

Agilent G3835AA MassHunter Mass Profiler Professional Software

Quick Start Guide

For Research Use Only. Not for use in diagnostic procedures.

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What is Agilent Mass Profiler Professional?

Agilent Mass Profiler Professional (MPP) software is a powerful chemometrics platform designed to exploit the high information content of mass spectra (MS) data and can be used in any MS-based differential analysis to determine relationships among two or more sample groups and variables. MPP provides advanced statistical analysis and visualization tools for GC/MS, LC/MS, CE/MS, and ICP-MS data analysis. MPP also integrates smoothly with Agilent MassHunter Workstation, Spectrum Mill, and ChemStation software and is the only platform that provides integrated identification/annotation of compounds and integrated pathway analysis for metabolomic and proteomic studies. The system also enables automated sample class prediction that revolutionizes mass spectrometer-based qualitative analysis of unknown samples in many applications. MPP is ideally suited for applications characterized by complex sample matrices such as metabolomics, proteomics, natural products, food, beverages, flavors, fragrances, and environmental analyses.



Features of Mass Profiler Professional

- Allows differential analysis of two or more sample sets from one or multiple MS analysis platforms in a single project.
- Designed for both mass spectrometrists and statisticians, with guided and advanced workflows.
- Provides comprehensive statistical tools including ANOVA, PCA, volcano plots, hierarchical trees, SOMs, QT clustering, and five different methods for class prediction.
- Generates inclusion lists for subsequent MS/MS-based analyses to facilitate identification of compounds of interest.
- The ID Browser allows integrated identification and annotation of compounds using LC/MS Personal Compound Database Libraries and GC/MS libraries (NIST and Agilent Fiehn Metabolomics).
- Allows import and export of data in several formats e.g. to further extend and customize statistical analysis and visualization capabilities using R-Scripts (see *Agilent GeneSpring GX R-integration package - Installation and Application Guide*).
- Integrates smoothly with Spectrum Mill to enable TOF/Q-TOF based discovery and QQQ-based verification of protein biomarkers.
- Integration with GeneSpring allows the correlation of pathways between MS (metabolomics, proteomics) and microarray data (transcriptomics) in one project, enabling true integrated biology studies.
- Class prediction models from GC/MS, LC/MS, CE/MS and ICP/MS data can be used with the standalone automated Sample Class Prediction (SCP) software to enable high-throughput routine classification of unknown samples.

What's new in MPP 14.9?

General Improvements

- Improved support for CEF files generated using MassHunter Unknown Analysis.
- Support for already log transformed data while creating Generic MPP experiment.

Venn Diagram Improvements

- Improved Venn analysis that supports:
 - Cross experiment analysis based on chosen entity annotation
 - Entity matching Inspector to review analysis to be performed.
 - Support for MPP entity lists in Venn based on LC/GC compound alignment.
 - Support for >4 entity list in Venn. Summary of unique and shared regions of Venn presented as table.

Normality Tests

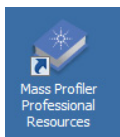
- Helpful in choosing appropriate downstream statistics.
- Filter entities based on Shapiro Wilk / D'Agostino Pearson test of normality for further statistical analysis.

Custom R-script Support

- Data normalization and correlation analysis using custom R-Script supported for most experiment types of GeneSpring/MPP.
- Four custom R scripts have been included.

Where to Find More Information

Resource App



The Mass Profiler Professional software suite includes a Supplemental Disc that contains an installer for the Resource App. Make sure you install this app to access the documents that are described in this topic.

Online help

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

Help Menu Click **Help > Documentation Index** to access the release notes, quick start guide, and HTML and PDF versions of the *Mass Profiler Professional User Manual*.

Documents

Mass Profiler Professional

These documents are found in the Mass Profiler Professional Resource App.

- Mass Profiler Professional Familiarization Guide
- Mass Profiler Professional Application Guide
- Agilent MassHunter Mass Profiler Professional User Manual.

You can find a PDF copy in the MPP installation folder

C:\Program Files\Agilent\MassHunter\Workstation\Mass Profiler Professional\docs\manual\MS, if you installed MPP using the default directory structure.

Workflow Guides and Overviews

These documents are found in the Mass Profiler Professional Resource App.

- Agilent Metabolomics Workflow - Discovery Workflow Guide / Overview
- Integrated Biology with Agilent Mass Profiler Professional - Workflow Guide / Overview
- Class Prediction with Agilent Mass Profiler Professional Workflow Guide / Overview
- Agilent Lipidomics - Workflow Guide / Overview

MassHunter Qualitative and Quantitative Analysis

These documents are found in the MassHunter Data Analysis Resource App.

- MassHunter Qualitative Analysis Familiarization Guide for LC/MS
- MassHunter Qualitative Analysis Familiarization Guide for GC/MS
- MassHunter Quantitative Analysis Familiarization Guide

Training

These training programs and videos are found in the Mass Profiler Professional Resource App.

Interactive Training and Videos A set of three interactive training guides can be found and launched from the Resource page found on the MPP Supplemental disc.

- **Getting Started with MPP:** An interactive tutorial that helps you get started using MPP. The tutorial introduces you to the MPP user interface and uses example data to guide you through creating a project and an experiment, importing data, and performing a differential analysis. An overview and flow chart is also presented for many of the advanced operations available in the Workflow Browser. The tutorial guides you through the use of versions 14.5 and 14.8 and is equally valuable to familiarize you with earlier versions of MPP. (The MPP 14.8 tutorials apply also to MPP 14.9.)
- **MPP Training Videos:** An interactive interface to a substantial suite of brief training videos that cover how to use MPP to analyze your data. The training videos were generated using versions from 14.0 through 14.5 and are valuable regardless of the version of MPP you are using.
- **Using MassHunter Profinder to Prepare Data:** An interactive interface to a suite of brief training videos that cover how to use Profinder to prepare your data for an analysis using MPP. The training videos are valuable regardless of the version of MPP and Profinder you are using.

Road Show Slide Presentation

- Metabolome Analysis - From Sample Prep Through Data Analysis

Training Courses Visit www.agilent.com to view a listing of training courses for MPP.


Getting Started

How do I get started?

This *Quick Start Guide* helps you launch MPP, activate your license, review the MPP user interface, and create a project and an experiment that you import data into and then use to begin your analysis.

If you are already familiar with the MPP software, after you install MPP you can immediately start using the preloaded demonstration project called “Malaria.” The Malaria data is from a research study previously published (Agilent application note p/n 5990-6790). The study used cell culture. No samples were derived from humans and Agilent does not imply any diagnostics in humans.

Start and explore Mass Profiler Professional

- 1 Double-click the **Mass Profiler Professional** icon  located on your desktop, or click **Start > All Programs > Agilent > MassHunter Workstation > Mass Profiler Professional > Mass Profiler Professional** (Windows 7), or click **Start > Agilent > Mass Profiler Professional** (Windows 10).
- 2 Activate your license. The first time you start MPP you are prompted to enter your **Mass Profiler Professional Order ID** before you can use the software (see [“Activate your license”](#) on page 7).
- 3 Complete your user registration. After you activate your license you are prompted to complete a **Registration** that is used to notify you of software updates and improve interactions you may have with customer support (see [“Register a user”](#) on page 9).
- 4 Review the following three sections in this *Quick Start Guide*:
 - “User Interface” on page 11
 - “Basic Tasks” on page 16
 - “Advanced Tasks” on page 25
- 5 Review the [Mass Profiler Professional Familiarization Guide](#) (see [“Documents”](#) on page 4). This guide helps you quickly create a project, create an experiment, import and organize data, and create an initial differential expression using pre-installed demonstration data - *Malaria Demo*.
- 6 Review the [Mass Profiler Professional Application Guide](#) (see [“Documents”](#) on page 4). This guide provides you with more detail about the MPP software and helps you create a project, create an experiment, import and organize data, and create an initial differential expression with your own data.
- 7 Review the [“Interactive Training and Videos”](#) on page 5 at any time to help you become familiar with preparing your data and using MPP to analyze your data.

- 8 Perform advanced analyses to meet your project needs using the operations available in the Workflow Browser (see “Workflow Browser” on page 14).

License Management and Registration

Activate your license

The first time you start MPP you enter your Order ID. License activation information is entered in the **Mass Profiler Professional License Activation** dialog box. An Internet network connection is required.

- 1 Mark **Mass Profiler Professional Order ID**. If you have additional software product licenses, such as for Pathway Architect or GeneSpring GX, mark your additional products (Figure 1).
- 2 Type your **Mass Profiler Professional Order ID** exactly as written, for example ABC1-2345-6789. If you have additional software product licenses, such as for Pathway Architect or GeneSpring GX, type your additional product Order IDs.
- 3 Click **OK**.

The Mass Profiler Professional software automatically validates your license and starts Mass Profiler Professional.

Mass Profiler Professional License Activation

Please choose your license type: Individual license

Order ID

You should have valid OrderIDs to activate Mass Profiler Professional over the web. To get OrderIDs, write to the support team at informatics_support@agilent.com.

Mass Profiler Professional OrderID

GeneSpring GX OrderID

Pathway Architect OrderID

Example: ABC1-2345-6789

Cloud or VM Installation

Proxy settings

Use proxy

proxy

port

Authenticate

user

password

Help OK Cancel

Figure 1 Mass Profiler Professional License Activation dialog box

Move your license to another PC

MPP licensing is automatically enforced. You may move a license to another computer by surrendering it on the current computer and then activating it on the new computer. If you need to uninstall MPP, it is always best to surrender the existing license before un-installing MPP so that the license is available to be moved to another computer.

To surrender your license:

- 1 Click **Help** > **License Manager** in the menu bar.

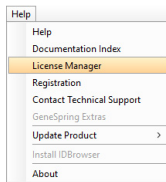


Figure 2 License Manager is available from the Help menu.

- 2 Click **Surrender** in the **License Manager** dialog box.

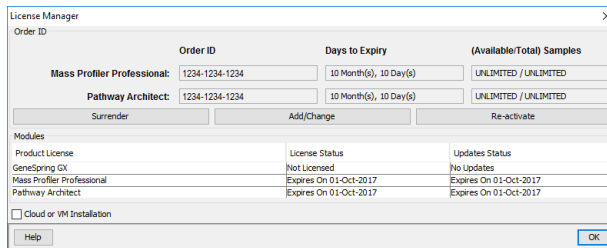


Figure 3 License Manager dialog box

- 3 Mark **Mass Profiler Professional** and any additional product Order IDs to surrender.

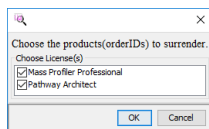


Figure 4 Order ID surrender product selection dialog box

4 Click **OK**.

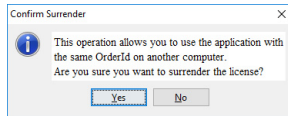


Figure 5 Confirm Surrender dialog box

5 Click **Yes** in the **Confirm Surrender** dialog box.

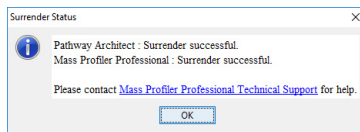


Figure 6 Surrender Status dialog box

6 Click **OK** in the **Surrender Status** dialog box.

Because your license is no longer active on the current computer, MPP software immediately closes after you click **OK**.

7 Activate your license Order ID on the new computer by following the steps in "[Activate your license](#)" on page 7.

Register a user

When you begin to use MPP for the first time you are prompted to register a user in the **Registration** dialog box. You must register and confirm your registration email within 7 days. After 7 days the **Registration** dialog box appears when you start MPP. An Internet network connection is required.

- 1** Type the requested user information into the **Registration** dialog box ([Figure 7](#) on page 10).
- 2** Click **Submit**.
- 3** Check your email from a message from informatics_support@agilent.com. An example email is shown in [Figure 8](#) on page 10.
- 4** Click **Confirm email address**.

Getting Started

License Management and Registration

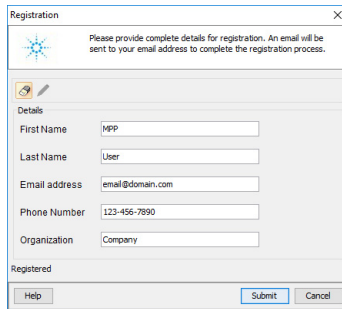


Figure 7 Registration dialog box with the status *Registered* shown in the lower left to indicate that the registration is confirmed

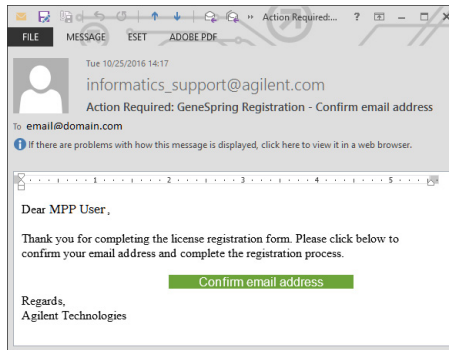




Figure 8 Example email from informatics_support@agilent.com

View or change your registration

You can view and change your registration at anytime.

- 1 Click **Help > Registration**.
- 2 View your current registration in the **Registration** dialog box (Figure 7).
- 3 Click **Cancel** to close the **Registration** dialog box without making changes, or Click the **Edit** registration icon  to enable editing of the registration fields.
- 4 Type new information into any of the registration fields. To add a new user you can first click the **Clear** icon  to erase the entries in all of the fields.
- 5 Click **Submit** when you have completed making your changes or updates.
- 6 Check your email from a message from **informatics_support@agilent.com**. An example email is shown in Figure 8.
- 7 Click **Confirm email address**.

User Interface

Main Functional Areas

The functional areas of Mass Profiler Professional are shown in [Figure 11](#) on page 12. The main MPP window consists of four parts: (1) the Menu Bar, (2) the Toolbar, (3) the Display Pane, and (4) the Status Bar.

Note: Help and detailed information regarding the various fields and statistical treatments are available by pressing **F1** or by referring to the *Mass Profiler Professional User Manual*.

1. Menu Bar The menu bar ([Figure 9](#)) provides actions that are used for managing your projects, experiments, pathways, and display pane views.

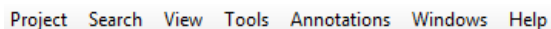


Figure 9 Menu bar

2. Toolbar The toolbar ([Figure 10](#)) is located below the menu bar and contains five sections of buttons for commonly used tasks:

Project section: New, Open, and Close

Experiment section: New, New MOA, and Add

Entity List section: Create entity list from selection, Inspect selected entity, and Import entity list (From File, From Dropbox, From Google Drive)

Plots, Statistics, and Pathways section: Scatter plot, Profile plot, Histogram plot (Single, Multiple), Matrix plot, Venn Diagram plot (Entity List, Pathway List), Box and Whisker plot, Violin plot, Heatmap plot, Mass versus RT plot, Data spreadsheet, Summary statistics, Create new pathway list, and Select data source for plots (Raw, Raw Scaled, Log2 Normalized, Log10 Normalized).

Sidebar section: Hide or show the sidebars that contain the Project Navigator, Workflow Browser, and Legend.

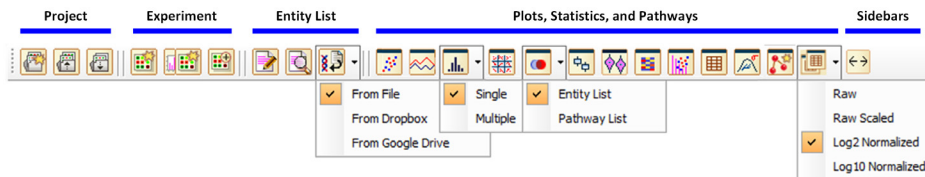


Figure 10 Toolbar and associated drop-down lists

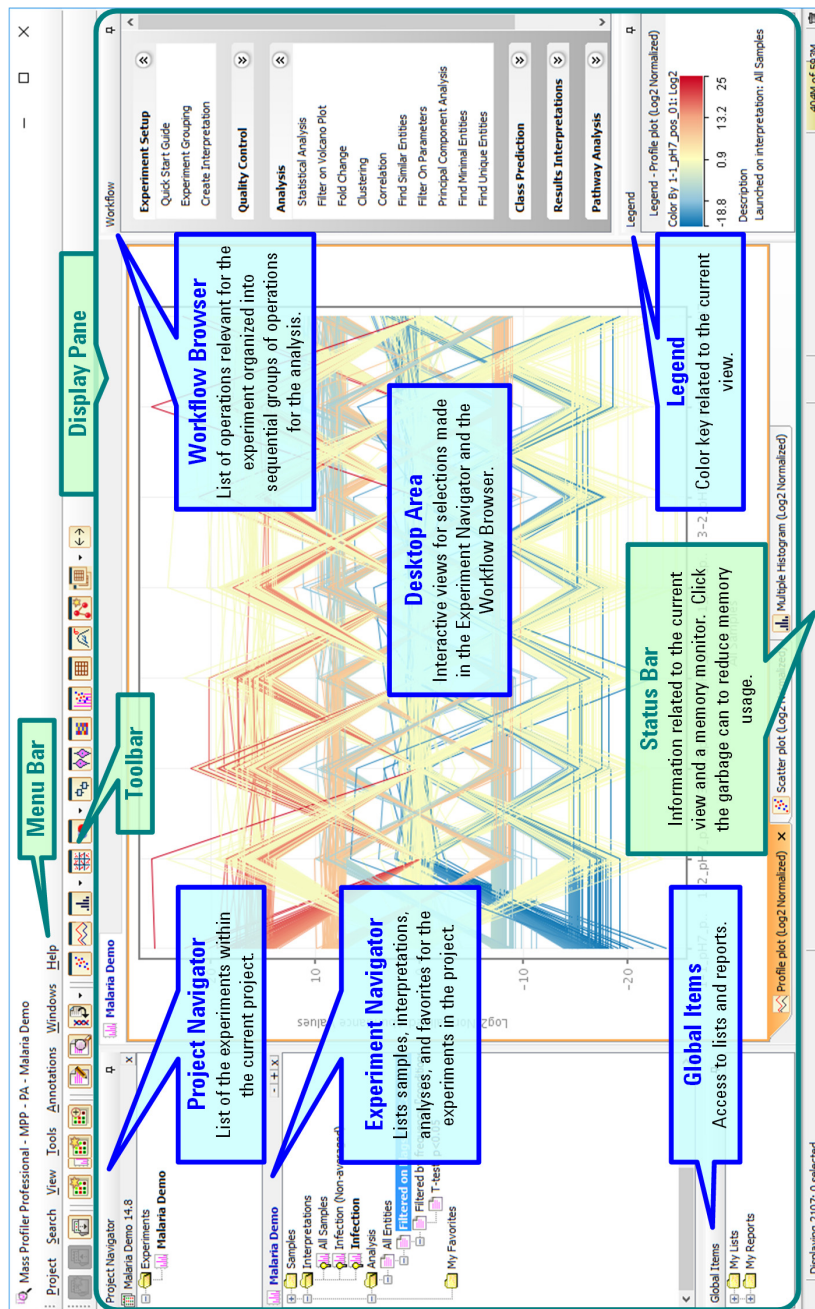


Figure 11 The main functional areas of the MPP software

Note: This figure is rotated on the page for printing.

3. Display Pane The display pane, see [Figure 11](#) on page 12, is further divided into six areas – Project Navigator, Experiment Navigator, Global Items, Desktop Area, Workflow Browser, and Legend.

Project Navigator

Displays the current project and lists all the experiments with the project.

Experiment Navigator

Displays information related to Samples, Interpretations, Analysis, and My Favorites in folders related to the selected experiment in the Project Navigator. Each experiment within a project has a separate experiment navigator pane.

Global Items

Displays list and report information for your project.

Desktop Area

Display of one or more interactive views associated with the experiments. Each view in the desktop area is marked with a tab and you can configure each view separately. Click **Windows > Tile** to arrange multiple views on the desktop. The current experiment, interpretation, and analysis are noted using bold font in the *Project Navigator* and *Experiment Navigator*.

A right-click anywhere in the active view shows you a menu of options ([Figure 12](#)) to customize the view, copy the view to the system clipboard, and export the view as an image file or as an HTML file.

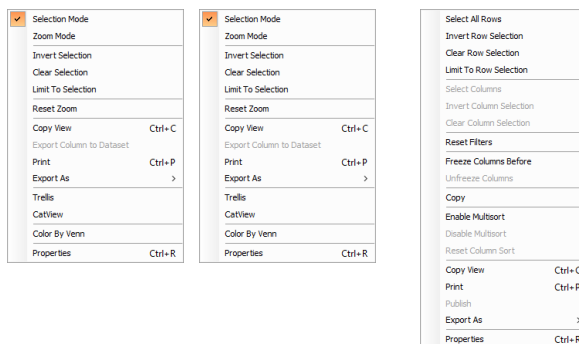


Figure 12 Right-click options within the desktop view automatically adjust to the type of view. These examples are from views containing plots and spreadsheets.

Workflow Browser

The Workflow Browser, [Figure 13](#), is organized into sequential groups of operations for the analysis of your data: Experiment Setup, Quality Control, Analysis, Class Prediction, Results Interpretations, Pathway Analysis (*optional*), NLP Networks (*optional*), and Utilities.

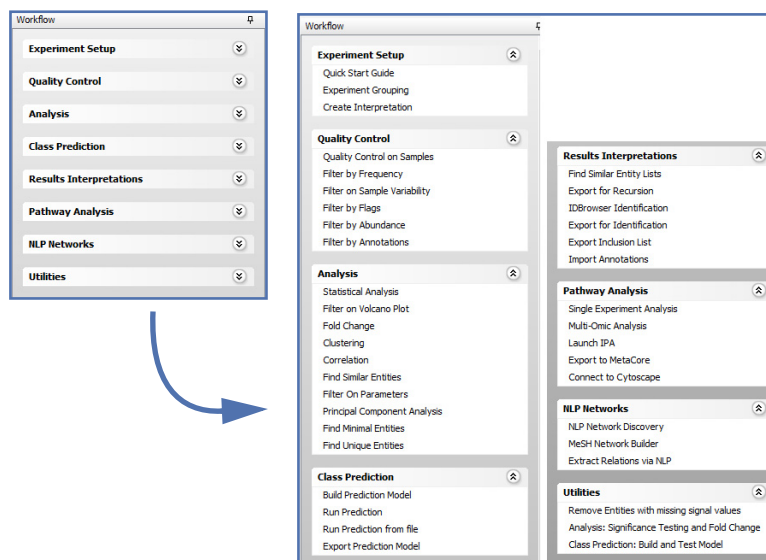


Figure 13 Workflow Browser view collapsed (left) and expanded to show the available operations (right)

Legend

The Legend ([Figure 14](#)) shows the key (scale) to the use of color in the active desktop view. Right-click on the Legend window to copy and export the legend as an image.

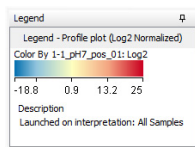


Figure 14 Legend

4. Status Bar The status bar (Figure 15) has three informative areas: the Status Area, the Ticker Area, and the Memory Monitor.

Status Area: Displays high-level information of the current view such as the number of rows and columns in table views and the number of entities or conditions selected in plot views.

Ticker Area: Displays the coordinates of the cursor in active plot views or the entity identification and value in table views.

Memory Monitor: Displays the total memory being used and the total memory allocated by MPP. You can click the **Garbage Can** icon  at any time to reduce the memory usage.



Figure 15 Status Bar



Basic Tasks

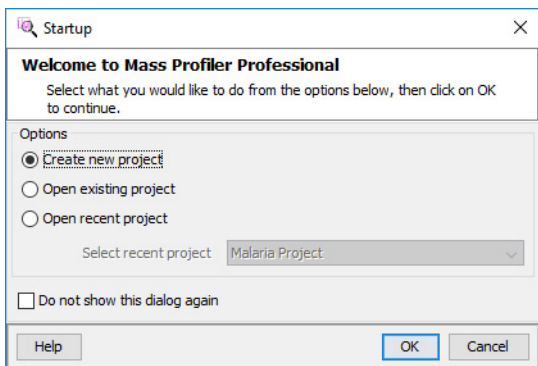
Set up a new project

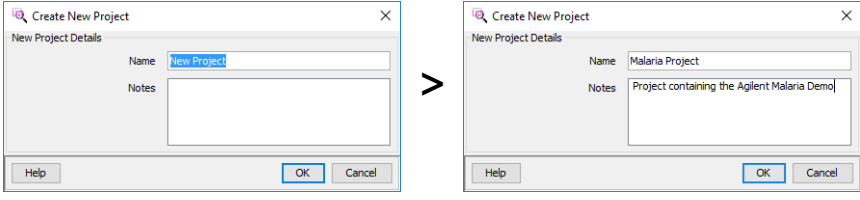


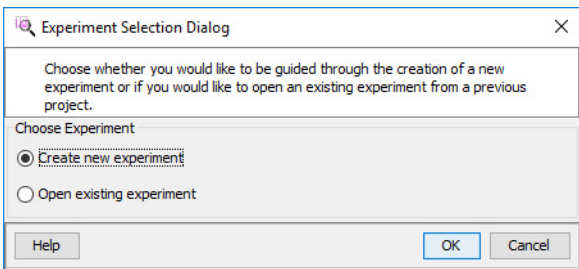
A project is a “container” for a collection of experiments, each experiment contains your samples, interpretations, and analyses. A project can have multiple experiments on different sample types and organisms.

Create a new project and experiment for your data

A new project and experiment is created through four sequential dialog boxes: (1) Startup, (2) Create New Project, (3) Experiment Selection, and (4) New Experiment. The Agilent *Malaria Demo* data supplied with MPP is used as an example in each step. You may substitute the malaria information with information for your data.

Steps	Detailed Instructions	Comments
1 Start Mass Profiler Professional.	<p>a Click the Mass Profiler Professional icon  on your desktop.</p>	<ul style="list-style-type: none"> The Startup dialog box helps you quickly set up a new project (this section) or continue your analysis with a previous project (see “Open a recent or existing project” on page 21).
2 Create a new project from the Startup dialog box.	<p>a Click Create new project. b Click OK.</p>	<ul style="list-style-type: none"> Create new project provides you with the option to create a new experiment or import an experiment from an existing project into the new project. After closing an open project, you may create a new project from the Menu bar, click Project > New Project, or from the Toolbar, click the New project  button.



Steps	Detailed Instructions	Comments
<p>3 Type descriptive information in the <i>New Project Details</i> section of the Create New Project dialog box.</p>	<p>a Type <code>Malaria Project</code> in Name. b Type <code>Project containing the Agilent Malaria Demo</code> in Notes. c Click OK.</p>	<ul style="list-style-type: none"> The project name and notes may be viewed and edited at any time using the Project Inspector by clicking Project > Inspect Project from the menu bar.
		
<p>4 Create a new experiment in the Experiment Selection Dialog dialog box.</p>	<p>a Click Create new experiment. b Click OK.</p>	<ul style="list-style-type: none"> You may create or add a new experiment to your project from the Menu bar, click Project > New Experiment, or from the Toolbar, click the New experiment  button, or click the Add experiment  button. If you click Open existing experiment, you are prompted for the experiment to add to the project as described in “Open a recent or existing project” on page 21.
		

Basic Tasks

Set up a new project

Steps	Detailed Instructions	Comments
5	Type and select information that guides the experiment creation in the New Experiment dialog box. <ol style="list-style-type: none">Type the descriptive name <code>Malaria Demo</code> in Experiment name. This name may be different from the project name.Select Mass Profiler Professional for Analysis type.Select Unidentified for the Experiment type.Select Analysis: Significance Testing and Fold Change for Workflow type.Type <code>Malaria LCMS ESI+ pH 7</code> in Experiment notes.Click OK.	<ul style="list-style-type: none">Experiment type determines how Mass Profiler Professional manages the data.Combined (Identified + Unidentified) is the proper Experiment type when you are unsure if the data has been identified in full or in part, or when other MassHunter software has been previously used to identify some of the compound features.Identified or Proteomics (Identified) is the proper Experiment type selection when the compounds have been identified by compound, formula, and/or CAS number.Unidentified is the proper Experiment type selection when the compounds have only been identified by their molecular features of neutral mass and retention time.

The screenshot shows the 'New Experiment' dialog box with the following values:

- Experiment name: `New Experiment`
- Analysis type: `Mass Profiler Professional`
- Experiment type: `Combined (Identified + Unidentified)`
- Workflow type: `Analysis: Significance Testing and Fold Change`
- Experiment notes: (empty text area)



The screenshot shows the 'New Experiment' dialog box with the following user-defined values:

- Experiment name: `Malaria Demo`
- Analysis type: `Mass Profiler Professional`
- Experiment type: `Unidentified`
- Workflow type: `Analysis: Significance Testing and Fold Change`
- Experiment notes: `Malaria LCMS ESI+ pH 7`

- Your new project is now set up.
- You are **immediately** guided through the steps to import and organize your data followed by the steps to create an initial analysis.

Import your data using the *MS Experiment Creation Wizard*

After you set up a project and create an experiment, the *MS Experiment Creation Wizard* guides you through the necessary steps to organize your experiment, import your data, define your experiment variables, and prepare your data for analysis. The *MS Experiment Creation Wizard* flow diagram is illustrated [Figure 16](#). The data preparation includes grouping, filtering, alignment, normalization, and baselining. The interactive training guide ***Getting Started with MPP*** (see “[Interactive Training and Videos](#)” on page 5) provides you through the steps to import and organize the *Malaria Demo* data. See the [Mass Profiler Professional Application Guide](#) for details to import non-Agilent data.

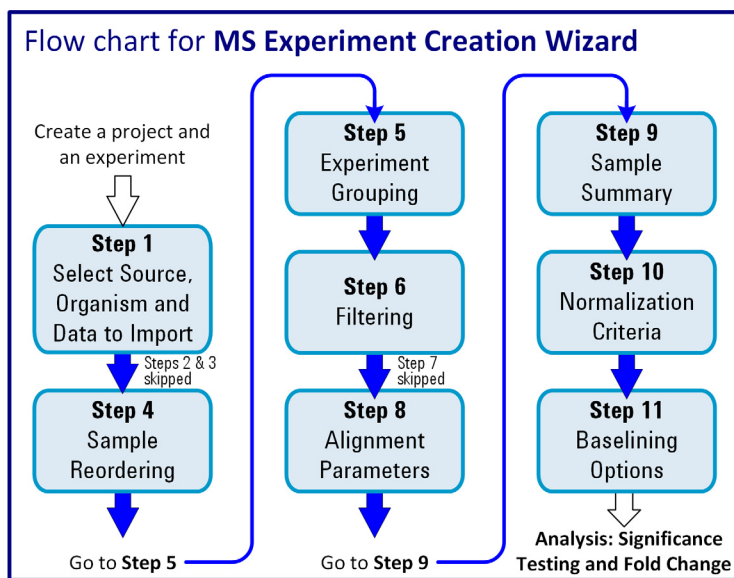


Figure 16 Steps in the *MS Experiment Creation Wizard* for the *Malaria Demo*.

Perform your initial differential analysis using the *Analysis: Significance Testing and Fold Change workflow*

The *Significance Testing and Fold Change Wizard* guides you through the steps necessary to enter parameters and values that improve the quality of your results and produce an initial differential expression for your analysis. The *Significance Testing and Fold Change Wizard* flow diagram is illustrated in [Figure 17](#). The [Mass Profiler Professional Familiarization Guide](#) (see “[Documents](#)” on page 4)

Basic Tasks

Perform your initial differential analysis using the Analysis: Significance Testing and Fold Change workflow

guides you through an initial differential analysis using the *Malaria Demo* data.

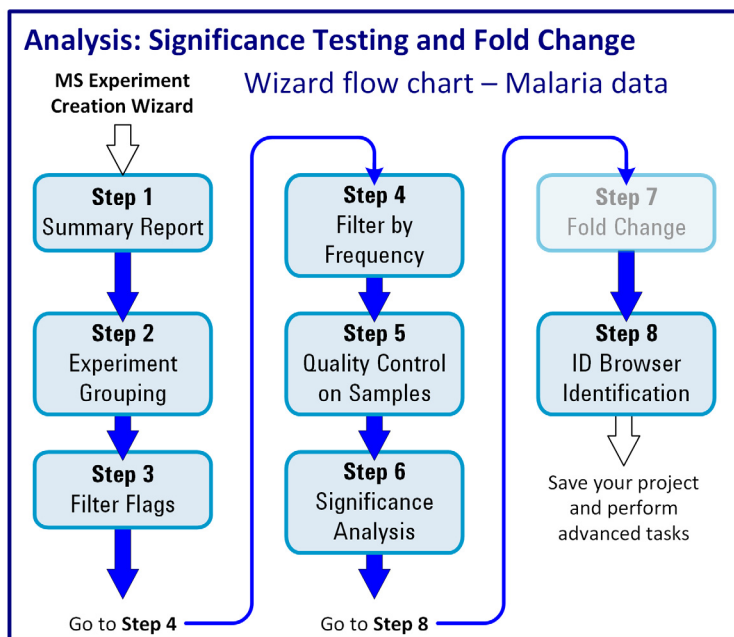



Figure 17 Steps in the “Analysis: Significance Testing and Fold Change Wizard” for the malaria data. Since Fold Change is combined with Step 6 for the malaria data, step 7 is skipped as a separate step.

Open a recent or existing project

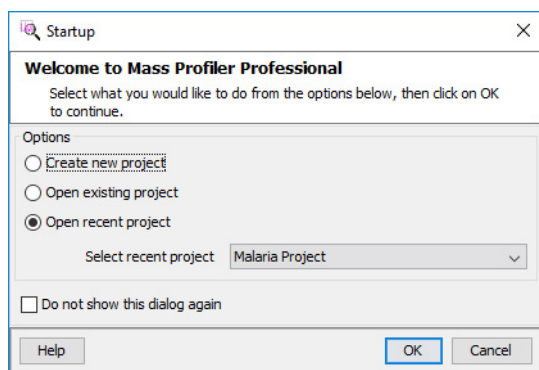
When you start Mass Profiler Professional the **Startup** dialog box allows you to quickly open a recent project, an existing project on your computer, or import an experiment from an existing project into a new project.

The steps presented are recommended if you are already familiar with the operations available in the Workflow Browser. If you are new to using Mass Profiler Professional start with “[Set up a new project](#)” on page 16 and then refer to the [Mass Profiler Professional Familiarization Guide](#) (see “[Documents](#)” on page 4).

Steps	Detailed Instructions	Comments
1 Start Mass Profiler Professional.	<p>a Click the Mass Profiler Professional icon  on your desktop.</p> <p>b Go to Step 2, Step 3, or Step 4.</p>	<ul style="list-style-type: none"> MPP begins with the Startup dialog box to help you quickly open a previous project: <p>Open recent project (go to Step 2) Open existing project (go to Step 3) Create new project (go to Step 4) and import an experiment from a previous project</p>

Open recent project:

- | | | |
|---|--|---|
| 2 Open a recent project in the Startup dialog box and select the Malaria project from the recent project list. | <p>a Click Open recent project.</p> <p>b Select Malaria Project from the Select recent project list.</p> <p>c Click OK.</p> | <ul style="list-style-type: none"> Open recent project opens the project and the experiment(s) that are stored in the project. If your project is not shown in the Select recent project list go to Step 3 and select it from the list of existing projects on your computer. A project is a container for a collection of experiments. A project can have multiple experiments on different sample types and organisms. You can now use the operations available in the Workflow Browser. |
|---|--|---|



Basic Tasks

Open a recent or existing project

Steps

Detailed Instructions

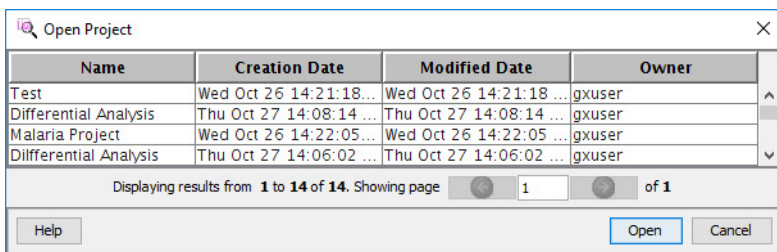
Comments

Open existing project:

- 3 Open an existing project in the **Startup** dialog box and select the Malaria project from the list of all of your existing projects.

- Click **Open existing project** in the **Startup** dialog box in Step 2 on [page 21](#).
- Click **OK**.
- Select the **Malaria Project** row from the **Open Project** dialog box.
- Click **Open**.

- **Open existing project** allows you to open a project that is no longer displayed in the recent project list.
- **Open existing project** opens the project and the experiment(s) that are stored in the project.
- When you have a large number of existing projects on your computer you may have to use the page navigation buttons in the **Open Project** dialog box.
- A selected project is highlighted by a color based on your PC's system settings.
- You can now use the operations available in the Workflow Browser.

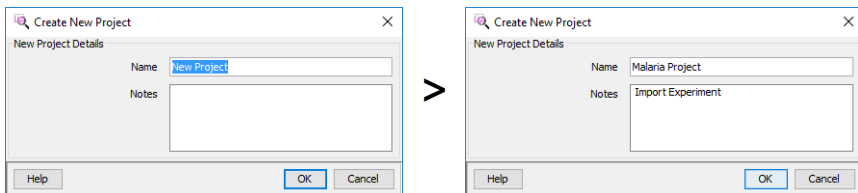


Create new project:

- 4 Create a new project in the **Startup** dialog box and import the experiment stored in the Malaria project into the new project.

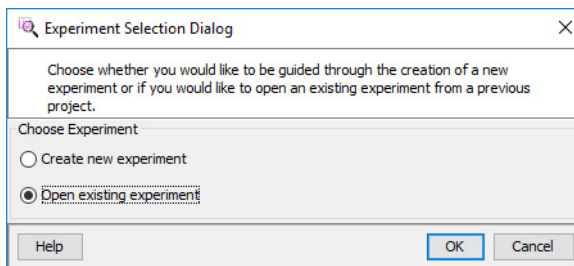
- Click **Create new project** in the **Startup** dialog box in step 2 on [page 21](#).
- Click **OK**.
- Type Malaria Project in **Name**.
- Type Import Experiment in **Notes**.
- Click **OK**.

- **Create new project** allows you to import an experiment from an existing project into the new project.
- See [“Set up a new project”](#) on page 16 for creating a new project and a new experiment.

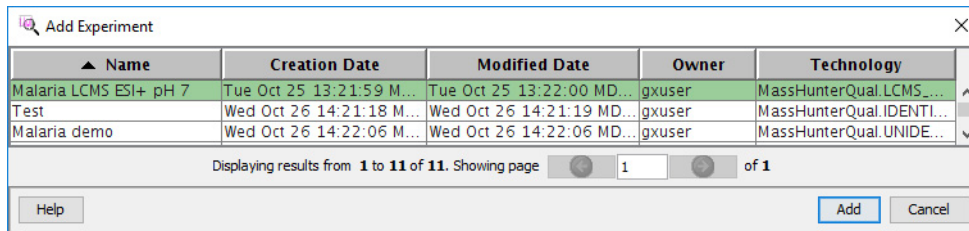


Steps	Detailed Instructions	Comments
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- f** Click **Open existing experiment** in the **Experiment Selection Dialog** dialog box.



- g** Select the **Malaria LCMS ESI+ pH 7** experiment in the **Add Experiment** dialog box
- h** Click **Add**.
- The selected experiment is shown highlighted using a background color.
 - The *Malaria LCMS ESI+ pH 7* experiment in the *Malaria* project is now imported into your new project and appears as if it was opened using **Open recent project**.
 - You can now use the operations available in the Workflow Browser.



Basic Tasks

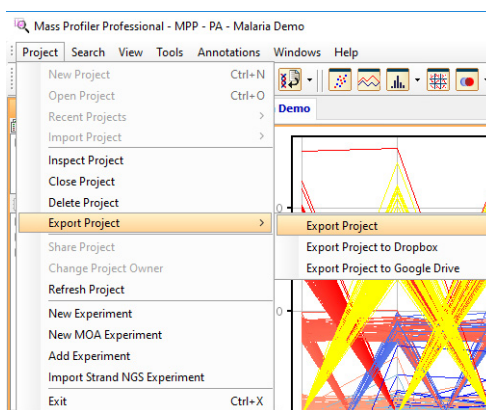
Save your project

Save your project

Save your current analysis as a TAR file for archiving, restoration of any future analysis to the current results, sharing the data with a collaborator, or sharing the data with Agilent customer support.

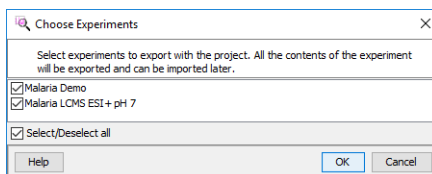
Steps	Detailed Instructions	Comments
1	Export your project to a TAR file.	

a Click **Project > Export Project**.



b Mark the check box next to the experiment you wish to save

c Click **OK**.



d Select or create the file folder.

e Type the **File** name.

f Click **Save**.

Advanced Tasks

Overview

The operations available in the Workflow Browser (see [Figure 13](#) on page 14) provide the tools necessary for analyzing features from your mass spectrometry data depending upon the need and aim of the analysis, the experiment design, and the focus of the study. This helps you create different interpretations to carry out the analysis based on the different filtering, normalization, and standard statistical methods.

Follow the procedures in the [Mass Profiler Professional Familiarization Guide](#) and [Mass Profiler Professional Application Guide](#) (see “Documents” on page 4) for increasingly detailed information to help you use MPP.

The [Agilent Metabolomics Workflow - Discovery Workflow Guide / Overview](#), , [Agilent Lipidomics - Workflow Guide / Overview](#), and the [Agilent MassHunter Mass Profiler Professional User Manual](#). (see “Documents” on page 4) provide you with techniques and explanations to perform advanced analysis tasks.

The interactive training guide ***MPP Training Videos*** (see “[Interactive Training and Videos](#)” on page 5) provides a substantial suite of brief training videos that cover how to use MPP to analyze your data.

Acknowledgment and Citations

BioCyc and KEGG

BioCyc Pathway/Genome Databases



Includes BioCyc Pathway/Genome databases from the Bioinformatics Research Group at SRI International®, used under license.

<http://www.biocyc.org/>

Citation based on use of BioCyc databases or the Pathway Tools software

If you use BioCyc databases or the Pathway Tools software in your research, cite relevant publications as described on the BioCyc website:

<http://biocyc.org/publications.shtml>

For example, users who publish research results in scientific journals based on use of data from the EcoCyc Pathway/Genome database should cite:

Keseler et al., *Nucleic Acids Research* **39**:D583-90, 2011.

Users who publish research results in scientific journals based on use of data from most other BioCyc Pathway/Genome databases should cite:

Caspi et al., *Nucleic Acids Research* **40**:D742-53, 2012.

KEGG Database



Includes KEGG (Kyoto Encyclopedia of Genes and Genomes) databases developed by Kanehisa Laboratories.

<http://www.genome.jp/kegg/>

Citation based on use of KEGG Database

If you use the KEGG database in your research, cite relevant publications as described on the KEGG website:

<http://www.genome.jp/kegg/kegg1.html>

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In this book

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G3835-90036



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