reassign plates, the original Worklist assignment will change. From this point, if you click Back to return to the plate assignment page, plate reassignments will be based on the changed Worklist.

To reassign plates based on the original Worklist assignment, first click Back to return to the Worklist Import page, then proceed to plate reassignment.

### **User Interface**

Study Worklist Import Study Wizard

Wo	orklist Impor	t Study Wizar	d				
1		A	cquisition	c.			
Pl	ate Assignme	nt					
		Plates in	worklist			Reassign	
►	p1				None		
		_	Back	Next	Finish	Canad	
			Back	Next	Finish	Cancel	

Figure 8. Worklist Import Study Wizard - Acquisition page

On the Worklist Quant page, you can specify whether or not to run a Quantitative Analysis method at the end of the study. You can also generate a Quantitative Analysis report and print it or save it to a file.

rklist Import Study	/ Wizard
	Worklist Quant
Quart Automatio	n
Quantitative Ana	lysis Method
Method:	SystemData quantmethod ani •
Method Path:	C\MassHunter\Methods
Generate R	leport
Template I	File: C:\MassHunter\Report Templates\Quant\en-US\Letter\ESTD\Results_No
	o default printer
Publish	
	Back Next Finish Cancel

Figure 9. Worklist Import Study Wizard - Worklist Quant page

The Worklist page is the same for all study types. The title of the window is different to show the Study type that is being created.

### User Interface

Study Worklist Import Study Wizard

	•	Sample Name	Sample Position	Method	Data
1	v	Sample1	P1-A1	C:\MassHunter\studies\1029	Sample1.d
2	v	Sample2	P1-A2	C:\MassHunter\studies\1029	Sample2.d

Figure 10. Worklist Import Study Wizard - Worklist page

# Study Worklist-Only Study Wizard

This wizard allows you to submit a Worklist-Only study based on an existing worklist. This wizard has three different pages. See **"To submit a Worklist-Only study"** on page 26.

On the Worklist Import page, you specify the worklist to use, the name of the Study, the Plate Assignment and the Submitter name.

Vorklist-Only Study Wizard
Sector Worklist Import
Worklat Fle Worklat Fle: pfh_Worklat wid Worklat File Path: [C:MassHunter/worklats\ @ Generate data files in study @ Copy methods in study
Study File Study Name: Date (MMDD'Y')  Worklast  Study File Study File Path: C:\MassHunter\studies  Field Assignment
Plates in worklist Reassign
▶ P1 None
Submitter: pfh 👻
Back Next Brish Cancel

Figure 11. Worklist-Only Study Wizard - Worklist Import page

On the Worklist Quant page, you specify whether to run a Quantitative Analysis method at the end of the study. You can also generate a Quantitative Analysis report and print it or save it to a file.

#### **User Interface**

Study Worklist-Only Study Wizard

-	/orklist Quant
Quant Automation	
Quantitative Analysis Me	thod
Method: PFH_)	Worklist_quantmethod.xml 👻
Method Path: C:\Ma	ssHunter\Methods
Taxalata Dia.	C:\MassHunter\Report Templates\Quant\en-US\Letter\ESTD\Results_No
Template File:	C:MassHunter/Report Templates/Quant/en-US/Letter/ESTD/Results_No
Print to default	L pinter
Print to default	L pinter

Figure 12. Worklist-Only Study Wizard - Worklist Quant page

The Worklist page is the same for all study types. The title of the window is different to show the Study type that is being created.

Work	list-Or	nly Study Wizard									
2	Sector Worklist										
	1	lnj Vol (μl)	Sample Name	Sample Position	Method						
1	V	As Method	Sample 1	P1-A1	PAH_Test.m						
4	1				•						
				Worklist							
		Ba	ck Next	Finish Can	cel						

Figure 13. Worklist-Only Study Wizard - Worklist page

# **Bioanalysis Study Wizard**

The Bioanalysis Study Wizard allows you to submit a worklist based upon a Bioanalysis input file. See **"To submit a Bioanalysis study"** on page 28. This wizard has four pages. A Bioanalysis Study has to have an internal standard.

This wizard is only available if the Bioanalysis Study Creator is enabled. See **"To enable a study using the Study Creator Enabler program"** on page 22.

The four wizard pages are:

- Bioanalysis Study Wizard Import page (Figure 14 on page 15)
- Bioanalysis Study Wizard Acquisition page (Figure 15 on page 16)
- Bioanalysis Study Wizard Quantitation and Reporting page (Figure 16 on page 16)
- Bioanalysis Study Wizard Worklist page (Figure 12 on page 14)

Bioanalysis Study Wizard
Sector Import
Import File
Import File: BioAnalysis_Example.TXT
Import File Path: C:\MassHunter\worklist_import\
Study File
Study Name: Date (MMDDYY) 💌 Blank
☑ Use separator between name items Separator:
Study File Path: C:\MassHunter\studies
Submitter: pfh
Back Next Finish Cancel

Figure 14. Bioanalysis Study Wizard - Import page

### User Interface

**Bioanalysis Study Wizard** 

Bioanalysis Study Wizar	d		
∕	Acquisition		
Sample Information	ı ————		
- Acquisition Meth	od		
Method:	Default.m	•	
Method Path:	C:\MassHunter\methods\		
Data File			
Data File:	Date (YYYYMMDD)	Sample Name 💌 Counter	
	Use separator between n	me items Separator:	
Plate Assignment			
Pla	ates in worklist	Reassign	
	Back Next	Finish Cancel	]

Figure 15. Bioanalysis Study Wizard - Acquisition page

Bioanalysis Study Wizard	
Quantitation and Reporting	
Quart Method Generation <sup>©</sup> Reference Data File <sup>©</sup> Preliminary Quart Method <sup>©</sup> Reference Data File by Calibration Level <sup>¶</sup> T = CmpdX:1	
Back Next Finish Cancel	

Figure 16. Bioanalysis Study Wizard - Quantitation and Reporting page

# **Optimizer Automation Study Wizard**

The Optimizer Automation Study Wizard allows you to submit a study based upon an XLS or XLSX file.

The Optimizer Automation study type is only available if the study is enabled. See **"To enable a study using the Study Creator Enabler program"** on page 22.

The two wizard pages are:

- Optimizer Automation Study Wizard Import page (Figure 17 on page 17)
- Optimizer Automation Study Wizard Optimize page (Figure 18 on page 18)

Optimizer Automation	n Study Wizard
∕	Import
Import File	
Import Fi	ile: ADME_Optimizer_Study_07120-1.xds
Import Fi	ile Path: C:\MassHunter\worklist_import\
Study File	
Study N	ame: Date (MMDDYY)   Optimizer
	☑ Use separator between name items Separator:
Study Fil	le Path: C:\MassHunter\studies
Map File	
Map File	e: OptimizerAutomation.xml
Map File	Path: C:\MassHunter\Configuration\study_creators\DDS\worklist_imp
Submitte	er: Your Name
	Back Next Finish Cancel

Figure 17. Optimizer Automation Study Wizard - Import page

### User Interface

**Optimizer Automation Study Wizard** 

Optimizer Automation Study Wizard									
Soptimize Optimize									
Optimizer Input									
Optimizer Database: C:\MassHunter\Databases\Optimizer									
Optimizer Project: OptimizerProject 1									
Positive Method: C:\MassHunter\Methods\Default.m									
Negative Method:									
Re-optimize compounds optimized more than 1 day(s) ago									
Edit Optimization Parameters									
Validation errors:									
Back Next Finish Cancel									

Figure 18. Optimizer Automation Study Wizard - Optimize page

### Getting Started

**Optimizer Automation Study Wizard** 

# Getting Started

### **Basic Tasks**

- "To start the Study Manager program" on page 20
- "To exit the Study Manager program" on page 21
- "To enable a study using the Study Creator Enabler program" on page 22
- "To switch users when Compliance is enabled" on page 23

### **Submitting Studies**

- "To submit a Worklist Import study" on page 24
- "To submit a Worklist-Only study" on page 26
- "To submit a Bioanalysis study" on page 28
- **"To submit an Optimizer Automation study"** on page 30
- "To resubmit a study from the Completed Studies tab" on page 31

### **Running a Study**

- **"To run a study"** on page 32
- "To stop the Study Queue" on page 33

### Modifying the Pending Studies Table

- "To delete a Pending Study" on page 34
- "To edit a worklist" on page 34
- "To rearrange the pending studies in the Study Queue" on page 35

### **Other Activities**

- "To select what occurs after an error happens" on page 36
- "To check the Logbook" on page 36
- "To use the keyboard to access the Ribbon" on page 37
- "To lock the console" on page 37
- **"To add a standby script"** on page 38

**Basic Tasks** 

To start the Study Manager program

# Basic Tasks

# To start the Study Manager program

Follow this procedure to start the Study Manager program.

The instructions below include the following assumptions:

- The hardware and software are installed.
- The instrument is configured.
- Use instructions in the Installation Guide to configure the instrument for the first time and any time you change the LC configuration.
- Do not run the Study Manager when tuning the instrument or running optimization manually.

After installation, you see all of the Agilent MassHunter Workstation software icons on your Desktop.

1 To start the Study Manager program, double-click the Agilent MassHunter Workstation program group.

Organize 🔻 Include in library 👻 Share with 👻 Burn New folder							
🔆 Favorites							
🥽 Libraries	Acq Tools	Qualitative Analysis	Qualitative Analysis	Acq System Launcher	Acq System Logbook	Data Acquisition	Offline Method
🝓 Homegroup		B.05.00 Tools	B.06.00 Tools				Editor
🖳 Computer	ş 🔊			<b>H</b>			Ì
🗣 Network	Offine Worklist Editor	Optimizer for Peptides	Optimizer	Qualitative Analysis B.05.00	Qualitative Analysis B.06.00	Source Optimizer	Study Manage

2 Double-click the Study Manager icon (

You can also click Programs> Agilent> MassHunter Workstation> Study Manager from the Windows Start menu.



# To exit the Study Manager program

You can close the Study Manager program from two different places.

- Click in the upper right corner of the program window.
- Click the Study Manager button and then click Exit Study Manager.

If the Study Manager queue is **Running**, then it continues to run even if you close the Study Manager user interface. To stop the Study Queue, you click one of the **Stop** commands.

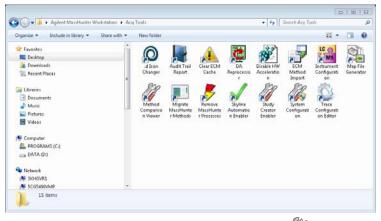
	MassHunter Study Manager – 🗖									
	Home Settinos									
		<b>&gt;</b>		Logbook	Lock Help ions Help					
	Submit									
(iiii	Logbook			inment:		Est.	Time Remainin	g (min)		
Þ	Lock Console						0.0			
	Lo	ock Session 🔞	Exit Study Mana	iger				No. 10		
Pendi	ing Studies Comp	pleted Studies								
	Name	Path	Submitter	Plate Assignment	Est. Study Duration	Est. Start Time	Sample Count			
1 +	102411_test4.s	C:\MassHunter\s	PFH	P1	00:00.00		1			
2		C:\MassHunter\s		None	00:00.00		1			
3	102411_test5.s	C:\MassHunter\s	PFH	P1	00:00.00		1			
4	102411_worklisti	C:\MassHunter\s	PFH	None 00:00.00			1			
For Help, Press F1 Pending Studies: 4 NUM CAPS SCRL										

21

# To enable a study using the Study Creator Enabler program

By default, all study types are enabled. If you want to hide one of the Study Types, you can disable the Study Type first.

- 1 To start the Study Creator Enabler program, double-click the Agilent MassHunter Workstation program group.
- 2 Double-click the Acq Tools icon.



3 Double-click the Study Creator Enabler icon (2017).

### NOTE

Do not enable the Bioanalysis study until you have installed the Quantitative Analysis and the Quantitative Analysis Reporting programs. Excel must also be installed.

- 4 Check the **Enabled Study Creators** list. If the Study Type that you want to use is not in this list, then do the following:
  - a Click the Study Type that you want to enable in the Available Study Creators list. Click is to copy this Study Type to the Enabled Study Creators list.
  - a Click the Study Type that you want to disable in the **Enabled Study** Creators list. Click the button to remove this Study Type from the Enabled Study Creators list
- 5 Click OK.

### **Basic Tasks**

To switch users when Compliance is enabled

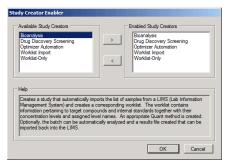


Figure 19. Study Creator Enabler Program

### To switch users when Compliance is enabled

You use the Mass Hunter Data Acquisition program in User Management and Audit Trail or Compliance mode to keep track of who is making changes on the system. You keep track of who is modifying methods and worklists, who is submitting studies and more. You do not need to stop the Study Queue to switch users.

- 1 Close the Study Manager program:
  - Click X in the upper right corner of the program window.
  - Click the Study Manager button and then click Exit Study Manager.

If the Study Manager queue is **Running**, then it continues to run even if you close the Study Manager user interface.

- **2** Open the Study Manager program. The MassHunter Workstation Logon dialog box opens.
  - Double-click the Study Manager icon ().
  - Click Programs> Agilent> MassHunter Workstation> Study Manager from the Windows Start menu.
- **3** Enter your User Name, Password and Domain.
- 4 Click OK.

Submitting a Study To submit a Worklist Import study

# Submitting a Study

- "To submit a Worklist Import study" on page 24
- "To submit a Worklist-Only study" on page 26
- "To submit a Bioanalysis study" on page 28
- "To submit an Optimizer Automation study" on page 30

# To submit a Worklist Import study

Follow this procedure to add a Worklist Import study to the queue.

- 1 Click **Submit** (submit) in the Ribbon. The "Select Study Creator" dialog box is opened.
- 2 Select Worklist Import as the study type.
- **3** Click **OK**. The Worklist Import Study Wizard opens (**Figure 7** on page 10). The Worklist Import page appears.
- 4 (optional) Change the **Import File Path**. Click \_\_\_\_\_ next to the Import File Path box to change the path.
- **5** Select the **Import File** to use for this study from the list. The list contains all worklists that are in the Import File Path.
- 6 Mark or clear the **Generate data files in study** check box. If this box is marked, then the data files that are generated when this study runs are placed in the study folder. Otherwise, the data files are placed in the worklist location.

However, if the data file specified in the worklist includes a full data file path (for example, *c*:\*mydata*\*a.d*), then the data file is created in that folder.

- 7 (optional) Mark the Copy methods in study check box.
- 8 Select how to name a Study. The Study name has two parts to set. If you select **Custom**, then you can type your own value in this box. This name appears in the Pending Studies table in the Name column.
- **9** Mark or clear the **Use separator between name items** check box. If you mark this box, then type the character to use to separate the three parts of the data file name in the **Separator** box.

### Submitting a Study

To submit a Worklist Import study

- 10 (optional) Change the Study File Path. Click \_\_\_\_\_ next to the Study File Path to change the path.
- 11 (optional) Change the Map File Path. Click \_\_\_\_ next to the Map File Path box to change the path.
- 12 Select the Map File to use for this study from the list. The list contains all worklists that are in the Import File Path. The Map File is used to map the columns in the Import File to the columns in the worklist.
- 13 (optional) Enter the name of the Submitter. This name appears in the Pending Studies table in the Submitter column. If Compliance is turned on, then this box is automatically set to the name of the user who has logged in when submitting the study, and this box cannot be changed.
- 14 Click Next. The Worklist Import Study Wizard Acquisition page (Figure 8 on page 11) is opened.
- 15 Select the Plate Assignment. The combo box shows all plates that are available. If the plate is already in the Study Queue, then it appears as In Use. You can still select a plate that appears In Use, but the plate should be replaced before the submitted study is executed.

Plate assignment will cause the sample positions in the worklist to be updated. The plate number found in the worklist corresponding to the selected plate will be replaced by the plate reassigned to it. The well position is not changed. All samples in the worklist with that plate number will be replaced by the plate assigned. The vial positions are not changed. Multiple well plates are supported.

- 16 Click Next. The Worklist Import Study Wizard Worklist Quant page (Figure 9 on page 11) is opened.
- 17 (optional) Mark the **Quant Automation** check box. If you mark this check box, then select the **Quantitative Analysis Method**.
- 18 (optional) Mark the Generate Report check box. If you mark this check box, then select the Template File to use for the report. You can also mark the Print to default printer check box and the Publish check box.
- **19** Click **Next**. The Worklist Import Study Wizard Worklist page (**Figure 10** on page 12) is opened.

20 Review the worklist for this study. Make any necessary changes.

**21** Click **Finish**. The study is submitted to the Pending Studies table.

# To submit a Worklist-Only study

Follow this procedure to add a worklist-only study to the queue.

- 1 Click the **Submit** icon (submit) in the Ribbon. The "Select Study Creator" dialog box is opened.
- 2 Select **Worklist-Only** as the study type.
- **3** Click **OK**. The Worklist-Only Study Wizard opens. (**Figure 11** on page 13). The Worklist Import page appears.
- 4 (optional) Change the **Worklist File Path**. Click \_\_\_\_\_ next to the Worklist File Path box to change the path.
- **5** Select the **Worklist File** to use for this study from the list. The list contains all worklists that are in the Worklist File Path.
- 6 Mark or clear the **Generate data files in study** check box. If this box is marked, then the data files that are generated when this study runs are placed in the study folder. Otherwise, the data files are placed in the worklist location.

However, if the data file specified in the worklist includes a full data file path (for example, *c*:\*mydata*\*a.d*), then the data file is created in that folder.

- 7 (optional) Mark the Copy methods in study check box.
- 8 Select how to name a Study. The Study name has two parts to set. If you select **Custom**, then you can type your own value in this box. This name appears in the Pending Studies table in the Name column.
- **9** Mark or clear the **Use separator between name items** check box. If you mark this box, then type the character to use to separate the three parts of the data file name in the **Separator** box.
- **10** (optional) Change the **Study File Path**. Click \_\_\_\_\_ next to the Study File Path to change the path.
- 11 Select the Plate Assignment. The combo box shows all plates that are available. If the plate is already in the Study Queue, then it appears as In Use. You can still select a plate that appears In Use, but the plate should be replaced before the submitted study is executed.

Plate assignment will cause the sample positions in the worklist to be updated. The plate number found in the worklist corresponding to the selected plate will be replaced by the plate reassigned to it. The well position is not changed. All samples in the worklist with that plate number will be replaced by the plate assigned. The vial positions are not changed. Multiple well plates are supported.

- 12 (optional) Type the **Submitter**. This name appears in the Pending Studies table in the Submitter column. If Compliance is turned on, then this box is automatically set to the name of the user who has logged in when submitting the study, and this box cannot be changed.
- **13** Click **Next**. The Worklist-Only Study Wizard Worklist Quant page (**Figure 12** on page 14) is opened.
- 14 (optional) Mark the **Quant Automation** check box. If you mark this check box, then select the **Quantitative Analysis Method**.
- 15 (optional) Mark the Generate Report check box. If you mark this check box, then select the Template File to use for the report. You can also mark the Print to default printer check box and the Publish check box.
- **16** Click **Next**. The Worklist-Only Study Wizard Worklist page (**Figure 13** on page 14) is opened.
- 17 Review the worklist for this study. Make any necessary changes.
- **18** Click **Finish**. The study is submitted to the Pending Studies table.

# To submit a Bioanalysis study

Follow this procedure to add a study to the queue. If Compliance for Quantitative Analysis is enabled, the user that submits the study also has to have the correct permissions in the Quantitative Analysis program. You can only submit a Bioanalysis study for a Triple Quadrupole instrument.

A Bioanalysis study has to contain at least one internal standard.

- 1 Click the **Submit** icon (Submit) in the Ribbon. The "Select Study Creator" dialog box is opened.
- 2 Select **Bioanalysis** as the study type.
- **3** Click OK. The Bioanalysis Study Wizard is opened. The Worklist Import page appears (**Figure 14** on page 15)
- 4 (optional) Change the Import File Path. If the Import File is not in the folder that appears, click \_\_\_\_\_ to change the path.
- **5** Select an Import File.
- **6** (optional) Change the Study File Path. Click \_\_\_\_\_ to change the path.
- 7 Select how to name the files in the Study in the Study File section.
- 8 Mark or clear the Use separator between name items check box. If you mark this box, then type the character to use to separate the two parts of the Study name in the Separator box.
- **9** (optional) Type the Submitter. This is the name of the person submitting the study. If Compliance is turned on, then this box is automatically set to the name of the user who has logged in when submitting the study, and this box cannot be changed.
- Click Next. The Bioanalysis Study Wizard Acquisition page appears (Figure 15 on page 16).
- 11 (optional) Change the **Method Path**. If the method is not in the folder that is shown, click \_\_\_\_\_ to change the path.
- 12 Select a Method.
- 13 Select how to name a **Data File**. The Data File name has three parts to set. If you select **Custom**, then you can type your own value in this box.
- 14 Mark or clear the Use separator between name items check box. If you mark this box, then type the character to use to separate the three parts of the data file name in the Separator box.
- 15 Select the Plate Assignment. The combo box shows all plates that are available. If the plate is already in the Study Queue, then it appears as In Use.

To submit a Bioanalysis study

You can still select a plate that appears **In Use**, but the plate should be replaced before the submitted study is executed.

Plate assignment will cause the sample positions in the worklist to be updated. The first plate number found in the worklist will be replaced by the plate assigned. The well position is not changed. All samples in the worklist with that plate number will be replaced by the plate assigned. The vial positions are not changed.

- **16** Click **Next**. The Bioanalysis Study Wizard Quantitation and Reporting page appears (**Figure 16** on page 16).
- 17 Click the Quant Method Generation button that you want to use.

If you click Reference Data File, select an existing data file to use.

If you click **Preliminary Quant Method**, select the quant method that is used as a starting point. If you acquired a data file previously, you may have created a Quant Method already.

If you click **Reference Data File by Calibration Level**, select the Calibration Level. The sample with the corresponding calibration level will be used as the reference data file.

- 18 Mark or clear the Generate LIMS Output check box.
- 19 Click Next. The Bioanalysis Study Wizard Worklist page appears.
- 20 Review the worklist for this study. Make any necessary changes.
- **21** Click **Finish**. The study is submitted to the Pending Studies table.

# To submit an Optimizer Automation study

Follow this procedure to add a study to the queue.

- 1 Click the **Submit** icon (2) in the Ribbon. The "Select Study Creator" dialog box is opened.
- 2 Select **Optimizer Automation** as the study type.
- **3** Click OK. The Optimizer Automation Study Wizard is opened. The Import page appears.(**Figure 17** on page 17)
- 4 (optional) Change the Import File Path. If the **Import File** is not in the folder that appears, click \_\_\_\_\_ to change the path.
- **5** Select an Import File. The Import File for this study is an Excel *XLS* or *XLSX* file.
- 6 Select how to name the files in the Study in the Study File section. The Study name has two parts to set. If you select **Custom**, then you can type your own value in this box. This name appears in the Pending Studies table in the Name column.
- 7 Mark or clear the **Use separator between name items** check box. If you mark this box, then type the character to use to separate the three parts of the data file name in the **Separator** box.
- 8 (optional) Change the Study File Path. Click \_\_\_\_\_ to change the path.
- 9 (optional) Select a **Map File**. You can change the **Map File** using the Map File Generator program. See the online Help for more information.
- **10** (optional) Type the Submitter. This is the name of the person submitting the study. If Compliance is turned on, then this box is automatically set to the name of the user who has logged in when submitting the study, and this box cannot be changed.
- 11 Click Next. The Optimizer Automation Study Wizard Optimize page (Figure 18 on page 18) appears.
- 12 (optional) Change the **Optimizer Database**. To change the selected Optimizer Database, click \_\_\_\_\_ to select a different database.
- 13 Select an Optimizer Project. If you have no projects in this Optimizer Database, click Edit Optimization Parameters and set up a project.
- 14 Select an optimizer method. You must select a **Positive Method** or a **Negative Method**. If you do not have any methods, click **Edit Optimization Parameters** and add one or more methods.

#### Submitting a Study

To resubmit a study from the Completed Studies tab

- 15 (optional) Mark the Re-optimize compounds optimized more than X day(s) ago check box. If you mark this check box, then you also need to select how many days to wait until you re-optimize a compound. If you want to re-optimize all compounds in the study, you enter 0 days.
- 16 Click Finish. The software validates the Optimizer Project. If an error exists in the Optimizer project, the errors are listed in the Validation errors section. To fix problems, click Edit Optimization Parameters to open the MassHunter Optimizer program. The currently selected database and project are automatically loaded. You need to fix any errors in the Optimizer project before you can submit the study.

# To resubmit a study from the Completed Studies tab

You can resubmit a study from the Completed Studies table. It is submitted at the end of the Pending Studies table.

- 1 Click the **Completed Studies** tab.
- 2 (optional) Right-click the study in the Completed Studies table and click Edit Worklist from Study. You use this command if you want to review and update the worklist before resubmitting it.
- **3** Right-click the study in the **Completed Studies** table and click **Resubmit**. A copy of the study is submitted to the **Pending Studies** table. The study is still shown in the Completed Studies table.

If you restart a study from the beginning, all data files and other generated files are deleted. You are given a warning before you resubmit a study.

4 Click the **Pending Studies** tab. The study is added to the end of the Pending Studies table.

To run a study

# Starting and Stopping the Study Queue

Use the following procedures to start and stop the Study Queue. The Study Queue includes the current study and the studies in the Pending Studies table.

- "To run a study" below
- "To stop the Study Queue" below

### To run a study

Follow this procedure to start running studies in the Study Queue.

- 1 Click the **Start** icon ( see ) in the Home tab in the Ribbon.
- 2 Click on one of the commands that is displayed.
- Start Starts the next pending study.
- **Resume Stopped Study** Continues the stopped study from the place where it was stopped.
- Restart Stopped Study Starts the stopped study from the beginning. This option is only available if the current study is Stopped. This option is not available if the data is acquired in Locked Mode because you cannot overwrite a data file that is acquired in Locked Mode.
- Skip Stopped Study This command is only available if the current study is stopped. The stopped study is moved to the Completed Studies table, and the first study in the Pending Studies table is started.

# To stop the Study Queue

Follow this procedure to stop running studies in the Study Queue.

- 1 Click the **Stop** icon ( <sup>sop</sup> ) in the Home tab in the Ribbon.
- 2 Click on the of the commands that is displayed.
  - **Stop Immediately** Stops the current run in the current study. The current study becomes a stopped Study. None of the stop commands are available after you click this command.
  - Stop After Current Run Stops the current study after the current run completes. The current study becomes a stopped study. The Stop Immediately command is still available after you click this command.
  - Stop After Current Study Stops the study queue after the current study completes. The current study is moved to the Completed Studies table if it finishes successfully. The Stop Immediately and the Stop After Current Run commands are still available after you click this command.

33

To delete a Pending Study

# Modifying the Pending Studies Table

Use the following procedures to change the order of the studies in the Pending Studies table in MassHunter Study Manager.

- "To delete a Pending Study" below
- "To edit a worklist" below
- "To rearrange the pending studies in the Study Queue" on page 35

# To delete a Pending Study

Use this procedure to delete a study from the Pending Studies table.

- 1 Submit a study to the queue. Follow the instructions in one of the following:
  - "To submit a Worklist Import study" on page 24
  - "To submit a Worklist-Only study" on page 26
  - "To submit a Bioanalysis study" on page 28
  - "To submit an Optimizer Automation study" on page 30
- 2 Right-click the study in the Pending Studies table. Click **Delete** in the shortcut menu. You can also press the **Delete** key on the keyboard.
- 3 Click Yes in the "Are you sure you want to delete the study" message box.

# To edit a worklist

Follow this procedure to edit a worklist for a pending study. You can edit a worklist from two different locations.

- 1 Right-click a pending study in the Pending Studies table or right-click the current study in the Current Study pane and click **Edit Worklist from Study**. The Study Submitter dialog box is opened.
- 2 (optional) Make changes to the worklist.
- 3 Click Save.

#### Modifying the Pending Studies Table To rearrange the pending studies in the Study Queue

You can also edit the worklist when you submit a study. The Worklist page of the appropriate study wizard is automatically displayed during this process.

You cannot edit an **Optimizer Automation** study. The **Edit Worklist From Study** command is not available for this Study Type.

# To rearrange the pending studies in the Study Queue

Follow this procedure to reorder the studies that are in the Pending Studies table. The first line in the Pending Studies table is the first pending study in the queue. The second line in the Pending Studies table is second in the queue, and so on. If you have more than one pending study in the Study Queue, you can rearrange the order of the studies.

- 1 Submit more than one study to the queue. Follow the instructions in one of the following:
  - "To submit a Worklist Import study" on page 24
  - "To submit a Worklist-Only study" on page 26
  - "To submit a Bioanalysis study" on page 28
  - "To submit an Optimizer Automation study" on page 30
- 2 Right-click one of the rows in the Pending Studies table.
- **3** Click **Move to Top**, **Move Up** or **Move Down** to move the selected study to the top of the Study Queue, one row up or one row down.

The first study in the Pending Studies table only has the **Move Down** command. The last study in the Pending Studies table only has the **Move to Top** and **Move Up** commands.

#### Other actions

To select what occurs after an error happens

# Other actions

Use the following procedures to set up compounds for use in MassHunter Study Manager.

- "To select what occurs after an error happens" below
- "To check the Logbook" below
- "To use the keyboard to access the Ribbon" on page 37
- "To lock the console" on page 37
- "To add a standby script" on page 38

### To select what occurs after an error happens

Use this procedure to change what happens after an error occurs.

- 1 Click the **Settings** tab in the Ribbon. The Study Settings Tab in the Ribbon appears (**"Settings Tab in the Ribbon"** on page 5).
- 2 Mark or clear the **Stop Study Queue on error** check box in the Study Queue Settings box. This box controls what happens to the study and the Study Queue when a study has an error.

If the check box is clear, then the study queue does not stop if the study encounters an error. The study stops executing and is moved to the Completed Studies table. If it is marked, then the Study Queue is stopped, and the study becomes a stopped study.

### To check the Logbook

Use this procedure to check the system and instrument events that occurred that are reported in the System Logbook.

- 1 Click the **Home** tab in the Ribbon. The Home Tab in the Ribbon appears.

A study log is created for each study. Each study has its own log, and it contains the messages that you normally see in the status window during the study execution. You right-click the row in the Completed Studies table and click **View Log**. The Study Log dialog box is opened which contains information about the study selected in the Completed Studies table.

## To use the keyboard to access the Ribbon

Use this procedure if you want to use the icons in the Ribbon using only the keyboard.

- 1 Press the **Alt** key. A series of letters appear on the different tabs and on the Office Button.
- 2 Type the letter of one of the tabs. A series of letters appear on each icon in that tab in the Ribbon.
- **3** Type the letter that is next to the icon that you want to use. If the icon contains a menu, the menu is displayed along with a letter for each item in the menu. Otherwise, the action occurs as if the icon was clicked.
- 4 (optional) Type the letter that is next to the command that you want to use.

## To lock the console

Use this procedure to lock the console. If the console is locked, you cannot modify a method or worklist in the Data Acquisition program.

- 1 Click the **Home** tab in the Ribbon. The Study Home Tab in the Ribbon appears.
- 2 Click the Lock Console icon in the Ribbon.

### To add a standby script

Use this procedure to add a standby script. A standby script is executed if the Study Queue has been idle for the number of minutes you entered to wait for. This section is only available if the **Lock Console when Study Queue Starts** check box is marked.

- 1 Click the **Settings** tab in the Ribbon. The **"Settings Tab in the Ribbon"** on page 5 appears.
- 2 Mark the **Enable standby script execution on idle** check box under Script Configuration.
- **3** Click \_\_\_\_\_ to change the **Standby Script**. The Select Script dialog box is opened.
- 4 Select a Script and enter any necessary parameters. Click OK.
- **5** Enter the number of minutes to wait in the **Wait for** box. The Study Queue needs to be idle for this number of minutes before this script is executed.

Task 1. Submit and run a Worklist Import Study

# Familiarization Exercise

### Task 1. Submit and run a Worklist Import Study

In this task you submit one study to the Pending Studies table. This study is based upon an example file that is provided on the installation disk in the **Support\Data** folder.

Task 1. Submitting and running a Worklist Import study

Steps	Detailed Instructions	Comments	
1 Open the Study Manager program and clear the items in the Pending Studies table (if necessary).	<ul> <li>a Double-click the Agilent MassHunter Study Manager icon,</li> <li>b Right-click any line in the Pending Studies table, and then click <b>Delete</b>.</li> </ul>	• Before deleting any studies from the Pending Studies table, make sure that no one else is using the system.	
2 Copy the example files in the Support\Data folder to the MassHunter folder.	<ul> <li>a Copy SystemData.txt to the \MassHunter\ worklist_import folder.</li> <li>b Copy SystemDataMap.xml to the \ MassHunter\StudyExamples folder.</li> </ul>	•	
3 Submit the Worklist Import study.	<ul> <li>a Click the Submit icon, in the Ribbon.</li> <li>b (optional) Select Worklist Import in the Select Study Creator dialog box. Click OK.</li> <li>c Select SystemData.txt as the Import File. Change the Import File Path if necessary.</li> <li>d (optional) Mark the Generate data files in study check box.</li> <li>e (optional) Mark the Copy methods in study check box.</li> <li>f Select Date (MMDDYY) as the first part of the Study Name.</li> <li>g Select Custom Name as the second part of the Study Name.</li> <li>h Then type <i>iii</i> as the Submitter.</li> <li>i Type <i>iii</i> as the Submitter.</li> </ul>	<ul> <li>If you enabled another study type, then you first need to select the type of study. See "To enable a study using the Study Creator Enabler program" on page 22.</li> <li>"<i>iii</i>" are your initials.</li> <li>The Plate Assignment is specific to your instrument setup.</li> <li>The example worklists are included on the installation disk in the Support\Data folder.</li> </ul>	

Task 1. Submit and run a Worklist Import Study

Steps	Detailed Instructions	Comments	
	Worklist Import Study Wizard		]
	Sector Worklist I	mport	
		mData bit	
		assHunter\worklist_import\	
	Use	MMDDYY)  pfh Test 1  separator between name items Separator:	
	Map File Map File: System	DataMap.xm	
	Submitter: pfh	•	
	Back	Next Finish Cancel	
	<ul> <li>k (optional) Reassig worklist.</li> <li>I Click Next.</li> </ul>	gn the Plates in	
	Worklist Import Study Wizard Acquisition	חנ	
	Plate Assignment Plates in worklist	Reassign None	
	Back	Next Finish Cancel	

Figure 21. The Worklist Import Study Wizard - Acquisition page

Task 1. Submit and run a Worklist Import Study

Detailed Instructions	Comments
<ul> <li>m (optional) Mark the Quant Automation check box.</li> <li>n If you mark the Quant Automatic check box, then select the Quantitative Analysis Method.</li> <li>o (optional) Mark the Generate Recheck box. If you mark this check select the Template File.</li> <li>p (optional) Mark the Print to defar printer check box.</li> <li>q (optional) Mark the Publish check</li> </ul>	eport sk box, ault
box. Select the file type to use.	
Quart Automation     Quartitative Analysis Method     Method:	Ver-US-VLetter/ESTD/Results_No
Pint to default pinter Publish	
	<ul> <li>m (optional) Mark the Quant Automation check box.</li> <li>n If you mark the Quant Automatic check box, then select the Quantitative Analysis Method.</li> <li>o (optional) Mark the Generate Riccheck box. If you mark this check select the Template File.</li> <li>p (optional) Mark the Print to definition printer check box.</li> <li>q (optional) Mark the Publish check box. Select the file type to use.</li> <li>r Click Next.</li> </ul>

Task 1. Submit and run a Worklist Import Study

Detailed Instructions Comments
<ul> <li>s Review the worklist in the Worklist Import Study Wizard - Worklist page.</li> <li>t (optional) Right-click the box in the upper left corner and click Worklist Run Parameters. Change the Method Path. Fix any other problems. Click OK.</li> <li>u Click Finish.</li> <li>You need to enter the Sample Position, Method and Data File for each of the three samples.</li> </ul>
Worklist Import Study Wizard
🔶 Worklist
🔽 Sample Name Sample Position Method Data F
1 v Sample1 P1-A1 pfhSulfamix_dMRM.m Sample1.d
2         ν         Sample2         P1-A2         pfhSulfamix_dMRM.m         Sample2.d           3         ν         Sample3         P1-A3         pfhSulfamix_dMRM.m         Sample3.d
Vorklist
Back Next Finish Cancel

Task 1. Submit and run a Worklist Import Study

Steps			Detailed Instructions	Comments
Ļ	Start running the stu Queue.	dy in the Study	<ul> <li>a Click the Start icon, O in the I</li> <li>b Click either Start or set ume St</li> <li>Study.</li> </ul>	····
C	₹ Home Settings	MassHunter	itudy Manager	- = X
	Start Stop Status Study Execution	Submit Logbool Study Submission Study	Console Actions Help	The study is removed from the
	rrent Study Name:	Path:		Pending Studies queue, and it
l	111711_pfh Test1.s	C:\MassHunter\stu	dies Est. Time Remaining (n	becomes the Current Study. If you
	Submitter:	Plate Assignment:		add another study, it is added to the
	PFH Ratus:	None		-
1	Acquisition: Running Sample P1-A1, 1	of 3		Pending Studies queue and started when the Current Study completes.
Pe	nding Studies Completed Studies	Submitter Plate Assignme	nt Est. Study Duration Est. Start Time Sample Count	
or I	Help, Press F1		Pending Studies: 0 NUM CAR	'S SCRL

Task 2. Submit and run multiple worklist-only studies

### Task 2. Submit and run multiple worklist-only studies

In this task you submit four different studies to the Pending Studies table. These studies are based upon four different worklists that are provided on the installation disk in the **Support\Data** folder. These worklists are created for the electrospray demo mix and contain three dilutions (level 1 to 3). You can rename the method that was used for the Triple Quadrupole Familiarization Guide exercises to the method used in these worklists.

Steps	Detailed Instructions	Comments		
1 Open the Study Manager program and clear the items in the Pending Studies table (if necessary).	<ul> <li>a Double-click the Agilent MassHunter Study Manager icon, </li> <li>b Right-click any line in the Pending Studies table, and then click <b>Delete</b>.</li> </ul>	• Before deleting any studies from the Pending Studies table, make sure that no one else is using the system.		
<ol> <li>Submit the first study.</li> <li>This study is a worklist-only study using the worklist GroupA.wkl.</li> </ol>	<ul> <li>a Click the Submit icon, in the Ribbon.</li> <li>b (optional) Select Worklist-Only in the Select Study Creator dialog box. Click OK.</li> <li>c Select Example_Worklist1.wkl as the Worklist file. Change the Worklist File Path if necessary.</li> <li>d (optional) Mark the Generate data files in study check box.</li> <li>e (optional) Mark the Copy methods in study check box.</li> <li>f Select Custom as the first part of the Study Name.</li> <li>g Then type <i>iii</i> Test1 in the Study Name.</li> <li>h Select Date (MMDDYY) as the second part of the Study Name.</li> <li>i Type <i>iii</i> as the Submitter.</li> <li>j (optional) Select the Plate Assignment.</li> <li>k Click Next.</li> </ul>	<ul> <li>If you enabled another study type, then you first need to select the type of study. See "To enable a study using the Study Creator Enabler program" on page 22.</li> <li>"iii" are your initials.</li> <li>The Plate Assignment is specific to your instrument setup.</li> <li>The example worklists are included on the installation disk in the Support\Data folder.</li> </ul>		

Task 2. Submit and run multiple worklist-only studies

Task 2. Submitting a	and running mu	tiple worklist-on	v studies	(continued)

Steps	Detailed Instruction	s Comments
	Worklist-Only Study Wizard	
	Sector Work	list Import
		Example_Worklist1.wkd  C:\MassHurter\worklist  Generate data files in study  Copy methods in study
	5	Ah Test 1
	Plate Assignment Plates in ▶ P1	worklist Reassign None
	Submitter: p	fh 🗸
	Bac	k Next Finish Cancel
	Figure 25. The V	Norklist-Only Study Wizard - Worklist Import page

Task 2. Submit and run multiple worklist-only studies

s	Detailed Instructions Comments
teps	<ul> <li>I (optional) Mark the Quant Automation check box. If you mark the Quant Automation check box, then select the Quantitative Analysis Method.</li> <li>m (optional) Mark the Generate Report check box. If you mark this check box, select the Template File.</li> <li>n (optional) Mark the Print to default printer check box.</li> <li>o (optional) Mark the Publish check box. Select the file type to use.</li> <li>p Click Next.</li> </ul>
	Worklist-Only Study Wizard
	Worklist Quant       Image: Constraint of the second s
	Template File: C:\MassHunter\Report Templates\Quant\en-US\Letter\ESTD\Results_No
	Back Next Finish Cancel

Task 2. Submit and run multiple worklist-only studies

Detailed Instructions Comments			
<ul> <li>q Review the worklist in the Worklist-Only Study Wizard - Worklist page.</li> <li>r (optional) Right-click the box in the upper left corner and click Worklist Run Parameters. Change the Method Path. Fix any other problems. Click OK.</li> <li>r Click Finish.</li> <li>The Method Path is set to D:\ MassHunter\methods. If that is not the correct path, then right-click the upper left corner of the table and clice Worklist Run Parameters. Then, change the method path to the correct location and click OK.</li> </ul>			
Worklist-Only Study Wizard			
Sector Worklist			
▼         Inj Vol (µl)         Sample Name         Sample Position         Method         Data File           1         N As Method         Owned 1         Di Matoria         Di M			
1         ν         As Method         Sample1         P1-A1         PAH_Testm         test2.d           2         ν         As Method         Sample1         P1-A2         PAH_Testm         test3.d			
۲			
Worklist Back Net Finish Cancel			

Figure 27. Worklist-Only Study Wizard - Worklist page

Task 2. Submit and run multiple worklist-only studies

Steps	Detailed Instructions	Comments
3 Submit the second study. The second study uses the worklist Example_Worklist2.wkl.	<ul> <li>a Click the Submit icon, in the Ribbon.</li> <li>b (optional) Select Worklist-Only in the Select Study Creator dialog box. Clice OK.</li> <li>c Select GroupB.wkl as the Worklist fill</li> <li>d Type iii Test2.s as the first part of the Study Name.</li> <li>e Type iii as the Submitter.</li> <li>f Select the Plate Assignment.</li> <li>g Click Next.</li> <li>h Review the Worklist Quant page.</li> <li>i Click Next.</li> <li>j Review the worklist in the Worklist-Only Study Wizard - Worklist page.</li> <li>k (optional) Right-click the box in the upper left corner and click Worklist Run Parameters. Change the Method Path. Fix any other problems. Click OK.</li> <li>l Click Finish.</li> </ul>	<ul> <li>you start executing the first study in the Pending Studies table. As each</li> <li>study finishes, the next study is started. You can execute these four different worklists sequentially without having to individually start them.</li> </ul>
4 Submit the third study. The third study uses the Example_Worklist3.wkl.	<ul> <li>a Click the Submit icon, in the Ribbon.</li> <li>b (optional) Select Worklist-Only in the Select Study Creator dialog box. Clice OK.</li> <li>c Select GroupC.wkl as the Worklist find Type iii Test3.s as the first part of the Study Name.</li> <li>e Type iii as the Submitter.</li> <li>f Select the Plate Assignment.</li> <li>g Click Next.</li> <li>h Review the worklist in the Worklist-Only Study Wizard - Worklist page.</li> <li>i (optional) Right-click the box in the upper left corner and click Worklist Run Parameters. Change the Methor Path. Fix any other problems. Click OK.</li> <li>j Click Finish.</li> </ul>	sk le. st

Task 2. Submit and run multiple worklist-only studies

Steps			Detail	led Instructio	ns		Com	iments
Pending Studies	Completed Studies							
Name	Path	Submitter	Plate Assignment	Est. Study Duration	Est. Start Time	Sample Count		
1 PFH Test1.s	C:\MassHunter\	PFH	None	00:24.00		6		
2 PFH Test2.s 3 PFH Test3.s	C:\MassHunter\ C:\MassHunter\	PFH PFH	None None	00:24.00 00:24.00		6		
4 PFH Test4.s		PFH	None	00:24.00		6		
For Help, Press F1					Pending Str	udies: 4 NUM CA	PS SCRL	
Figure 28.	The Pendi	ng Studies	table with fo	our different s	tudies sub	mitted		
Queue.	ning the studie r studies will b		b Cli	ick the <b>Start</b> ic ick either <b>Sta</b> udy		in the Ribbon. I <b>me Stopped</b>	Pi	he first study is removed from the ending Studies table. The formation for this study is visible in he Current Study pane.
			MassHunter Stud	dy Manager			_ = X	
Home	Settings							
Start Stop	Running <sub>Status</sub>	Submit	(	Lock Help Console				The first study, PFH Test1
Stud	/ Execution	Study Submi	ssion Study Ac	tions Help				appears in the Current Study
Name: pfh Test 1_0212	212 s	Pat	n: <b>\MassHunter\studie</b>		Est	Time Remaining (	min)	pane.
Submitter:			e Assignment:		Lot.			<del>-</del>
pfh		P1				4		The second study that you
Status:								added, PFH Test2, is now
Acquisition: Ru	nning Sample P1-A1,	1 of 1					- I	the first study in the Pending
Pending Studies	Completed Studies							Studies table.
Name	Path	Submitter	Plate Assignment	Est. Study Duration	Est. Start Time	Sample Count		
1 pfh Test2_0	2121 C:\MassHunter\s.	pfh	P1	00:04.00	2/12/2012 7:05:	8 1		
2 _ pth lest3_0	2121 C:\MassHunter\s.	pfh	P1	00:04.00	2/12/2012 7:09:	5 I		
For Help, Press F1					Pending St	udies: 2 NUM CA	PS SCRL	
Figure 29.	Running th	an Study O			. onang or		2 Sont	1
i iyule 29.	nunning ti	ic Study Q	ucue					

Task 2. Submit and run multiple worklist-only studies

# Bioanalysis Study and Compliance

If User Management and Audit Trail or Compliance Mode is enabled, then the person submitting the study must be allowed to perform the following commands in the MassHunter Qualitative Analysis program:

#### **Group Batch Analysis**

- CmdNewBatchTable
- CmdImportSamplesFromWorklist
- CmdSaveBatchTable
- CmdCloseBatchTable
- CmdAnalyze

#### **Group Method Development**

- CmdImportMethodFromSample
- CmdImportMethodFromFile
- CmdImportMethodFromAcquisition (DDS)
- CmdSetMethodTargetCompoundAttribute
- CmdStartMethodEditing
- CmdSaveMethodAs
- CmdEndMethodEditing
- CmdRemoveMethodCalibration
- CmdAddMethodCalibration

#### **Group Report**

• GenerateReport

An easy way to implement this is to create a Group in Windows called Bioanalysis. Then, add all users that run Bioanalysis studies to that group. Then, using the ATM Configuration program, right-click the **Required User Role** box and add a role called Bioanalysis. Finally, for all of the commands listed, select them as ones someone in that user role can perform.

### In this guide

This Quick Start Guide describes how to use the MassHunter Study Manager software. This guide applies to MassHunter Data Acquisition for Triple Quad (Model K6460 and K6420) mass spectrometer.

For In Vitro Diagnostic Use

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