MassHunter Study Manager for Ultivo LC/TQ

Quick Start Guide

What is MassHunter Study Manager?

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, four different studies can be created:

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

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.

Documents

Agilent Bioanalysis Workflow Guide This guide shows you how to submit a Bioanalysis study.

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 8
- **"Study Worklist-Only Study Wizard"** on page 12
- **"Bioanalysis Study Wizard"** on page 14
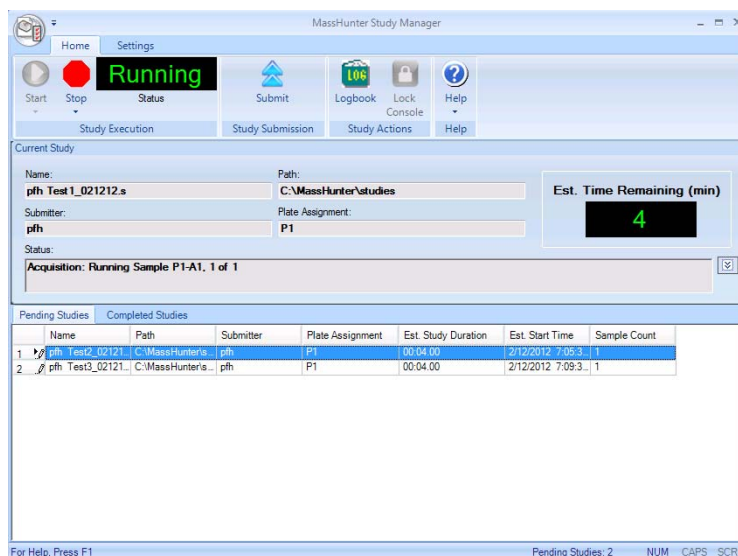- **"Optimizer Automation Study Wizard"** on page 16

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 31. 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 20.
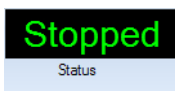
Status   Shows the state of the Study Queue. It can be **Stopped**, **Stopping**, **Running** or **Idle**. The state is **Stopped** if a user directly stopped the queue or the study encountered an error (and the **Stop Study Queue on error** check box is marked.) The state is **Stopping** if a user clicks 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 Ultivo LC/TQ. You can submit the following studies:

- **"To submit a Worklist Import study"** on page 23
- **"To submit a Worklist-Only study"** on page 25
- **"To submit a Bioanalysis study"** on page 27
- **"To submit an Optimizer Automation study"** on page 29

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 of the current study. See "To lock the console" on page 36.

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

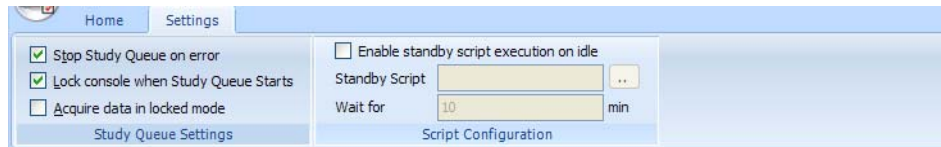The following toolbar buttons are available in the Settings tab in the Ribbon in the MassHunter Study Manager:

Figure 2   Settings Tab in the Ribbon
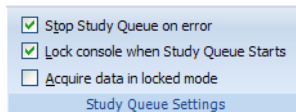
Study Queue Settings

Figure 3

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 Start   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 unlock the console only 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 when Study 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.
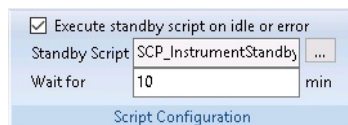
Figure 4   Script configuration options

Execute standby script on idle or error   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 31. 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.
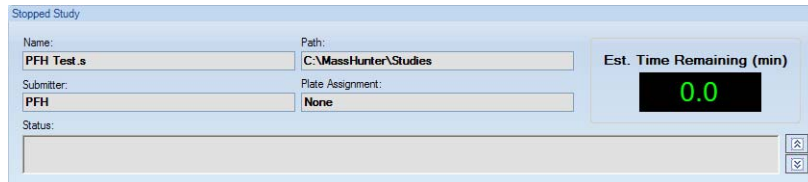
Figure 5   Current/Stopped Study Pane

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 31 and **"To rearrange the pending studies in the Study Queue"** on page 34.

Figure 6   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 30.

Figure 7   Completed Studies tab

Select Study Creator Dialog Box

This dialog box appears when you click the **Submit** icon ( )in the Home tab in the Ribbon if you have enabled more than one study type. For more information on submitting a study, see:
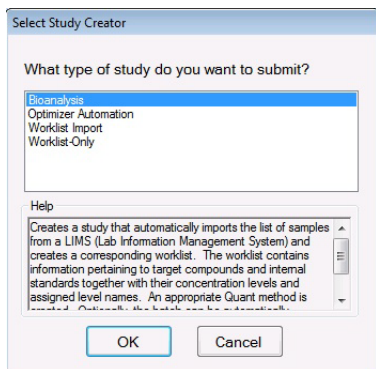
- **"To submit a Worklist Import study"** on page 23
- **"To submit a Worklist-Only study"** on page 25

The following study types are only available for an **Ultivo LC/TQ** Data Acquisition system.

- **"To submit a Bioanalysis study"** on page 27
- **"To submit an Optimizer Automation study"** on page 29

Study types are only available if they are enabled. See **"To enable a study using the Study Creator Enabler program"** on page 21. If you only have one Study type enabled, then this dialog box is not shown.
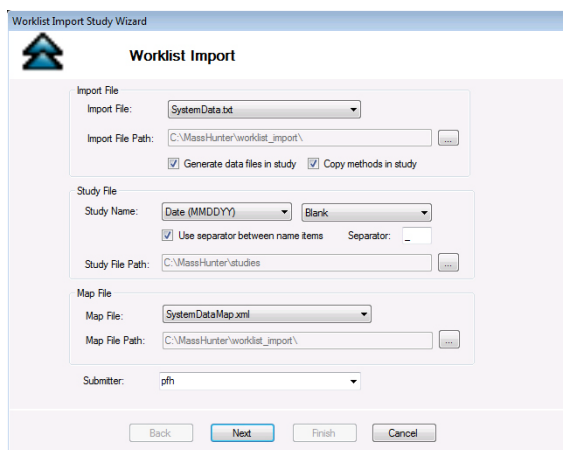
Figure 8 "Select Study Creator" Dialog Box for Ultivo LC/TQ Data Acquisition
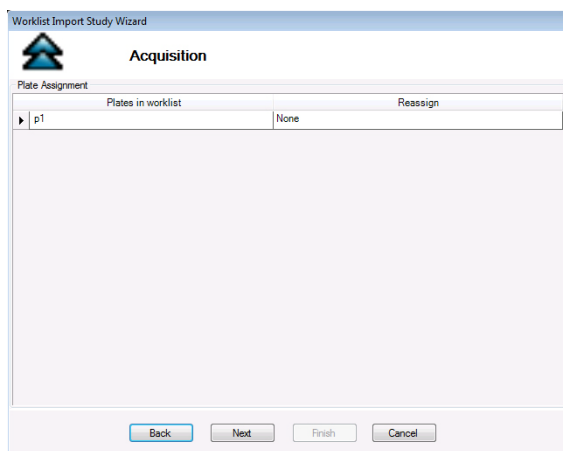
Study Worklist Import Study Wizard

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 Import study"** on page 23.

Figure 9   Worklist Import Study Wizard - Worklist Import page

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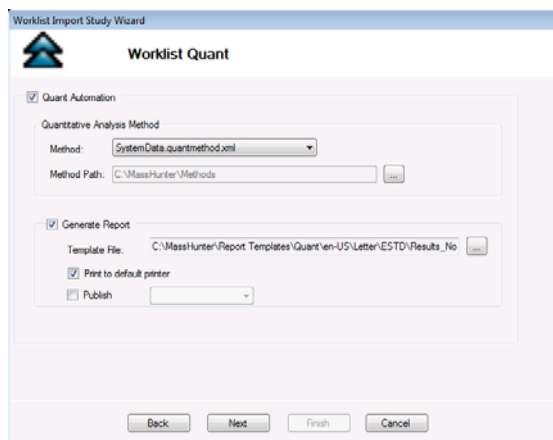

Figure 10   Worklist Import Study Wizard - Acquisition page

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 11   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.

Figure 12   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 25.

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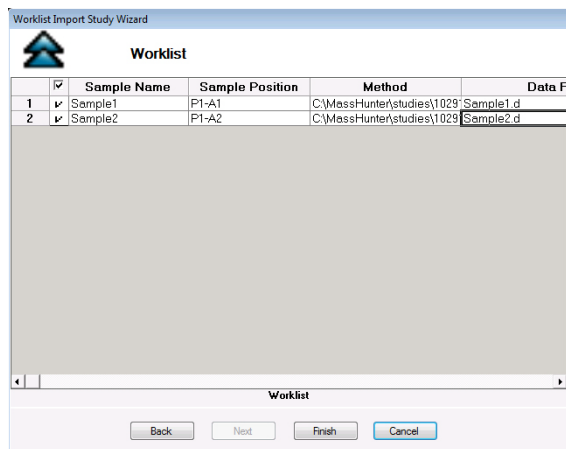

Figure 13   Worklist-Only Study Wizard - Worklist Import page

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.
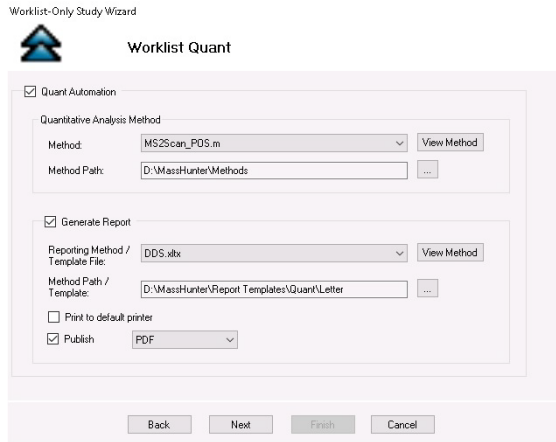
Figure 14   Worklist-Only Study Wizard - Worklist Quant page

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.
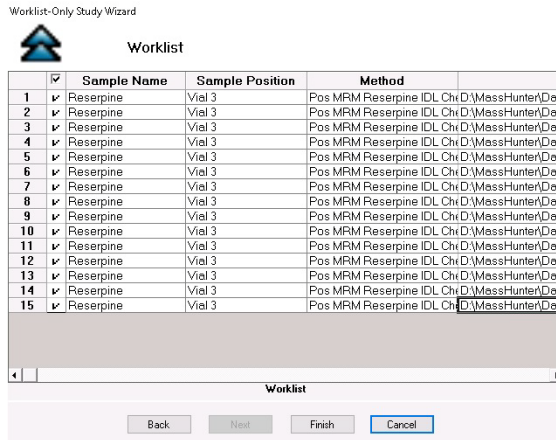
Figure 15   Worklist-Only Study Wizard - Worklist page

Bioanalysis Study Wizard
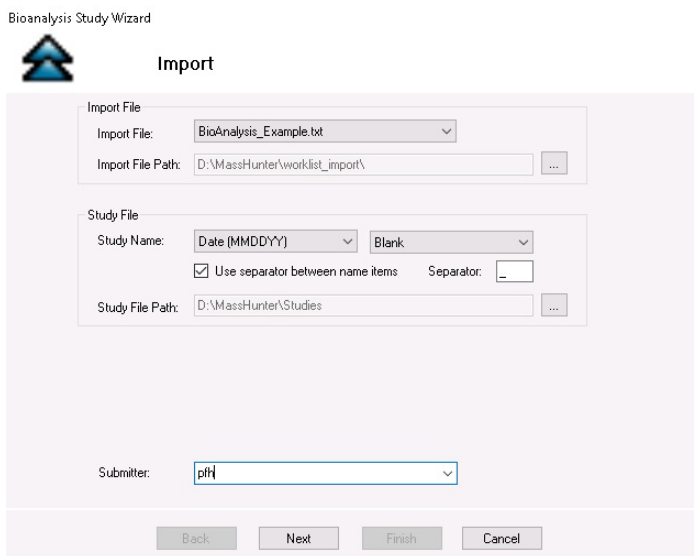
The Bioanalysis Study Wizard allows you to submit a worklist based upon a Bioanalysis input file. See **"To submit a Bioanalysis study"** on page 27. This wizard has four pages. A Bioanalysis Study has to have an internal standard.

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 21.

The four wizard pages are:

- Bioanalysis Study Wizard Import page(**Figure 16** on page 14)
- Bioanalysis Study Wizard Acquisition page(**Figure 17** on page 15)
- Bioanalysis Study Wizard Quantitation and Reporting page(**Figure 18** on page 15)
- Bioanalysis Study Wizard Worklist page (**Figure 14** on page 13)

Figure 16   Bioanalysis Study Wizard - Import page

Figure 17   Bioanalysis Study Wizard - Acquisition page

Figure 18   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 21.

The two wizard pages are:

- Optimizer Automation Study Wizard - Import page (**Figure 19** on page 16)
- Optimizer Automation Study Wizard - Optimize page (**Figure 20** on page 17)

Figure 19   Optimizer Automation Study Wizard - Import page
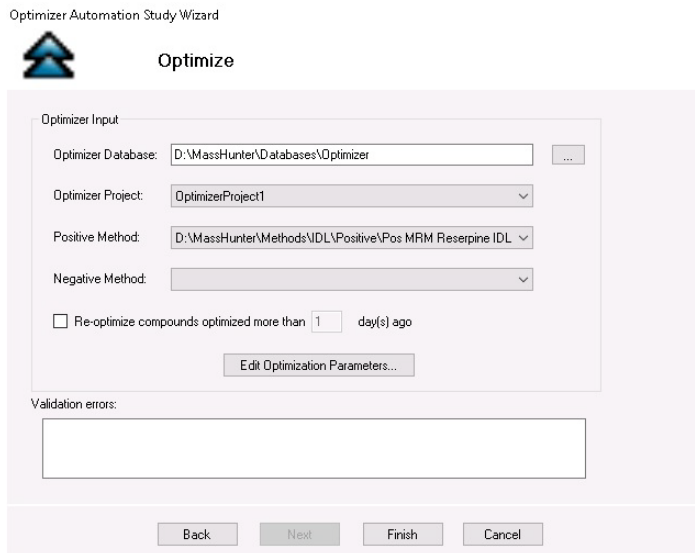
Figure 20   Optimizer Automation Study Wizard - Optimize page

Getting Started

Basic Tasks

Submitting Studies

Running a Study

Modifying the Pending Studies Table

Other Activities

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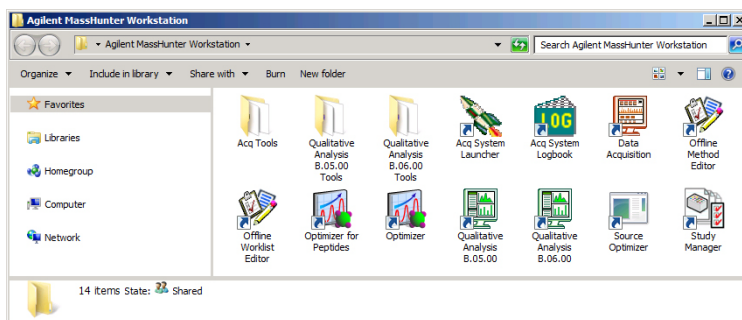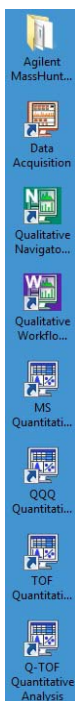
2 Double-click the **Study Manager** icon ().

You can also click the start button and then **Agilent MassHunter LCMS Acq > Study Manager**.

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.

Study Manager button
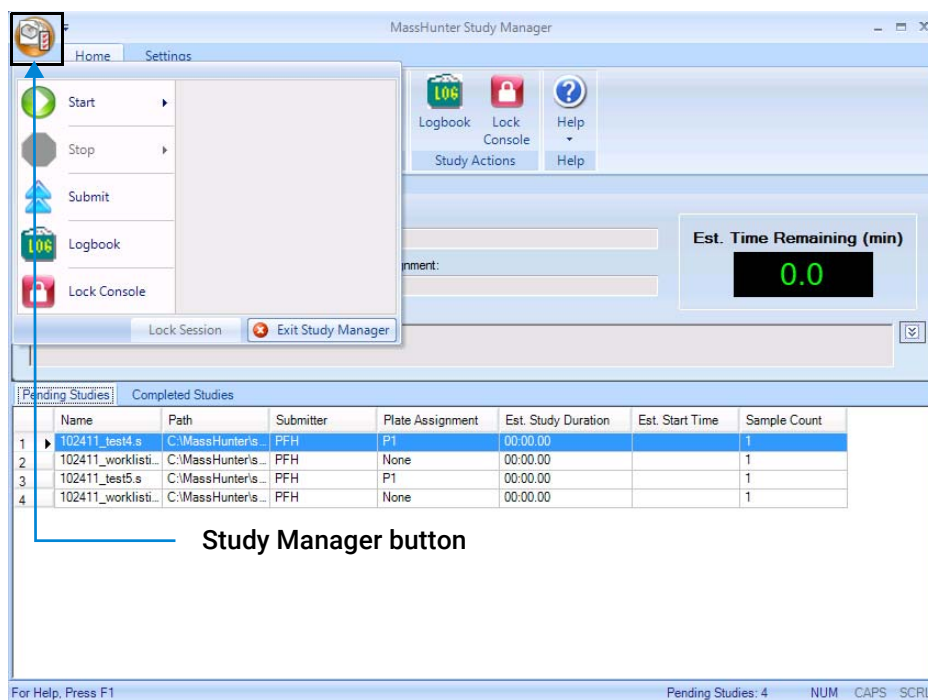
To enable a study using the Study Creator Enabler program

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 ( ).

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 the ⟨ > ⟩ button to copy this Study Type to the **Enabled Study Creators** list.

   b 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.

Figure 21   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

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

1 Click the **Submit** icon (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 9** 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\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 (*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 10** on page 10) 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 11** 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 12** on page 11) 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 13** on page 12). 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\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 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 14** on page 13) 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 15** on page 13) 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 the **Ultivo LC/TQ** instrument.

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

1 Click the **Submit** icon ( ) 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 is shown (**Figure 16** on page 14)

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 17** on page 15).

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.

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 18** on page 15).

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.

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 the **Ultivo LC/TQ** instrument.

1 Click the **Submit** icon ( ) 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 is shown.(**Figure 19** on page 16)

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 Optimizer Automation Study Wizard - Optimize page (**Figure 20** on page 17) 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.

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

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 ( ) 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 (⬢ stop) 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.

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 34

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 23
- **"To submit a Worklist-Only study"** on page 25
- **"To submit a Bioanalysis study"** on page 27
- **"To submit an Optimizer Automation study"** on page 29

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 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.

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 23
- **"To submit a Worklist-Only study"** on page 25
- **"To submit a Bioanalysis study"** on page 27
- **"To submit an Optimizer Automation study"** on page 29

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

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 36
- **"To lock the console"** on page 36
- **"To add a standby script"** on page 37

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 is shown (**"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 is shown.

2 Click the **Logbook** icon ( ) in the **Study Actions** section in the Home tab.

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 is shown.

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 Start** check box is marked.

1 Click the **Settings** tab in the Ribbon. The **"Settings Tab in the Ribbon"** on page 5 is shown.

2 Mark the **Execute standby script on idle or error** 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. Submitting and running 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.
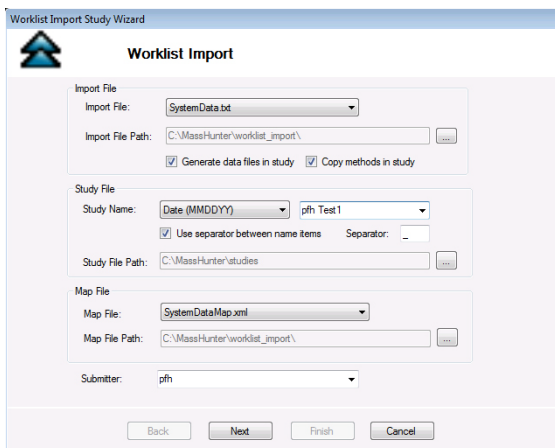
Steps	Detailed Instructions	Comments
1 Open the Study Manager program and clear the items in the Pending Studies table (if necessary).	**a** Double-click the **Agilent MassHunter Study Manager** icon, . **b** Right-click any line in the Pending Studies table, and then click **Delete**.	• Before deleting 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.	**a** Copy **SystemData.txt** to the **\MassHunter\worklist_import** folder. **b** Copy **SystemDataMap.xml** to the **\MassHunter\StudyExamples** folder.	

Steps	Detailed Instructions	Comments
3 Submit the Worklist Import study.	**a** Click the **Submit** icon, [Submit icon], in the Ribbon. **b** (*optional*) Select **Worklist Import** in the **Select Study Creator** dialog box. Click **OK**. **c** Select **SystemData.txt** as the **Import File**. Change the **Import File Path** if necessary. **d** (*optional*) Mark the **Generate data files in study** check box. **e** (*optional*) Mark the **Copy methods in study** check box. **f** Select **Date (MMDDYY)** as the first part of the Study Name. **g** Select **Custom Name** as the second part of the Study Name. **h** Type *iii* Test1 in the **Study Name**, where *iii* are your initials. **i** Type *iii* as the **Submitter**. **j** Click **Next**.	• 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 21. • The Plate Assignment is specific to your instrument setup. • The example worklists are included on the installation disk in the **Support\Data** folder.

Figure 22 The Worklist Import Study Wizard - Worklist Import page

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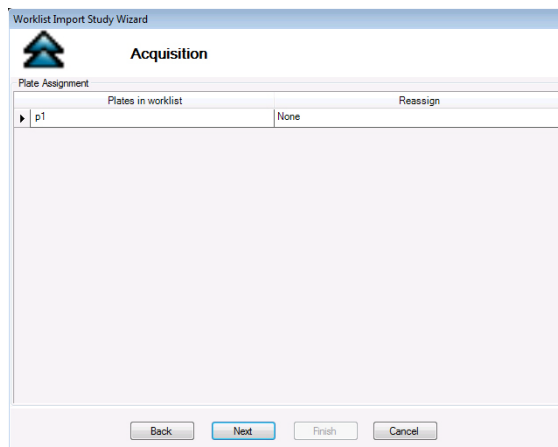
l Click **Next**.

| Steps	Detailed Instructions	Comments

Figure 23   The Worklist Import Study Wizard - Acquisition page

m (*optional*) Mark the **Quant Automation** check box.

n If you mark the **Quant Automation** check box, then select the **Quantitative Analysis Method**.

o (*optional*) Mark the **Generate Report** check box. If you mark this check box, select the **Template File**.

p (*optional*) Mark the **Print to default printer** check box.

q (*optional*) Mark the **Publish** check box. Select the file type to use.

r Click the **Next** button.
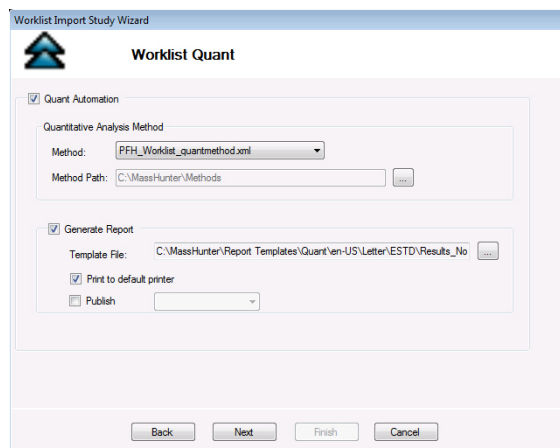
Steps	Detailed Instructions	Comments
	Figure 24 The Worklist Import Study Wizard - Worklist Quant page	
	s Review the worklist in the **Worklist Import Study Wizard - Worklist** page. **t** (*optional*) Right-click the box in the upper left corner and click **Worklist Run Parameters**. Change the **Method 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.

Steps	Detailed Instructions	Comments
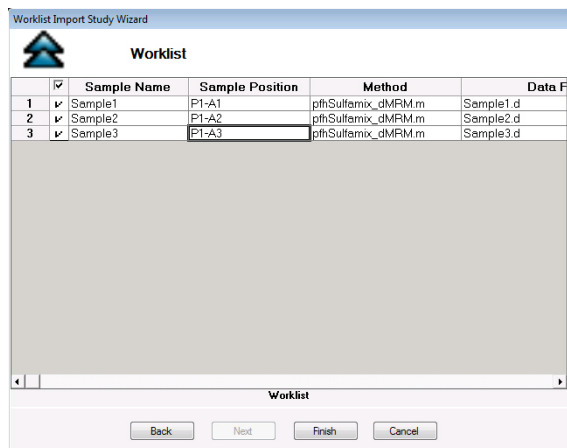
Figure 25   Worklist Import Study Wizard - Worklist page

Steps	Detailed Instructions	Comments
4 Start running the study in the Study Queue.	**a** Click the **Start** icon, , in the Ribbon. **b** 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.
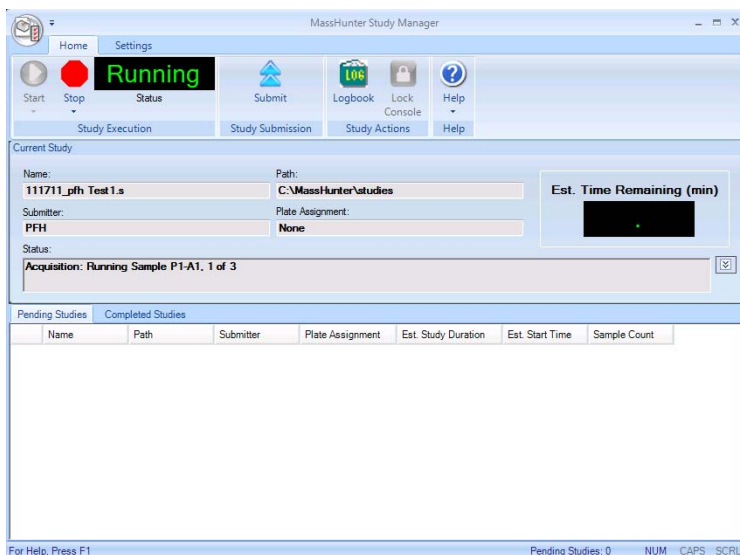
The study is removed from the Pending Studies queue, and it becomes the Current Study. If you add another study, it is added to the Pending Studies queue, and it is started when the Current Study completes.

Figure 26   Running the Study Queue

Task 2. Submitting and running 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 Ultivo LC/TQ 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).	**a** Double-click the **Agilent MassHunter Study Manager** icon, . **b** Right-click any line in the Pending Studies table, and then click **Delete**.	• Before deleting any studies from the Pending Studies table, make sure that no one else is using the system.
2 Submit the first study. • This study is a worklist-only study using the worklist **GroupA.wkl**.	**a** Click the **Submit** icon, , in the Ribbon. **b** (*optional*) Select **Worklist-Only** in the Select Study Creator dialog box. Click **OK**. **c** Select **Example_Worklist1.wkl** as the Worklist file. Change the Worklist File Path if necessary. **d** (*optional*) Mark the **Generate data files in study** check box. **e** (*optional*) Mark the **Copy methods in study** check box. **f** Select **Custom** as the first part of the Study Name. **g** Then type iii Test1 in the **Study Name**. **h** Select **Date (MMDDYY)** as the second part of the Study Name. **i** Type *iii* as the **Submitter**. **j** (*optional*) Select the Plate Assignment. **k** Click **Next**.	• 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 21. • "*iii*" are your initials. • The Plate Assignment is specific to your instrument setup. • The example worklists are included on the installation disk in the **Support\Data** folder.

Steps	Detailed Instructions	Comments

Figure 27 The Worklist-Only Study Wizard - Worklist Import page

| | **l** (*optional*) Mark the **Quant Automation** check box. If you mark the **Quant Automation** check box, then select the **Quantitative Analysis Method**.
 m (*optional*) Mark the **Generate Report** check box. If you mark this check box, select the **Template File**.
 n (*optional*) Mark the **Print to default printer** check box.
 o (*optional*) Mark the **Publish** check box. Select the file type to use.
 p Click the **Next** button. | • You do not have to run the Quant Automation. If you do mark this check box, then you must select a Quantitative Analysis method. |

Steps	Detailed Instructions	Comments
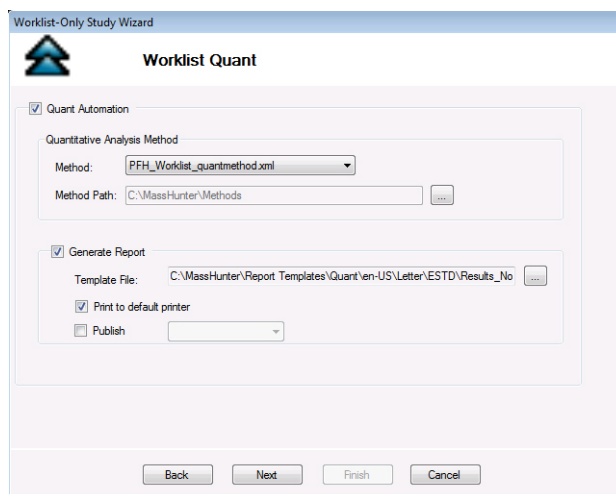
Figure 28   The Worklist-Only Study Wizard - Worklist Import page

|		
	q Review the worklist in the **Worklist-Only Study Wizard - Worklist** page. **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**. **s** Click **Finish**.	• 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 click **Worklist Run Parameters**. Then, change the method path to the correct location and click **OK**.

Steps	Detailed Instructions	Comments
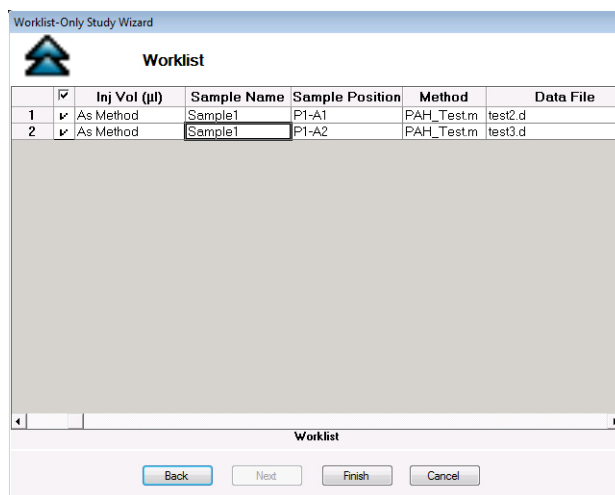
Figure 29   Worklist-Only Study Wizard - Worklist page

3 Submit the next two studies.
  • The second study uses the worklist **Example_Worklist2.wkl**.
  • The third study uses the **Example_Worklist3.wkl**.

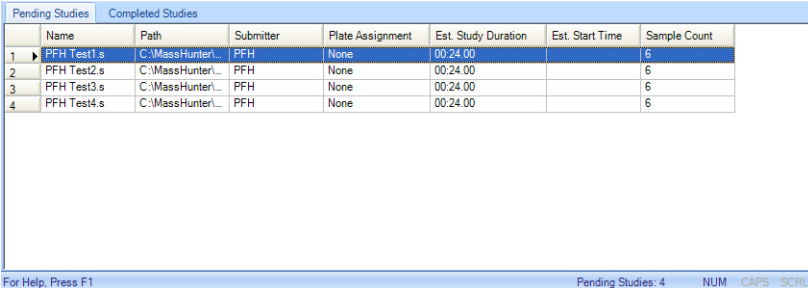**a** Click the **Submit** icon, , in the Ribbon.
b (*optional*) Select **Worklist-Only** in the Select Study Creator dialog box. Click **OK**.
c Select **GroupB.wkl** as the Worklist file.
d Type *iii* `Test2.s` as the first part of the **Study Name**.
e Type *iii* as the **Submitter**.
f Select the **Plate Assignment**.
g Click **Next**.
h Review the **Worklist Quant** page.
i Click **Next**.
j Review the worklist in the Worklist-Only Study Wizard - Worklist page.
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**.
l Click **Finish**.

• Study Manager lets you put many different studies in the Pending Studies table. When you click **Start**, 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.

Steps	Detailed Instructions	Comments
	a Click the **Submit** icon, ![Submit], in the Ribbon.	• This section describes submitting the third study.
	b (*optional*) Select **Worklist-Only** in the Select Study Creator dialog box. Click **OK**.	
	c Select **GroupC.wkl** as the Worklist file.	
	d Type *iii* `Test3.s` as the first part of the **Study Name**.	
	e Type *iii* as the **Submitter**.	
	f Select the **Plate Assignment**.	
	g Click **Next**.	
	h Review the worklist in the **Worklist-Only Study Wizard - Worklist** page.	
	i (*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**.	
	j Click **Finish**.	

Figure 30   The Pending Studies table with four different studies submitted

Steps	Detailed Instructions	Comments
4 Start running the studies in the Study Queue. • All four studies will be run.	**a** Click the **Start** icon, , in the Ribbon. **b** Click either **Start** or **Resume Stopped Study**.	• The first study is removed from the Pending Studies table. The information for this study is visible in the Current Study pane.
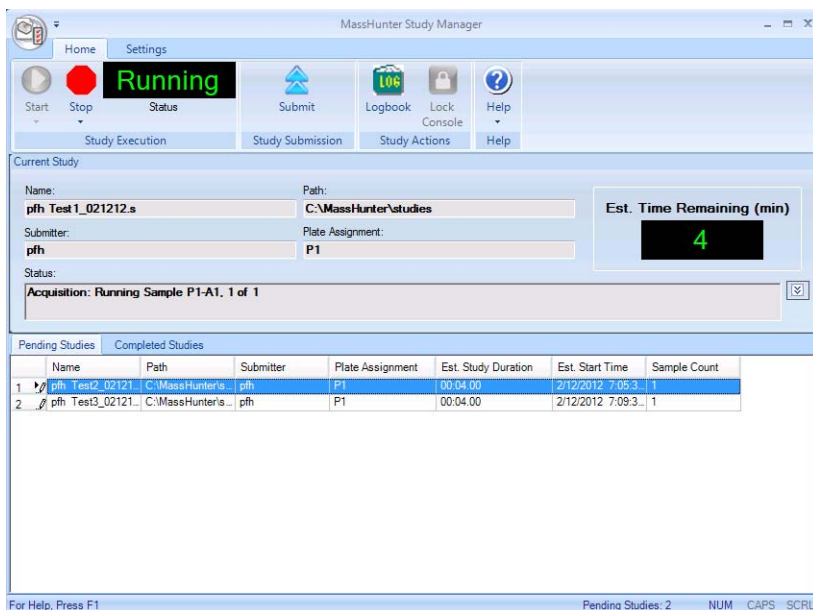
The first study, PFH Test1 is shown in the Current Study pane.

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

Figure 31 Running the Study Queue

Task 3. Submitting 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 the *Agilent Bioanalysis Workflow Guide* for more information on finishing this task. You can find this guide on the **www.agilent.com** web site.

Task 4. Submitting an Optimizer Automation Study

See **"To submit an Optimizer Automation study"** on page 29.

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 version C.01.00 of MassHunter Study Manager for Ultivo LC/TQ or higher until superseded.

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