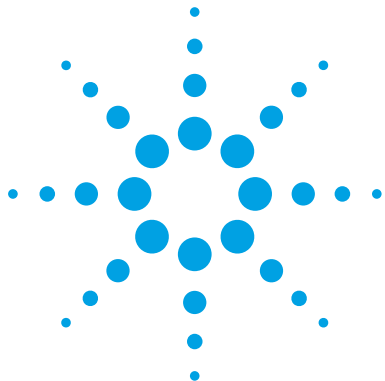




MassHunter Walkup Custom Sample Import

Programmer Guide

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When a user submits samples to Walkup, the user specifies in the Sample List table a list of samples. The list includes the sample names, the Walkup method to use, and other information.

Walkup includes the feature “Manual Sample Import” to allow you to simplify and automate this process. This feature leads to fewer errors and provides convenience to the user.

With Manual Sample Import, Walkup can read the data in an Import File to fill the Sample List table. A Sample Map File is used to interpret the data in the Import File. The Import File can be created manually, or automatically by a Laboratory Information Management System (LIMS). Instead of typing the



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sample information into the Sample List Table, the user just selects an Import File from a folder that contains Import Files for all the samples to be submitted.

One disadvantage of using Import Files is that the user cannot easily see the content of the Import File, so the user can easily select the wrong one and end up submitting the wrong samples.

In Walkup C.02.02, a feature called “Custom Sample Import” was introduced.

Custom Sample Import allows you to write a simple program to help your users to easily submit samples, reduce unnecessary typing and eliminate potential errors. Custom Sample Import also allows sample submission to follow the practices of your organization's workflows.

Two examples of how custom Sample Import Programs can be used are described in this guide.

Sample Submission Stored in a LIMS

Some organizations use a LIMS to keep track of the samples to be submitted by each user. Typically, the LIMS generates an Import File for each user in advance and places it in a central folder. The user then logs onto Walkup and starts the sample submission process. After selecting the appropriate workflow, the user selects an Import File from the central folder. The user must be careful to select the correct Import File. After the Import File is loaded, the Sample List Table is populated.

With the Custom Sample Import feature, and the appropriately written Custom Sample Import program, the LIMS no longer needs to generate the Import File for each user in advance. The user also does not need to select an Import File. After the submitter enters his or her user name and selects the appropriate workflow, Walkup launches the Custom Sample Import program to query the LIMS with the user's name to find the list of samples to be submitted by the user. This program can be written to automatically create an Import File and tell Walkup to import this file into the Sample List table. This Custom Sample Import program can be written in any Windows programming language.

The user can verify if the samples are correct and then load the sampler with the appropriate samples to complete the sample submission process. The user does not have to be aware of any Import File because the Import Files are hidden from the user. The list of samples are basically transferred from LIMS to Walkup just by supplying the user's name.

Super Method

If an analysis requires running multiple Walkup methods on a sample, the user needs to remember the multiple methods that are required for a given analysis. Manual sample submission done this way is tedious and error-prone.

With the Custom Sample Import feature, you can create a configuration file that lists all the Walkup methods required for an analysis, creating effectively a “super method.” When a user submits a sample with the appropriate workflow, the custom Sample Import Program can read the configuration file and display a list of super methods that can be run. After a super method is selected, the custom Sample Import Program can generate an Import File that contains each Walkup method associated with the super method. This Import File is then read by Walkup to populate the Sample List table.

The custom Sample Import Program to do the steps just described is installed with Walkup as an example. See [“Example Application - Super Method”](#) on page 9.

Setting up and using Custom Sample Import

To set up custom sample import

- 1 Create an Import Map File.

You do this in the same way as creating an import map file for the manual sample import process. Do this step in the **Import Map Configuration View**.

- 2 Create a custom Sample Import Program.

This program can be written in any programming language, as long as it can run in Microsoft Windows. See “[Working with Custom Sample Import](#)” on page 6 for more details.

- 3 Create a Workflow and configure it for Custom Sample Import.

In the **Workflow Configuration View**, add a new workflow. Enter whatever workflow columns are required for your analysis.

The image shows two overlapping windows from a software application. The top window, titled "Workflow Columns", contains a table with four columns: "Column Display Name", "Column Type", "Mandatory", and "Custom Val". The first row is highlighted in orange and contains the text "Custom Column" in the "Column Display Name" and "Column Type" fields. Below the table is a text input field with the placeholder "Click here to add new column in Workflow." To the right of the table are two buttons: "Move Up" (with an upward arrow) and "Move Down" (with a downward arrow). The bottom window, titled "Custom Sample Import", has a checked checkbox labeled "Allow Custom Sample Import". Below this, there are two fields: "Import Map" with a dropdown menu showing "Samples Demo Map", and "Sample Import Program" with a text box containing the path "C:\Program Files (x86)\Agilent\MassHunter\Walkup\bin\CustomSampleImportSuperMethod.exe" and a browse button. At the bottom of this window are "Save" and "Cancel" buttons.

- 4 Select the option **Allow Custom Sample Import**. Select the appropriate **Import Map** and custom **Sample Import Program**.

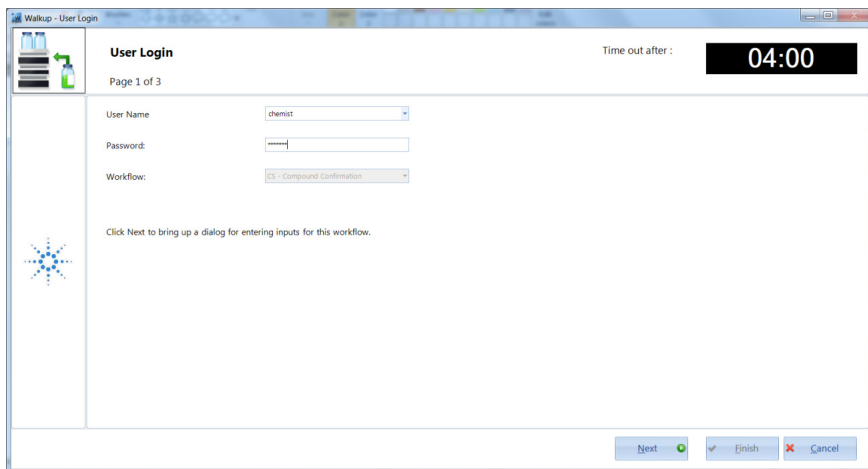
- 5 Click **OK**.

Once you have verified and saved the configuration, users can use the new workflow to submit samples for custom sample import.

To submit samples for custom sample import

- 1 In the Walkup Console, click **Submit Samples**.

The screen below will be displayed.



- 2 Enter the user name and password and select the new workflow. The **Number of Samples** and **Import Samples** options are hidden.
- 3 Click **Next**.

At this time, Walkup:

- Disables **Next** and **Cancel** buttons.
- Launches the custom **Sample Import Program** configured for this workflow.
- Depending on the custom **Sample Import Program**, a dialog can appear to query the user for more information. Once the user closes the dialog (if any), the custom Sample Import Program creates the Import File and passes it to Walkup.
- Displays the second page of the Sample Submission form, which shows the samples to be submitted.

From this point on, Walkup behaves the same as for manual sample submission.

Working with Custom Sample Import

Sample Import Parameter XML File

When the custom Sample Import program is launched, a Sample Import Parameter XML file is created that contains information entered by the user who started the sample submission.

This file is named **SampleImportParamsYYYY_MM_DD_HHMMSS.xxx**, where the variables are based on the time that the file is generated:

- *YYYY* is the year
- *MM* is the month
- *DD* is the day
- *HH* is the hour
- *MM* is the minutes
- *SS* is the second
- *xxx* is csv, .txt, .xls, .xlsx or .xslm, depending on the Import Map that is selected.

This format is used to make sure that the file name is unique. The full path of this file is passed as a command line argument to the custom Sample Import Program.

The default location of the generated file is:

Users\user\AppData\Local\Temp\Walkup\SampleImportFiles

The custom Sample Import Program does not need to know about the file naming convention because the full path name is passed to the program.

An example of the contents an Import File is shown below

```
<?xml version="1.0" encoding="UTF-8"?>
<SampleImportParameters>
  <UserName>chemist</UserName>
  <Workflow>Compound Confirmation</workflow>
  <SamplesFilePath>C:\Users\Walkup\AppData\Local\Temp\Walkup\
SampleImportFiles\
SampleInformation2015_01_12_112030.csv</SamplesFilePath>
  <MethodsAllowedPerSample>1</MethodsAllowedPerSample>
</ SampleImportParameters >
```

The XML tag <SamplesFilePath> contains the location where the Import File needs to be created by the custom Sample Import Program. The location is the same folder as where the Sample Import Parameter XML file is to be created.

Sample Custom Import Program Timeout

Walkup will wait for the custom Sample Import Program to complete its task to create the Sample Import file. However, after a specified “wait time” is reached, Walkup stops the Sample Import Program. (The wait time is configured by the **Cancel submission if no activity after** option in the **System Configuration View**).

If the custom Sample Import Program encounters an error and can't generate a valid Sample Import file, make sure that your custom Sample Import Program displays an error message. Once the message is closed, the program must return a non-zero process exit code.

If Walkup receives a non-zero exit code, Walkup remains on page 1 of Sample Submission and enables the Next button. The user can choose to cancel the submission or try again by clicking **Next**.

If the configured import map and import data file do not match, an error will be displayed. The error will be similar to the error displayed for manual sample import.

When the Sample Import file is successfully created, Walkup uses the file and Import Map to populate the Sample List table on page 2 of the Sample Submission form.

Sample Import Parameters and Import data file deletion

The Sample Import Parameters file and generated Sample Import file are deleted if sample submission succeeds, or if the user cancels the submission. If sample submission fails, these files will not be deleted, to allow an administrator to troubleshoot the error.

Configuration for Editing Sample Information in Custom Sample Import

Configuration for custom sample import is only needed in the Workflow configuration. By default, the sample information in the Sample List Table can be changed by the user. This can be disabled by user group but must be configured in the following screens:

- In the **System Configuration View**, select **Allow samples to be submitted from import file**.
- In the **Users and Groups Configuration View**, for each required group, select **Allow Import**, and clear the check box for **Allow users to modify import sample information**.

Restrictions

Unregistered Users Unregistered users are not allowed to submit by sample import. For unregistered users only workflows with custom sample import option disabled will be displayed. Unregistered users will not be able to use manual or custom sample import.

Default Initialization New Walkup workflows start with the option **Allow Custom Sample Import** disabled.

Upgrade Walkup workflows created before Walkup C.02.02 are upgraded with the option **Allow Custom Sample Import** disabled.

Impact on Import Export This new configuration is available while importing and exporting.

Example Application - Super Method

Example code is provided on the installation disc in the folder **Support\Custom Sample Import**.

The steps in this section describe how to use the example Sample Import Program to run a Super Method. See “[Super Method](#)” on page 3.

Step 1. Set up a workflow to use the example programs

- Create a new workflow:
 - Select **Allow Custom Sample Import**.
 - For **Import Map**, select **Samples Demo Map**.
 - For **Sample Import Program**, select the example **CustomSampleImportSuperMethod.exe** that is installed on your computer.

The screenshot shows two overlapping windows from a software application. The top window, titled 'Workflow Columns', contains a table with four columns: 'Column Display Name', 'Column Type', 'Mandatory', and 'Custom Val'. The first row is highlighted in orange and contains the text 'Custom Column' in both the 'Column Display Name' and 'Column Type' fields. Below this row, there is a text prompt: 'Click here to add new column in Workflow.' To the right of the table are two buttons: 'Move Up' (with an upward arrow) and 'Move Down' (with a downward arrow). The bottom window, titled 'Custom Sample Import', has a checked checkbox labeled 'Allow Custom Sample Import'. Below this, there are two fields: 'Import Map' with a dropdown menu showing 'Samples Demo Map', and 'Sample Import Program' with a text box containing the file path 'C:\Program Files (x86)\Agilent\MassHunter\Walkup\bin\CustomSampleImportSuperMethod.exe' and a file selection icon. At the bottom of this window are 'Save' and 'Cancel' buttons.

Step 2. Run the new workflow

- 1 Start the sample submission and select the new workflow.

The screenshot shows a window titled "Walkup - User Login". Inside, there's a "User Login" section with a "Page 1 of 3" indicator. A "Time out after:" timer shows "04:50". There's a "Register New User:" checkbox. Below it are input fields for "UserName:" (set to "chemist"), "Password:" (empty, with a note "Password is not required for current user."), "DepartmentID:" (set to "Dept1"), and "Workflow:" (set to "WorkFlow"). A blue star icon is on the left. At the bottom, there are "Next", "Finish", and "Cancel" buttons.

- 2 Click Next.

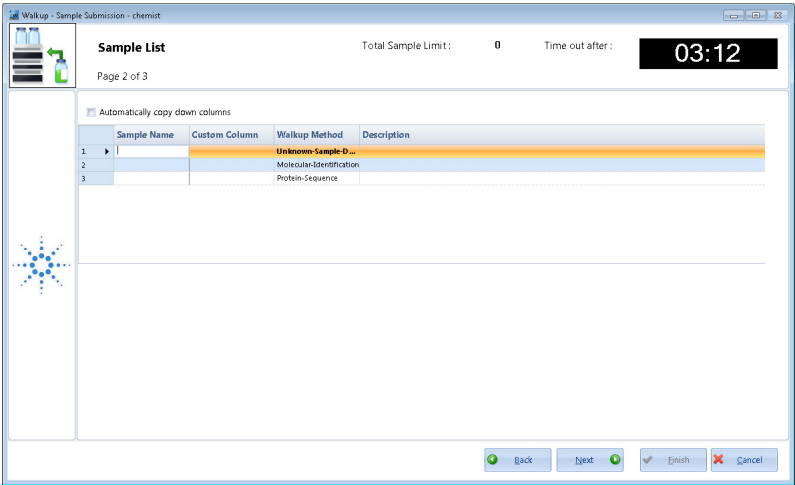
The SuperMethod dialog box is displayed.

The screenshot shows a "SuperMethod Selection" dialog box overlaid on the login form. The dialog has a "SuperMethod:" dropdown menu with "SuperMethod1" selected. There are "Ok" and "Cancel" buttons at the bottom. The background login form is partially visible, showing the "chemist" username and "Dept1" department.

- 3 Select the appropriate super method to use.

The Sample List table populates with the list of Walkup methods that correspond to a Super Method specified in the file **D:\MassHunter\Walkup\CustomSampleImportData\SuperMethodConfigurationExample.txt**. You can add additional Super Methods in this text file.

Example Application - Super Method
Step 2. Run the new workflow



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In This Book

This guide instructions to
do custom sample import
by creating a custom
Sample Import Program.

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