

# MassHunter Study Manager

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# 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 this product, five different studies can be created:

- Worklist-Only
- Worklist Import
- Bioanalysis
- Optimizer Automation
- Drug Discovery Screening

The Worklist-Only study and the Worklist Import study are the only Study Types supported with MassHunter Data Acquisition for Q-TOF and TOF.

## **Help**

**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

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

- “Home tab on the ribbon” on page 4
- “Settings tab on 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
- “Drug Discovery Screening Study Wizard” on page 17
- “Optimizer Automation Study Wizard” on page 19

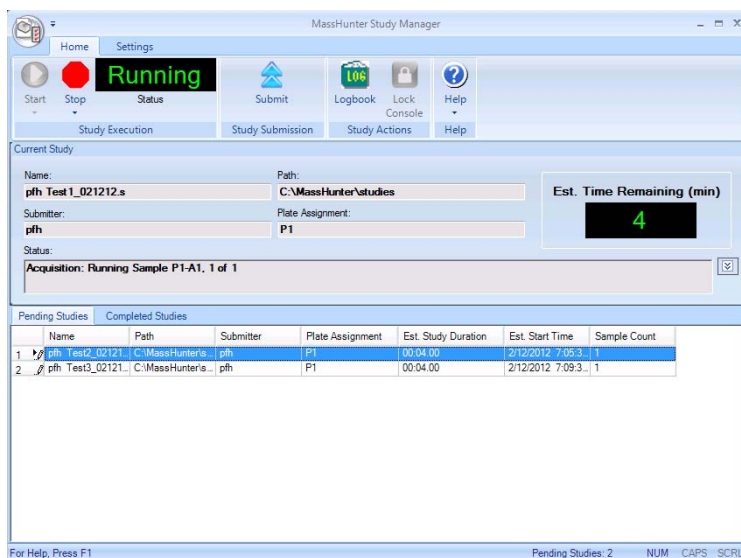


Figure 1. MassHunter Study Manager main window

## Home tab on the ribbon

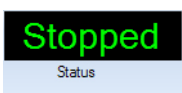
The following toolbar buttons are available on the MassHunter Study Manager toolbar:



**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 36. 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 23.



**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 26
- “To submit a **Worklist-Only study**” on page 28
- “To submit a **Bioanalysis study**” on page 30
- “To submit a **Drug Discovery Screening study**” on page 32
- “To submit an **Optimizer Automation study**” on page 34



**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 41.



**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

## User Interface

### Settings tab on the ribbon

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 of the current study. See “To lock the console” on page 42.



**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 on the ribbon

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

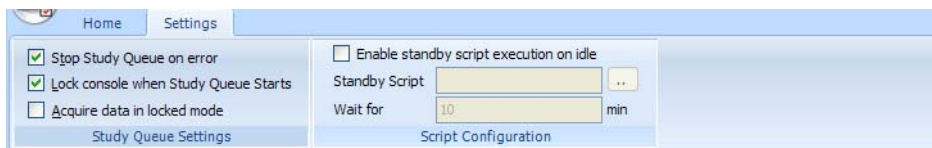
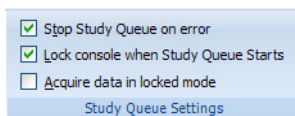


Figure 2. Settings Tab on the ribbon

### 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.

## User Interface

### Settings tab on the ribbon

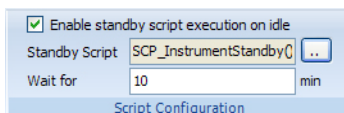
**Lock Console when Study Queue Starts** Toggles whether or not to automatically lock the console when you start the queue. If you lock the console, then no one can modify the method or the worklist in the Data Acquisition program while the study is running. The system automatically unlocks the console 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 **Lock Console**  on the Home tab. You should only unlock the console to make any required changes 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.



**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**.

## 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 36. 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.

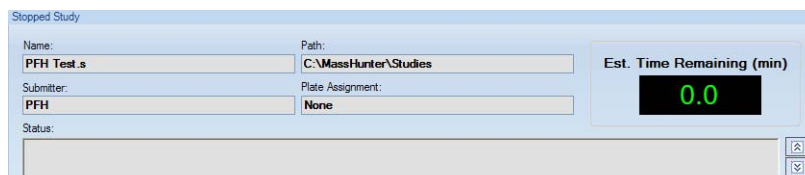


Figure 3. Current/Stopped Study Pane

## Pending Studies tab

On this tab, you can examine and rearrange the studies in the Pending Studies table. See **“To run a study”** on page 36 and **“To rearrange the pending studies in the Study Queue”** on page 40.

Pending Studies		Completed Studies					
	Name	Path	Submitter	Plate Assignment	Est. Study Duration	Est. Start Time	Sample Count
1	091310_Bioanalysis.s	C:\MassHunter\studi...	Your Name	P2	00:03.00	9/23/2010 1:56:5...	12
2	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 35.

	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	✔	Completed	1/4/2010 10:34:2...	1/4/2010 10:36:5...

Figure 5. Completed Studies tab



## Select Study Creator Dialog Box

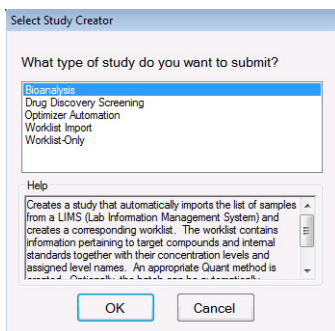
This dialog box appears when you click **Submit**  on the Home tab on the ribbon if you have enabled more than one study type. For more information on submitting a study, see:

- **“To submit a Worklist Import study”** on page 26
- **“To submit a Worklist-Only study”** on page 28

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

- **“To submit a Bioanalysis study”** on page 30
- **“To submit a Drug Discovery Screening study”** on page 32
- **“To submit an Optimizer Automation study”** on page 34

Study types are only available if they are enabled. See **“To enable a study using the Study Creator Enabler program”** on page 24. If you only have one Study type enabled, then this dialog box is not shown.



**Figure 6.** “Select Study Creator” Dialog Box for Triple Quadrupole Data Acquisition

## User Interface

### Study Worklist Import Study Wizard

The Worklist Import study and the Worklist-Only study are the only studies supported for Q-TOF and TOF instruments.

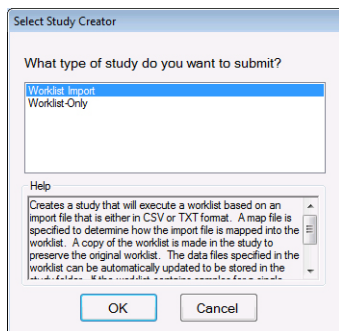


Figure 7. Select Study Creator Dialog Box for TOF/Q-TOF Data Acquisition software

## 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 28. This study is supported for QQQ, Q-TOF and TOF.

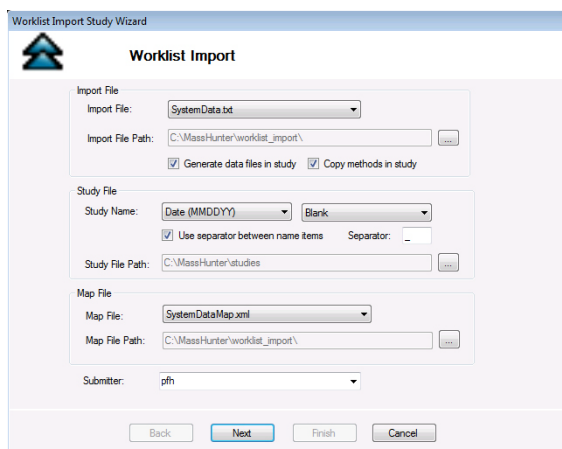
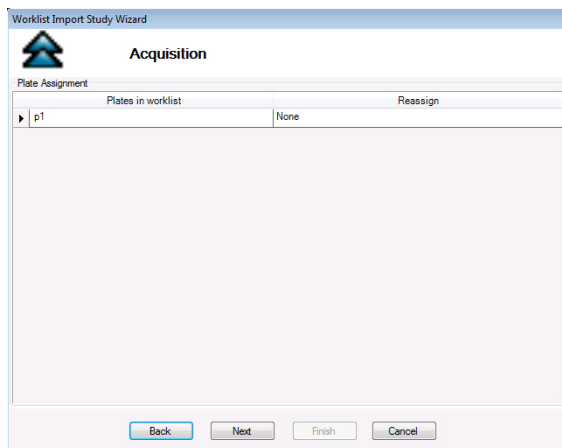


Figure 8. Worklist Import Study Wizard - Worklist Import page

## User Interface

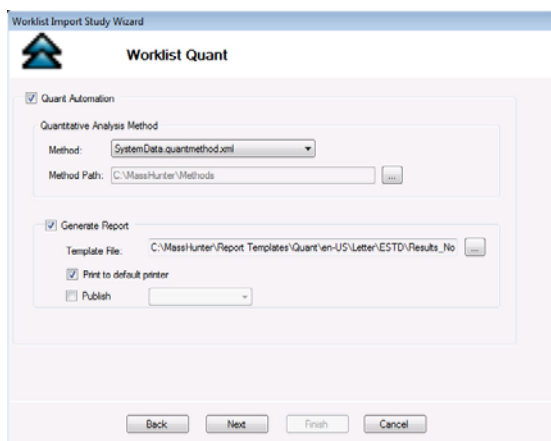
### Study Worklist Import Study Wizard

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



**Figure 9.** 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.



**Figure 10.** 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

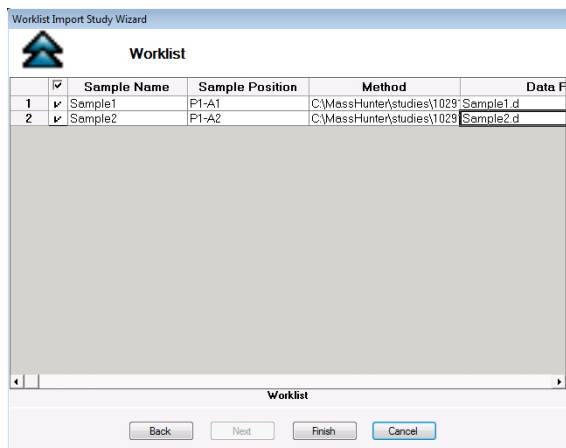


Figure 11. Worklist Import Study Wizard - Worklist page

## 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 28. This study is supported for QQQ, Q-TOF and TOF.

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

Plates in worklist	Reassign
P1	None

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

## User Interface

### Study Worklist-Only Study Wizard

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.

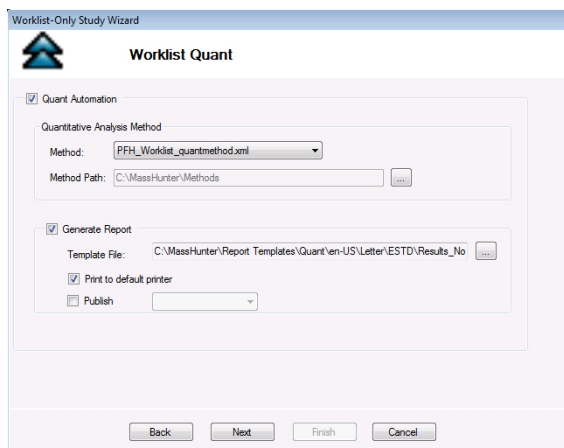


Figure 13. Worklist-Only Study Wizard - Worklist Quant page

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.

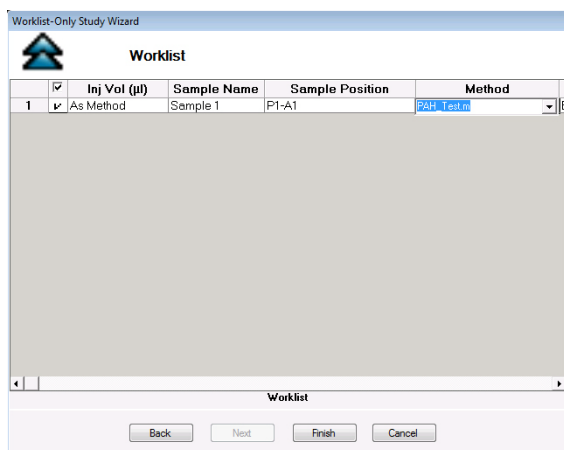


Figure 14. Worklist-Only Study Wizard - Worklist page

## 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 30. This wizard has four pages. A Bioanalysis Study has to have an internal standard.

This study type is not supported with the Q-TOF or TOF instruments.

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 24.

The four wizard pages are:

- Bioanalysis Study Wizard Import page(**Figure 15** on page 15)
- Bioanalysis Study Wizard Acquisition page(**Figure 16** on page 16)
- Bioanalysis Study Wizard Quantitation and Reporting page(**Figure 17** on page 16)
- Bioanalysis Study Wizard Worklist page (**Figure 13** on page 14)

The screenshot shows the 'Import' page of the Bioanalysis Study Wizard. The window title is 'Bioanalysis Study Wizard'. The page has a blue header with a blue arrow icon pointing up. Below the header, the title 'Import' is centered. The main area contains two sections: 'Import File' and 'Study File'. The 'Import File' section has a dropdown menu for 'Import File' with 'BioAnalysis\_Example.TXT' selected, and a text box for 'Import File Path' containing 'C:\MassHunter\worklist\_import\'. The 'Study File' section has a dropdown for 'Study Name' with 'Date (MMDDYY)' selected, a dropdown for 'Blank', a checked checkbox for 'Use separator between name items', a 'Separator' field, and a text box for 'Study File Path' containing 'C:\MassHunter\studies'. At the bottom, there is a 'Submitter' dropdown with 'pjh' selected. Below the form are four buttons: 'Back', 'Next', 'Finish', and 'Cancel'.

Figure 15. Bioanalysis Study Wizard - Import page

## User Interface

### Bioanalysis Study Wizard

The screenshot shows the 'Acquisition' page of the Bioanalysis Study Wizard. The window title is 'Bioanalysis Study Wizard'. The page is divided into three main sections: 'Sample Information', 'Data File', and 'Plate Assignment'.  
- **Sample Information:** Contains an 'Acquisition Method' section with a 'Method' dropdown set to 'Default.m' and a 'Method Path' text box containing 'C:\MassHunter\methods\' with a browse button.  
- **Data File:** Contains a 'Data File' section with three dropdowns: 'Date (YYYYMMDD)', 'Sample Name', and 'Counter'. Below these is a checked checkbox 'Use separator between name items' and a 'Separator' text box.  
- **Plate Assignment:** A table with two columns: 'Plates in worklist' and 'Reassign'.  
At the bottom, there are four buttons: 'Back', 'Next', 'Finish', and 'Cancel'.

Figure 16. Bioanalysis Study Wizard - Acquisition page

The screenshot shows the 'Quantitation and Reporting' page of the Bioanalysis Study Wizard. The window title is 'Bioanalysis Study Wizard'. The page is divided into two main sections: 'Quant Method Generation' and 'Result'.  
- **Quant Method Generation:** Contains three radio buttons: 'Reference Data File', 'Preliminary Quant Method', and 'Reference Data File by Calibration Level'. The third option is selected. Below it is a dropdown menu showing '1 = CmpdX:1'.  
- **Result:** Contains a checked checkbox 'Generate LIMS Output'.  
At the bottom, there are four buttons: 'Back', 'Next', 'Finish', and 'Cancel'.

Figure 17. Bioanalysis Study Wizard - Quantitation and Reporting page



## Drug Discovery Screening Study Wizard

The Drug Discovery Screening Study Wizard allows you to submit a study based upon an Excel .XLS or .XLSX file. This study type is not supported with the Q-TOF or TOF instruments.

The Drug Discovery Screening study type is only available if the study is enabled. See **“To enable a study using the Study Creator Enabler program”** on page 24.

The four wizard pages are:

- Drug Discovery Screening Study Wizard - Import page (**Figure 18** on page 17)
- Drug Discovery Screening Study Wizard - Acquisition page (**Figure 19** on page 18)
- Drug Discovery Screening Study Wizard - Optimize page (**Figure 20** on page 18)
- Drug Discovery Screening Study Wizard - Worklist page (**Figure 13** on page 14)

The screenshot shows the 'Import' page of the Drug Discovery Screening Study Wizard. The window title is 'Drug Discovery Screening Study Wizard'. The page is titled 'Import' and features a blue arrow icon. It contains three main sections: 'Import File' with fields for 'Import File' (DDS\_Example.xlsx) and 'Import File Path' (C:\MassHunter\worklist\_import\); 'Study File' with fields for 'Study Name' (Date (MMDDYY) and DDS), a checked 'Use separator between name items' checkbox, a 'Separator' field, and 'Study File Path' (C:\MassHunter\studies); and 'Map File' with fields for 'Map File' (DDS.xml) and 'Map File Path' (C:\MassHunter\Configuration\study\_creators\DDS\worklist\_imp). A 'Submitter' field is set to 'pjh'. At the bottom are 'Back', 'Next', 'Finish', and 'Cancel' buttons.

**Figure 18.** Drug Discovery Screening Study Wizard - Import page

## User Interface

### Drug Discovery Screening Study Wizard

The screenshot shows the 'Acquisition' page of the 'Drug Discovery Screening Study Wizard'. The window title is 'Drug Discovery Screening Study Wizard'. The page is divided into three main sections: 'Sample Information', 'Acquisition Method Parameters', and 'Plate Assignment'.  
1. 'Sample Information':  
- 'Acquisition Method': A dropdown menu showing 'Default.m'.  
- 'Method Path': A text box containing 'C:\MassHunter\methods\' and a browse button (...).  
2. 'Acquisition Method Parameters':  
- A checked checkbox 'Override Acquisition Dwell Time' with a spin box set to '50' and the unit 'ms'.  
- A spin box for 'Max. transitions per compound in method' set to '1'.  
3. 'Plate Assignment':  
- A table with two columns: 'Plates in worklist' and 'Reassign'.  
- A row with 'P1' in the first column and 'None' in the second column.  
At the bottom, there are four buttons: 'Back', 'Next', 'Finish', and 'Cancel'.

Figure 19. Drug Discovery Screening Study Wizard - Acquisition page

The screenshot shows the 'Optimize' page of the 'Drug Discovery Screening Study Wizard'. The window title is 'Drug Discovery Screening Study Wizard'. The page is divided into two main sections: 'Optimizer Input' and 'Validation errors'.  
1. 'Optimizer Input':  
- 'Optimizer Database': A text box containing 'C:\MassHunter\Databases\Optimizer' and a browse button (...).  
- 'Optimizer Project': A dropdown menu showing 'OptimizerProject1'.  
- 'Positive Method': A dropdown menu showing 'C:\MassHunter\Methods\Default.m'.  
- 'Negative Method': An empty dropdown menu.  
- A checked checkbox 'Re-optimize compounds optimized more than' with a spin box set to '1' and the unit 'day(s) ago'.  
- An 'Edit Optimization Parameters...' button.  
2. 'Validation errors':  
- An empty text box for displaying errors.  
At the bottom, there are four buttons: 'Back', 'Next', 'Finish', and 'Cancel'.

Figure 20. Drug Discovery Screening Study Wizard - Optimize page

## Optimizer Automation Study Wizard

The Optimizer Automation Study Wizard allows you to submit a study based upon an XLS or XLSX file. This study type is not supported with the Q-TOF or TOF instruments.

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 24.

The two wizard pages are:

- Optimizer Automation Study Wizard - Import page (**Figure 21** on page 19)
- Optimizer Automation Study Wizard - Optimize page (**Figure 19** on page 18)

Optimizer Automation Study Wizard

**Import**

Import File

Import File: ADME\_Optimizer\_Study\_07120-1.xls

Import File Path: C:\MassHunter\worklist\_import\

Study File

Study Name: Date (MMDDYY) Optimizer

Use separator between name items Separator: \_

Study File Path: C:\MassHunter\studies

Map File

Map File: OptimizerAutomation.xml

Map File Path: C:\MassHunter\Configuration\study\_creators\DDS\worklist\_imp

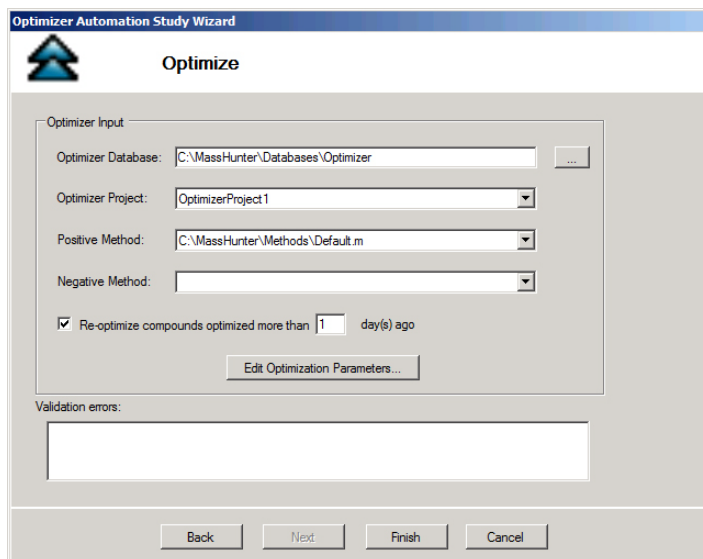
Submitter: Your Name

Back Next Finish Cancel

**Figure 21.** Optimizer Automation Study Wizard - Import page

## User Interface

### Optimizer Automation Study Wizard



The screenshot shows the 'Optimize' page of the 'Optimizer Automation Study Wizard'. The window title is 'Optimizer Automation Study Wizard'. The page features a blue header with a logo and the word 'Optimize'. Below the header is a section titled 'Optimizer Input' containing several fields: 'Optimizer Database' (text box with 'C:\MassHunter\Databases\Optimizer' and a browse button), 'Optimizer Project' (dropdown menu with 'OptimizerProject1'), 'Positive Method' (dropdown menu with 'C:\MassHunter-Methods\Default.m'), and 'Negative Method' (dropdown menu). There is a checked checkbox for 'Re-optimize compounds optimized more than 1 day(s) ago' and an 'Edit Optimization Parameters...' button. Below this is a 'Validation errors:' section with an empty text box. At the bottom are 'Back', 'Next', 'Finish', and 'Cancel' buttons.

Figure 22. Optimizer Automation Study Wizard - Optimize page

## Getting Started

### Basic Tasks

- [“To start the Study Manager program”](#) on page 22
- [“To exit the Study Manager program”](#) on page 23
- [“To enable a study using the Study Creator Enabler program”](#) on page 24
- [“To switch users when Compliance is enabled”](#) on page 25

### Submitting Studies

- [“To submit a Worklist Import study”](#) on page 26
- [“To submit a Worklist-Only study”](#) on page 28
- [“To submit a Bioanalysis study”](#) on page 30
- [“To submit a Drug Discovery Screening study”](#) on page 32
- [“To submit an Optimizer Automation study”](#) on page 34
- [“To resubmit a study from the Completed Studies tab”](#) on page 35

### Running a Study

- [“To run a study”](#) on page 36
- [“To stop the Study Queue”](#) on page 37

### Modifying the Pending Studies Table

- [“To delete a Pending Study”](#) on page 38
- [“To edit a worklist”](#) on page 39
- [“To rearrange the pending studies in the Study Queue”](#) on page 40

### Other Activities

- [“To select what occurs after an error happens”](#) on page 41
- [“To check the Logbook”](#) on page 41
- [“To use the keyboard to access the Ribbon”](#) on page 42
- [“To lock the console”](#) on page 42
- [“To add a standby script”](#) on page 43

## Basic Tasks

To start the Study Manager program

# Basic Tasks

## To start the Study Manager program

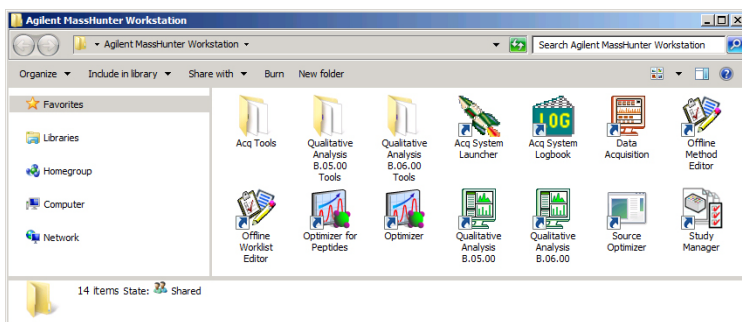
Follow this procedure to start the Study Manager program.


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.



- 2 Double-click the **Study Manager** icon ()


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

## Basic Tasks

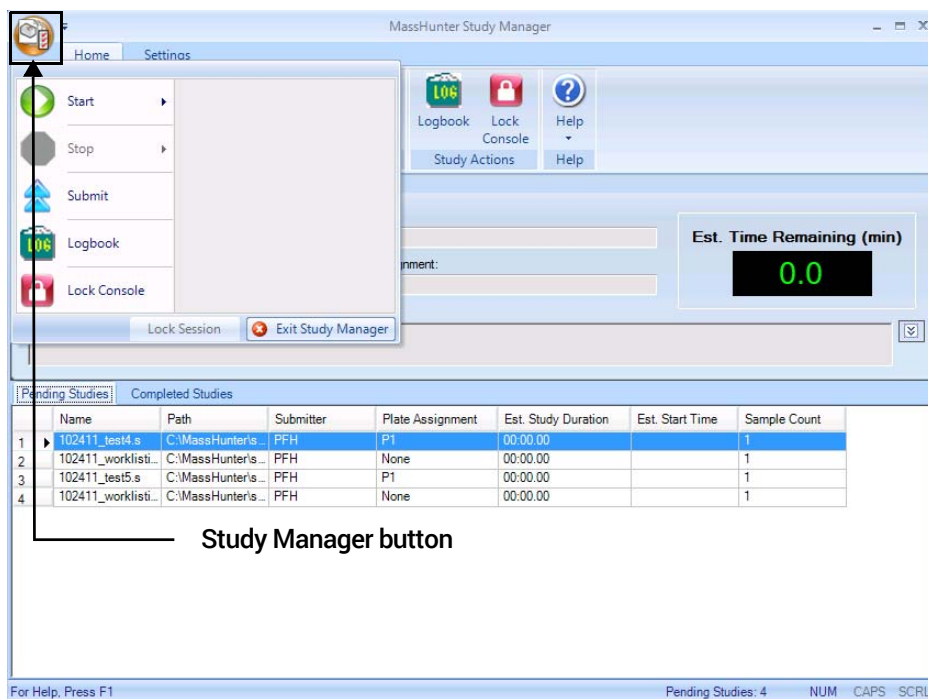
To exit the Study Manager program

# To exit the Study Manager program

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

- Click the  button 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.



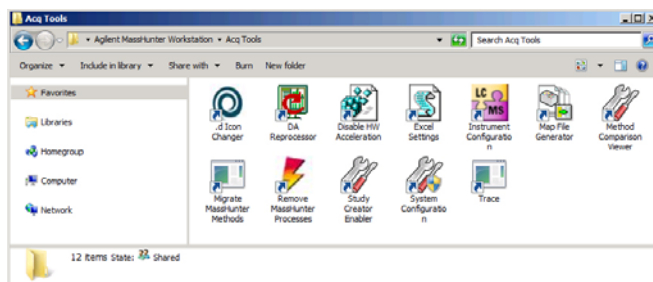
## Basic Tasks

To enable a study using the Study Creator Enabler program

# 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. NOTE: The **Disable HW Acceleration** program is only available with the TOF/Q-TOF Data Acquisition software.



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

## NOTE

Do not enable the **Bioanalysis** or the **Drug Discovery Screening** 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 the  button 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 the **OK** button.



## Basic Tasks

### To switch users when Compliance is enabled

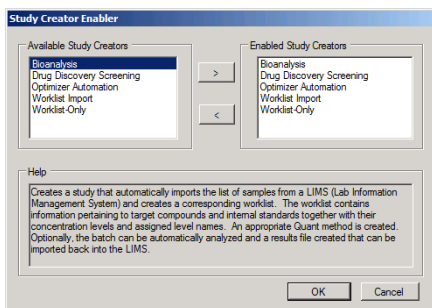




Figure 23. Study Creator Enabler Program

## To switch users when Compliance is enabled

You use the Compliance program 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 the  button 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 the **OK** button.

## Submitting a Study



To submit a Worklist Import study

# Submitting a Study

- “To submit a Worklist Import study” on page 26
- “To submit a Worklist-Only study” on page 28
- “To submit a Bioanalysis study” on page 30
- “To submit a Drug Discovery Screening study” on page 32
- “To submit an Optimizer Automation study” on page 34

## To submit a Worklist Import study

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

- 1 Click **Submit** () on 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 8** on page 10). The Worklist Import page is shown.
- 4 (optional) Change the **Import File Path**. Click the  button 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\1.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 is shown in the Pending Studies table in the Name column.

## Submitting a Study

To submit a Worklist Import study



- 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 the  button next to the Study File Path to change the path.
- 11 (optional) Change the **Map File Path**. Click the  button 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 is shown 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 9** 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 is shown as **In Use**. You can still select a plate that is shown **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 10** 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 11** 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.

## Submitting a Study

To submit a Worklist-Only study

### To submit a Worklist-Only study

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

- 1 Click **Submit** () on 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 12** on page 13). The Worklist Import page is shown.
- 4 (optional) Change the **Worklist File Path**. Click the  button 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\1.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 is shown 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 the  button 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 is shown as **In Use**. You can still select a plate that is shown **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

## Submitting a Study

### To submit a Worklist-Only study

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 is shown 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 13** 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 14** 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.





## Submitting a Study

To submit a Bioanalysis study

### 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  on 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 is shown (**Figure 15** on page 15)
- 4 (optional) Change the Import File Path. If the Import File is not in the folder that is shown, click the  button to change the path.
- 5 Select an Import File.
- 6 (optional) Change the Study File Path. Click the  button 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.
- 10 Click **Next**. The Bioanalysis Study Wizard - Acquisition page is shown (**Figure 16** on page 16).
- 11 (optional) Change the **Method Path**. If the method is not in the folder that is shown, click the  button 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.

## Submitting a Study

### To submit a Bioanalysis study

**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 is shown as **In Use**. You can still select a plate that is shown **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 is shown (**Figure 17** 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 is shown.

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





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

## Submitting a Study

To submit a Drug Discovery Screening study

### To submit a Drug Discovery Screening study

Follow this procedure to add a Drug Discovery Screening study to the queue. You can only submit a Drug Discovery Screening study for a Triple Quadrupole instrument.

- 1 Click **Submit**  on the ribbon. The “Select Study Creator” dialog box is opened.
- 2 Select **Drug Discovery Screening** as the study type.
- 3 Click OK. The Drug Discovery Screening Study Wizard is opened. (**Figure 18** on page 17) The Import page is shown.
- 4 (optional) Change the Import File Path. If the Import File is not in the folder that is shown, click the  button to change the path.
- 5 Select an Import File. The Import File for this study is an 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 is shown 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 two parts of the Study name in the **Separator** box.
- 8 (optional) Change the Study File Path. Click the  button 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 on this program.
- 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 Drug Discovery Screening Study Wizard - Acquisition page is shown (**Figure 19** on page 18).
- 12 (optional) Change the **Method Path**. If the method is not in the folder that is shown, click the  button to change the path.
- 13 Select a **Method**.



## Submitting a Study

### To submit a Drug Discovery Screening study





- 14 (optional) Mark the **Override Acquisition Dwell Time** check box. If you mark this check box, then select the dwell time to use for the MRM transitions in the acquisition method in the worklist.
- 15 Select the **Max. transitions per compound in method** value. The maximum number of MRM transitions to have for each compound in the optimized acquisition method. The number of transitions stored in the database per compound may be larger than this number.
- 16 Select the **Plate Assignment**. The combo box shows all plates that are available. If the plate is already in the Study Queue, then it is shown as **In Use**. You can still select a plate that is shown **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.
- 17 Click **Next**. The Drug Discovery Screening Study Wizard - Optimize page is shown (**Figure 20** on page 18).
- 18 Select the **Optimizer Database**. If there are no projects in the Optimizer Database, click **Edit Optimization Parameters** to set up a project in the MassHunter Optimizer program.
- 19 Select the **Optimizer Project**.
- 20 Select the **Positive Method** and/or the **Negative Method**. You must select at least one of these methods. If there are no methods in a project, click **Edit Optimization Parameters** to start the MassHunter Optimizer program. Then, add one or more methods to the project.
- 21 (optional) Mark the **Re-optimize compounds optimized more than X day(s) ago**. 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.
- 22 Click **Next**. If an error exists in the Optimizer project, the errors are listed in the Validation errors section. To fix any errors in the optimization settings, 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 the Drug Discovery Screening Study Wizard - Worklist page is shown.
- 23 Review the worklist for this study. Make any necessary changes.
- 24 Click **Finish**. The study is submitted to the Pending Studies table.

## Submitting a Study

To submit an Optimizer Automation study

### To submit an Optimizer Automation study

Follow this procedure to add a study to the queue. You can only submit an Optimizer Automation study for a Triple Quadrupole instrument.

- 1 Click **Submit** (  ) on 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 is shown. (Figure 21 on page 19)
- 4 (optional) Change the Import File Path. If the **Import File** is not in the folder that is shown, click the  button 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 is shown 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 Drug Discovery Screening Study Wizard - Optimize page (Figure 22 on page 20) is shown.
- 12 (optional) Change the **Optimizer Database**. To change the selected Optimizer Database, click the  button 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 the **Edit Optimization Parameters** button 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.

## Starting and Stopping the Study Queue

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 **Start** () on the Home tab on 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 **Stop** () on the Home tab on 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.

## Modifying the Pending Studies Table

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 40

## 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 26
  - “**To submit a Worklist-Only study**” on page 28
  - “**To submit a Bioanalysis study**” on page 30
  - “**To submit a Drug Discovery Screening study**” on page 32
  - “**To submit an Optimizer Automation study**” on page 34
- 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.

## Modifying the Pending Studies Table

To edit a worklist

### 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 the **Save** button.

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.

## Modifying the Pending Studies Table

To rearrange the pending studies in the Study Queue

### 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 26
  - “**To submit a Worklist-Only study**” on page 28
  - “**To submit a Bioanalysis study**” on page 30
  - “**To submit a Drug Discovery Screening study**” on page 32
  - “**To submit an Optimizer Automation study**” on page 34
- 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 42
- “To lock the console” on page 42
- “To add a standby script” on page 43

## To select what occurs after an error happens


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

- 1 Click the **Settings** tab on the ribbon. The Study Settings tab on the ribbon is shown (“**Settings tab on 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 on the ribbon. The Home Tab on the ribbon is shown.
- 2 Click **Logbook**  in the **Study Actions** section on the Home tab.

## Other actions

### To use the keyboard to access the Ribbon

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 on 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 on 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 on the ribbon. The Study Home Tab on the ribbon is shown.
- 2 Click the **Lock Console** icon on the ribbon.

## Other actions

### To add a standby script

## 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 on the ribbon. The “**Settings tab on the ribbon**” on page 5 is shown.
- 2 Mark the **Enable standby script execution on idle** check box under Script Configuration.
- 3 Click the  button 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.

## Familiarization Exercise



### 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. Submit and run 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).	<p><b>a</b> Double-click the Agilent MassHunter Study Manager icon, .</p> <p><b>b</b> Right-click any line in the Pending Studies table, and then click <b>Delete</b>.</p>	<ul style="list-style-type: none"><li>• Before deleting any studies from the Pending Studies table, make sure that no one else is using the system.</li></ul>
2 Copy the example files in the Support\Data folder to the MassHunter folder.	<p><b>a</b> Copy <i>SystemData.txt</i> to the \MassHunter\worklist_import folder.</p> <p><b>b</b> Copy <i>SystemDataMap.xml</i> to the \MassHunter\StudyExamples folder.</p>	
3 Submit the Worklist Import study.	<p><b>a</b> Click the <b>Submit</b> icon, , on the ribbon.</p> <p><b>b</b> (optional) Select <b>Worklist Import</b> in the <b>Select Study Creator</b> dialog box. Click <b>OK</b>.</p> <p><b>c</b> Select <b>SystemData.txt</b> as the <b>Import File</b>. Change the <b>Import File Path</b> if necessary.</p> <p><b>d</b> (optional) Mark the <b>Generate data files in study</b> check box.</p> <p><b>e</b> (optional) Mark the <b>Copy methods in study</b> check box.</p> <p><b>f</b> Select <b>Date (MMDDYY)</b> as the first part of the Study Name.</p> <p><b>g</b> Select <b>Custom Name</b> as the second part of the Study Name.</p> <p><b>h</b> Then type <i>iii Test1</i> in the <b>Study Name</b>.</p> <p><b>i</b> Type <i>iii</i> as the <b>Submitter</b>.</p> <p><b>j</b> Click Next.</p>	<ul style="list-style-type: none"><li>• If you enabled another study type, then you first need to select the type of study. See <b>“To enable a study using the Study Creator Enabler program”</b> on page 24.</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 <b>Support\Data</b> folder.</li></ul>

## Familiarization Exercise

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

Task 1. Submit and run a Worklist Import study (continued)

Steps	Detailed Instructions	Comments
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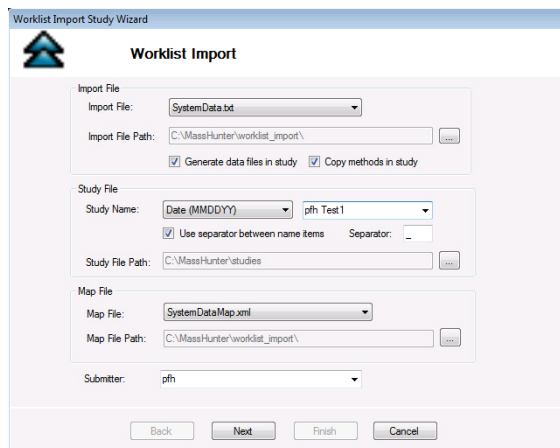


Figure 24. The Worklist Import Study Wizard - Worklist Import page

- k (optional) Reassign the Plates in worklist.
- l Click Next.

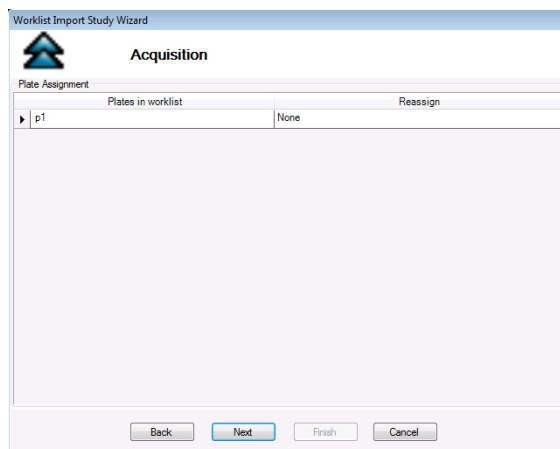


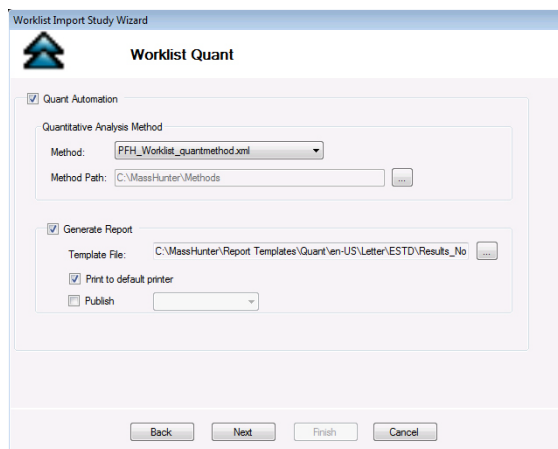
Figure 25. The Worklist Import Study Wizard - Acquisition page

## Familiarization Exercise

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

Task 1. Submit and run a Worklist Import study (continued)

Steps	Detailed Instructions	Comments
	<p><b>m</b> (optional) Mark the <b>Quant Automation</b> check box.</p> <p><b>n</b> If you mark the <b>Quant Automation</b> check box, then select the <b>Quantitative Analysis Method</b>.</p> <p><b>o</b> (optional) Mark the <b>Generate Report</b> check box. If you mark this check box, select the <b>Template File</b>.</p> <p><b>p</b> (optional) Mark the <b>Print to default printer</b> check box.</p> <p><b>q</b> (optional) Mark the <b>Publish</b> check box. Select the file type to use.</p> <p><b>r</b> Click the Next button.</p>	



**Figure 26.** The Worklist Import Study Wizard - Worklist Quant page

- s** Review the worklist in the Worklist Import Study Wizard - Worklist page.
- 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**.
- u** Click **Finish**.
- You need to enter the **Sample Position**, **Method** and **Data File** for each of the three samples.

## Familiarization Exercise

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

Task 1. Submit and run a Worklist Import study (continued)

Steps	Detailed Instructions	Comments
-------	-----------------------	----------

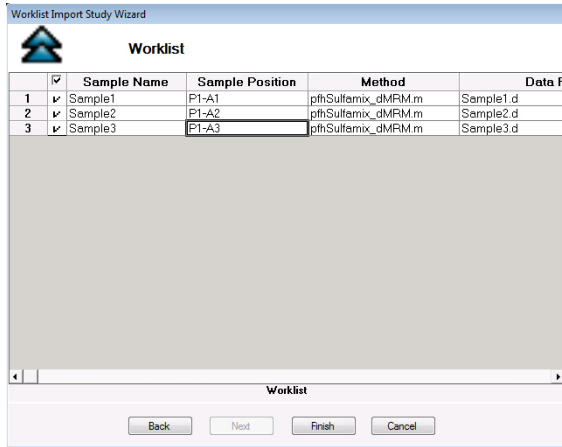



Figure 27. Worklist Import Study Wizard - Worklist page

- 4 Start running the study in the Study Queue.
- Click the **Start** icon,  , on the ribbon.
  - Click either **Start** or **Resume Stopped Study**.
- The study is removed from the Pending Studies table. The information for this study is visible in the Current Study pane.

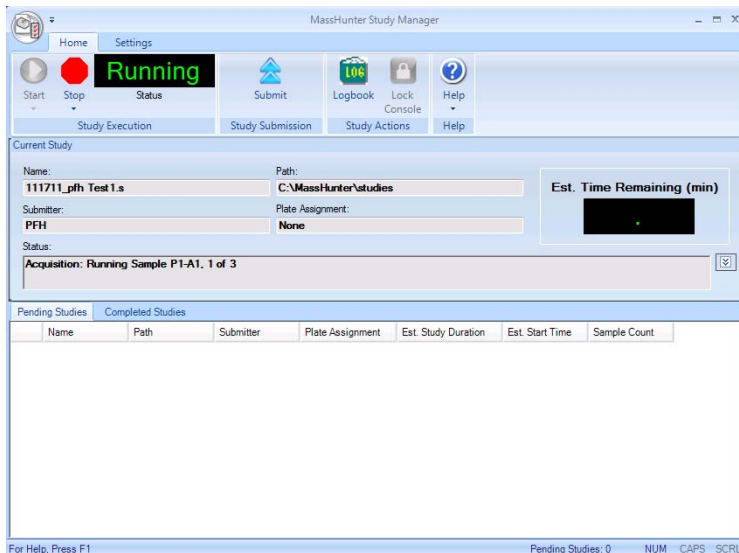


Figure 28. Running the Study Queue

The study is removed from the Pending Studies queue, and it becomes the Current Study. If you add another study, it is added to the Pending Studies queue and started when the Current Study completes.



## Familiarization Exercise

### 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 (sulfa drugs) and contain three dilutions (level 1 to 3). You can rename the method that was used for the Triple Quad Familiarization Guide exercises to the method used in these worklists.

#### Task 2. Submitting and running multiple worklist-only studies

Steps	Detailed Instructions	Comments
1 Open the Study Manager program and clear the items in the Pending Studies table (if necessary).	<p><b>a</b> Double-click the Agilent MassHunter Study Manager icon. </p> <p><b>b</b> Right-click any line in the Pending Studies table, and then click <b>Delete</b>.</p>	<ul style="list-style-type: none"><li>• Before deleting any studies from the Pending Studies table, make sure that no one else is using the system.</li></ul>
2 Submit the first study. <ul style="list-style-type: none"><li>• This study is a worklist-only study using the worklist GroupA.wkl.</li></ul>	<p><b>a</b> Click <b>Submit</b>, , on the ribbon.</p> <p><b>b</b> (optional) Select <b>Worklist-Only</b> in the Select Study Creator dialog box. Click <b>OK</b>.</p> <p><b>c</b> Select <b>Example_Worklist1.wkl</b> as the Worklist file. Change the Worklist File Path if necessary.</p> <p><b>d</b> (optional) Mark the <b>Generate data files in study</b> check box.</p> <p><b>e</b> (optional) Mark the <b>Copy methods in study</b> check box.</p> <p><b>f</b> Select <b>Custom</b> as the first part of the Study Name.</p> <p><b>g</b> Then type <i>iii</i> Test1 in the <b>Study Name</b>.</p> <p><b>h</b> Select <b>Date (MMDDYY)</b> as the second part of the Study Name.</p> <p><b>i</b> Type <i>iii</i> as the <b>Submitter</b>.</p> <p><b>j</b> (optional) Select the Plate Assignment.</p> <p><b>k</b> Click <b>Next</b>.</p>	<ul style="list-style-type: none"><li>• If you enabled another study type, then you first need to select the type of study. See <b>"To enable a study using the Study Creator Enabler program"</b> on page 24.</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 <b>Support\Data</b> folder.</li></ul>



## Familiarization Exercise

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

Task 2. Submitting and running multiple worklist-only studies (continued)

Steps	Detailed Instructions	Comments
-------	-----------------------	----------

Worklist-Only Study Wizard

### Worklist Import

**Worklist File**

Worklist File: Example\_Worklist1.wkd

Worklist File Path: C:\MassHunter\worklists\

Generate data files in study  Copy methods in study

**Study File**

Study Name: pfh Test 1 Date (MMDDYY)

Use separator between name items Separator: -

Study File Path: C:\MassHunter\studies

**Plate Assignment**

	Plates in worklist	Reassign
▶ P1		None

Submitter: pfh

Back Next Finish Cancel

Figure 29. The Worklist-Only Study Wizard - Worklist Import page

## Familiarization Exercise

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

Task 2. Submitting and running multiple worklist-only studies (continued)

Steps	Detailed Instructions	Comments
	<p><b>l</b> (optional) Mark the <b>Quant Automation</b> check box. If you mark the <b>Quant Automation</b> check box, then select the <b>Quantitative Analysis Method</b>.</p> <p><b>m</b> (optional) Mark the <b>Generate Report</b> check box. If you mark this check box, select the <b>Template File</b>.</p> <p><b>n</b> (optional) Mark the <b>Print to default printer</b> check box.</p> <p><b>o</b> (optional) Mark the <b>Publish</b> check box. Select the file type to use.</p> <p><b>p</b> Click the Next button.</p>	<ul style="list-style-type: none"><li>You do not have to run the Quant Automation. If you do mark this check box, then you must select a Quantitative Analysis method.</li></ul>

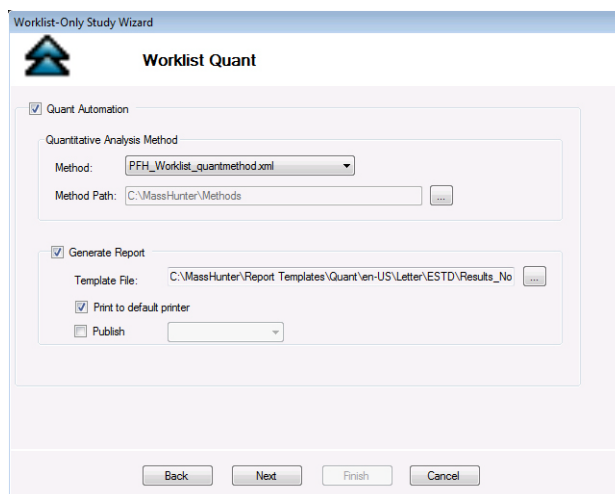


Figure 30. The Worklist-Only Study Wizard - Worklist Import page

## Familiarization Exercise

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

Task 2. Submitting and running multiple worklist-only studies (continued)

Steps	Detailed Instructions	Comments
	<p>q Review the worklist in the Worklist-Only Study Wizard - Worklist page.</p> <p>r (optional) Right-click the box in the upper left corner and click <b>Worklist Run Parameters</b>. Change the <b>Method Path</b>. Fix any other problems. Click <b>OK</b>.</p> <p>s Click <b>Finish</b>.</p>	<ul style="list-style-type: none"><li>The Method Path is set to <b>D:\MassHunter\methods</b>. If that is not the correct path, then right-click the upper left corner of the table and click <b>Worklist Run Parameters</b>. Then, change the method path to the correct location and click <b>OK</b>.</li></ul>

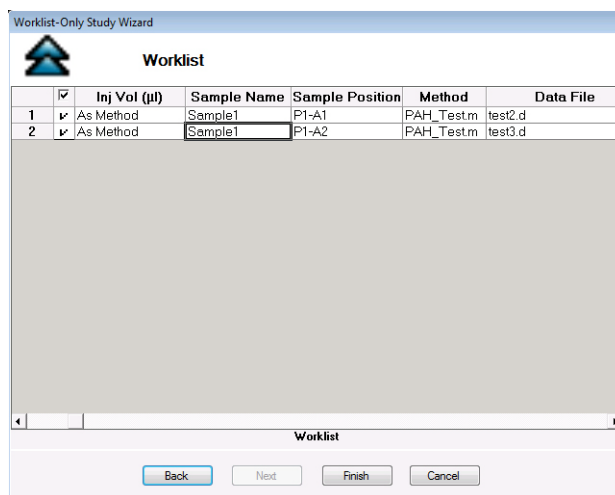




Figure 31. Worklist-Only Study Wizard - Worklist page

## Familiarization Exercise

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

Task 2. Submitting and running multiple worklist-only studies (continued)

Steps	Detailed Instructions	Comments
<p>3 Submit the next two studies.</p> <ul style="list-style-type: none"> <li>The second study uses the worklist Example_Worklist2.wkl.</li> <li>The third study uses the Example_Worklist3.wkl.</li> </ul>	<p><b>a</b> Click the <b>Submit</b> icon, , on the ribbon.</p> <p><b>b</b> (optional) Select <b>Worklist-Only</b> in the Select Study Creator dialog box. Click <b>OK</b>.</p> <p><b>c</b> Select <b>GroupB.wkl</b> as the Worklist file.</p> <p><b>d</b> Type <code>iii Test2.s</code> as the first part of the <b>Study Name</b>.</p> <p><b>e</b> Type <code>iii</code> as the <b>Submitter</b>.</p> <p><b>f</b> Select the <b>Plate Assignment</b>.</p> <p><b>g</b> Click <b>Next</b>.</p> <p><b>h</b> Review the <b>Worklist Quant</b> page.</p> <p><b>i</b> Click <b>Next</b>.</p> <p><b>j</b> Review the worklist in the Worklist-Only Study Wizard - Worklist page.</p> <p><b>k</b> (optional) Right-click the box in the upper left corner and click <b>Worklist Run Parameters</b>. Change the <b>Method Path</b>. Fix any other problems. Click <b>OK</b>.</p> <p><b>l</b> Click <b>Finish</b>.</p>	<ul style="list-style-type: none"> <li>Study Manager lets you put many different studies in the Pending Studies table. When you click <b>Start</b>, you start executing the first study in the Pending Studies table. As each study finishes, the next study is started. You can execute these four different worklists sequentially without having to individually start them.</li> </ul>
	<p><b>a</b> Click the <b>Submit</b> icon, , on the ribbon.</p> <p><b>b</b> (optional) Select <b>Worklist-Only</b> in the Select Study Creator dialog box. Click <b>OK</b>.</p> <p><b>c</b> Select <b>GroupC.wkl</b> as the Worklist file.</p> <p><b>d</b> Type <code>iii Test3.s</code> as the first part of the <b>Study Name</b>.</p> <p><b>e</b> Type <code>iii</code> as the <b>Submitter</b>.</p> <p><b>f</b> Select the <b>Plate Assignment</b>.</p> <p><b>g</b> Click <b>Next</b>.</p> <p><b>h</b> Review the worklist in the Worklist-Only Study Wizard - Worklist page.</p> <p><b>i</b> (optional) Right-click the box in the upper left corner and click <b>Worklist Run Parameters</b>. Change the <b>Method Path</b>. Fix any other problems. Click <b>OK</b>.</p> <p><b>j</b> Click <b>Finish</b>.</p>	<ul style="list-style-type: none"> <li>This section describes submitting the third study.</li> </ul>

## Familiarization Exercise

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


Task 2. Submitting and running multiple worklist-only studies (continued)

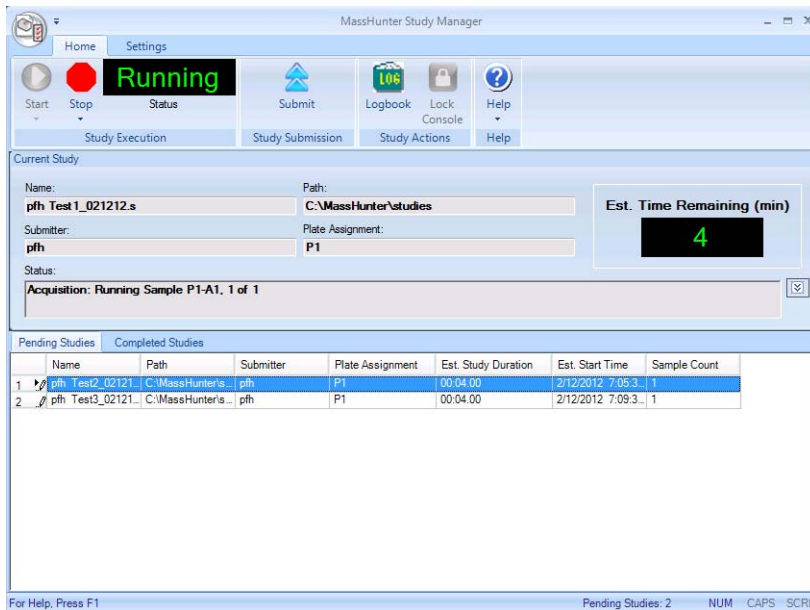
Steps	Detailed Instructions	Comments
-------	-----------------------	----------

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	C:\MassHunter\...	PFH	None	00:24.00		6
3	PFH Test3.s	C:\MassHunter\...	PFH	None	00:24.00		6
4	PFH Test4.s	C:\MassHunter\...	PFH	None	00:24.00		6

For Help, Press F1 Pending Studies: 4 NUM CAPS SCRL

**Figure 32.** The Pending Studies table with four different studies submitted

- |   |  |   |   |
|---|--|---|---|
| <p><b>4</b> Start running the studies in the Study Queue.</p> <ul style="list-style-type: none"> <li>All four studies will be run.</li> </ul> | <p><b>a</b> Click <b>Start</b>, on the ribbon.</p> <p><b>b</b> Click either <b>Start</b> or <b>Resume Stopped Study</b>.</p> |  | <ul style="list-style-type: none"> <li>The first study is removed from the Pending Studies table. The information for this study is visible in the Current Study pane.</li> </ul> |
|---|--|---|---|



The screenshot shows the MassHunter Study Manager interface. The 'Running' status is highlighted in green. The 'Current Study' pane shows details for 'pFH Test1\_021212.s', including its path, submitter, and plate assignment. The 'Est. Time Remaining (min)' is shown as 4. The 'Pending Studies' table at the bottom shows that the first study (PFH Test1.s) has been removed, and the second study (pFH Test2\_021212.s) is now the first in the queue.

Pending Studies		Completed Studies					
	Name	Path	Submitter	Plate Assignment	Est. Study Duration	Est. Start Time	Sample Count
1	pFH Test2_021212.s	C:\MassHunter\...	pFH	P1	00:04.00	2/12/2012 7:05:3...	1
2	pFH Test3_021212.s	C:\MassHunter\...	pFH	P1	00:04.00	2/12/2012 7:09:3...	1

For Help, Press F1 Pending Studies: 2 NUM CAPS SCRL

The first study, PFH Test1 is shown in the Current Study pane.

The second study that you added, PFH Test2, is now the first study in the Pending Studies table.

**Figure 33.** Running the Study Queue

## Familiarization Exercise

### Task 3. Submit a Bioanalysis Study

## Task 3. Submit a Bioanalysis Study

You can submit a study to the Pending Studies table based upon a LIMS input file. The input file is a text file created using a LIMS system. The output file is also a text file, but it is created by the MassHunter Quantitative Analysis program which is started automatically by the Study Manager program.

This output file can be loaded back into a LIMS system.

See **“To submit a Bioanalysis study”** on page 30.

## Task 4. Submit a Drug Discovery Screening Study

You can submit a study of multiple sample groups to be run in a single batch by reading an Excel spreadsheet. Each sample group can have a different set of compounds. An optimized acquisition method will be created for each sample group and used during data acquisition. A batch will be created for the samples in the study and a Quantitative Analysis method will be automatically created and applied to the batch after all samples are acquired.

See **“To submit a Drug Discovery Screening study”** on page 32.

## Task 5. Submit an Optimizer Automation Study

Optimization is also done as part of the Drug Discovery Screening study.

See **“To submit an Optimizer Automation study”** on page 34

# Bioanalysis Study and Compliance

If Compliance is enabled, then the person submitting the study must be allowed to perform the following user roles:

## 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 TOF/Q-TOF B.05.01 and Data Acquisition for Triple Quad LC/MS B.06.00 or higher until superseded.



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