Agilent G3835AA MassHunter Mass Profiler Professional Software

Familiarization Guide

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, ICP-MS, and NMR 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.

How do I get started with Mass Profiler Professional?

MPP comes preloaded with a demonstration experiment to show you the functionality of the product. A project called “Malaria” contains an experiment called “Malaria LCMS ESI+ pH 7.” You are encouraged to explore this demonstration project to get to know Mass Profiler Professional. Use the familiarization tutorial to create your first project and experiment with the software.

Agilent Technologies

Familiarization Tutorial: How do I do a new analysis?

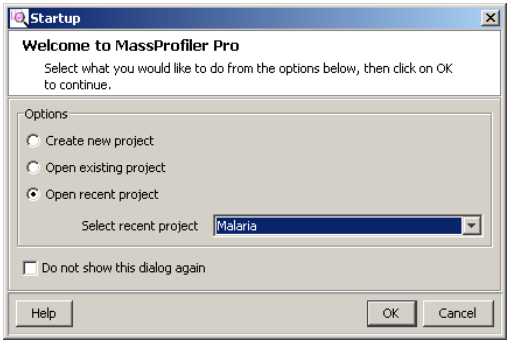
The steps of the familiarization tutorial are (1) Create a new project and experiment for your data, (2) Import and organize your data, (3) Perform your initial differential analysis, (4) Use MassHunter ID Browser to identify your compounds, and (5) Save your project

Exercise 1. Create a new project and experiment for your data

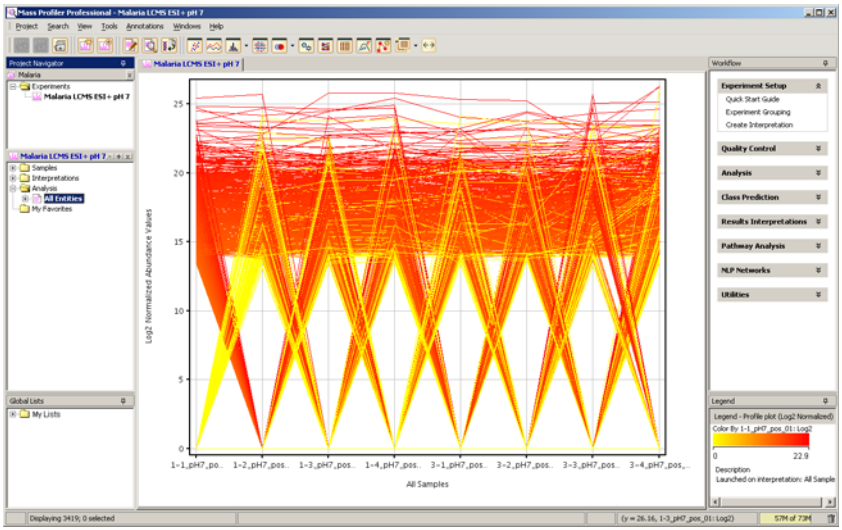
An easy way to start using the MPP software is to recreate the sample experiment from the demonstration project. The original *Malaria Demo* data you need is provided with the MPP installation. The data files are located in named folders within the main installation folder, usually found in **C:\Program Files\Agilent\MassHunter\Workstation\Mass Profiler Professional\samples** (Windows 7).

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. Follow the steps below to create a new experiment with the *Malaria Demo* data.

Steps	Detailed Instructions	Comments
1 Start Mass Profiler Professional.		
2 In the **Startup** dialog box, open a recent project or create a new project.	If you want to use the *Malaria* project: **a** Click **Open recent project**. **b** Select **Malaria** from the **Select recent project** list. **c** Click **OK**.	• The **Startup** dialog box helps you quickly set up a new project or continue your analysis with a previous project. • **Open recent project** opens the project and experiment(s) that are stored in the 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.

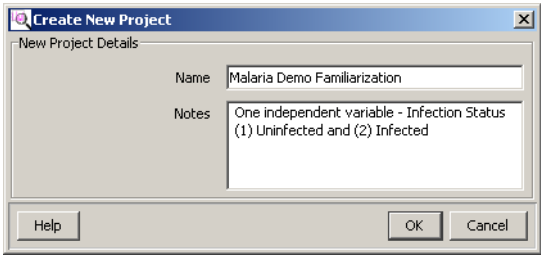


Steps	Detailed Instructions	Comments
	d Select an operation from the **Workflow Browser** to continue analyzing the *Malaria Demo* project.	• The **Workflow Browser** is found along the right sidebar and is organized in groups of operations.

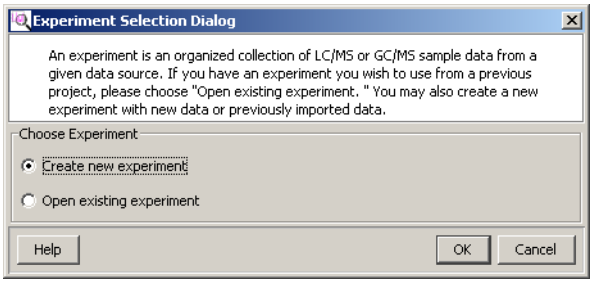


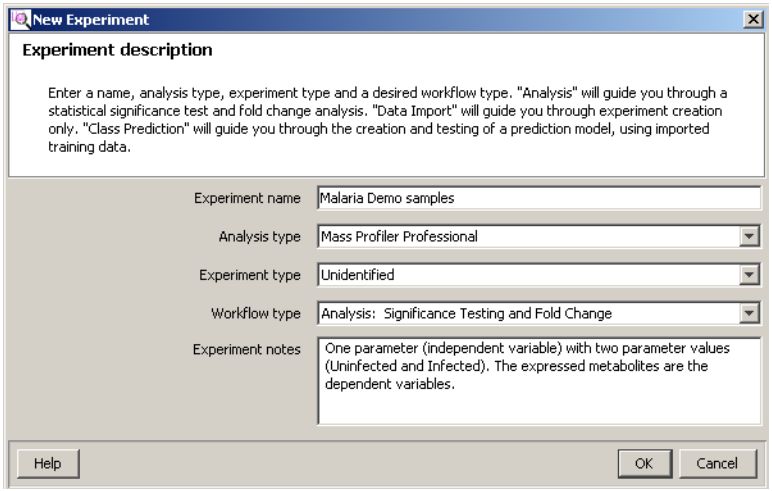
If you instead want to create a new project, click **Create new project** and go to Step 3, otherwise proceed to Exercise 4 on page 21.

3 In the **Create New Project** dialog box, enter your project information.	**a** Type `Malaria Demo Familiarization` in **Name**. **b** Type descriptive information in **Notes**. **c** Click **OK**.	• 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.



Steps	Detailed Instructions	Comments
4 In the **Experiment Selection Dialog** dialog box, create a new experiment.	**a** Click **Create new experiment**. **b** Click **OK**.	• If you click **Open existing experiment**, you are prompted for the experiment to add to the project. This is the same as clicking the **Add experiment** button  .
5 In the **New Experiment** dialog box, enter and select information that guides your experiment creation.	**a** Type a descriptive name for the experiment in **Experiment name**. **b** Select **Mass Profiler Professional** for **Analysis type**. **c** Select **Unidentified** for the **Experiment type**. **d** Select **Analysis: Significance Testing and Fold Change** for **Workflow type**. **e** Type descriptive information in **Experiment notes**. **f** Click **OK**.	• You may also create a new experiment from the Menu bar, click **Project > New Experiment,** or from the Toolbar, click the **New experiment** button  . • **Experiment type** determines how Mass Profiler Professional manages the data. • You select **Unidentified** when the compounds have only been identified by their molecular features of neutral mass and retention time. • You select **Identified** when the compounds have been identified by compound, formula, and/or CAS number. • You select **Combined (Identified + Unidentified)** when you are unsure if the data has been identified in full or in part, or when MassHunter Qualitative Analysis has been previously used to identify some of the compound features.





Exercise 2. Import and organize your data

After you set up a project and create an experiment, the **MS Experiment Creation Wizard** immediately 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 in Figure 1. The data preparation includes grouping, filtering, alignment, normalizing, and baselining.

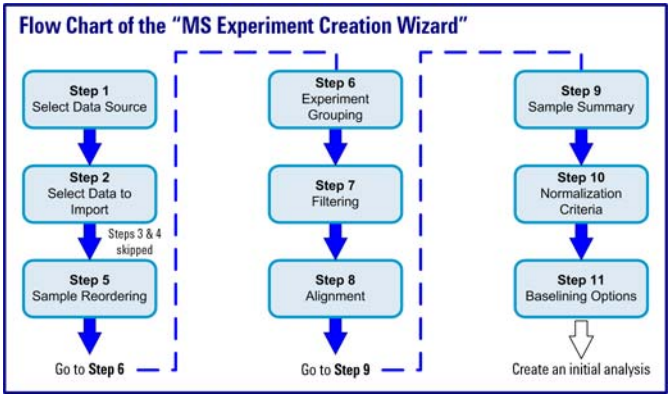
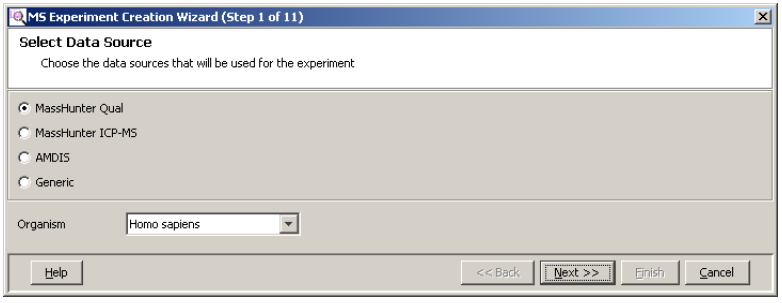
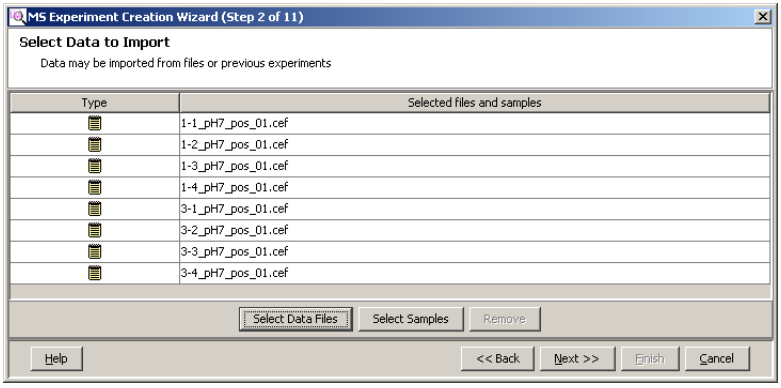


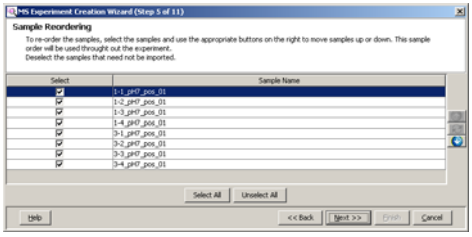
Figure 1 MS Experiment Creation Wizard

Steps	Detailed Instructions	Comments
1 Select the data source in the **MS Experiment Creation Wizard (Step 1 of 11)**.	**a** Click **MassHunter Qual** and select **Homo sapiens** for the **Organism** if you are using the *Malaria Demo* data set. **b** Click **Next**.	• If you are using your own data set, click the source of your sample files, and select the **Organism** of the sample files or select **None**. • Note that selecting an **Organism** is most important when you use the Pathway Analysis features of MPP.

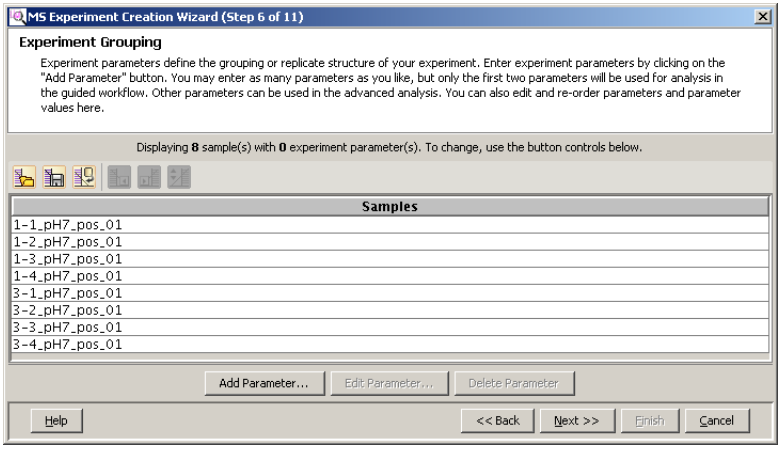


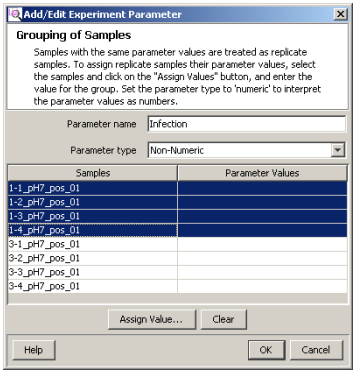
Steps	Detailed Instructions	Comments
2 Select the sample data to import in the **MS Experiment Creation Wizard (Step 2 of 11)**.	**a** Click **Select Data Files** to display the file selection dialog box. **b** Select all of the **.cef** files you want to import into the experiment. The example Malaria data files are: • 1-1_pH7_pos_01.cef • 1-2_pH7_pos_01.cef • 1-3_pH7_pos_01.cef • 1-4_pH7_pos_01.cef • 3-1_pH7_pos_01.cef • 3-2_pH7_pos_01.cef • 3-3_pH7_pos_01.cef • 3-4_pH7_pos_01.cef **c** Click **Open** to load the selected files. **d** Click **Next**.	• Note: The **Open** dialog likely already points to the **samples** directory in the main Mass Profiler Professional installation directory, but if not, browse to **C:\Program Files\Agilent\MassHunter\Workstation\Mass Profiler Professional\samples\Malaria Demo**. • A progress indicator is displayed while the files are being loaded into MPP.
3 Review and order the selected files that you are importing in the **MS Experiment Creation Wizard (Step 5 of 11)**.	**a** Review the order of your samples. The order does not need to be changed unless an entry is out of sequence. **b** Click **Next**.	• Note: This step presents you with the only opportunity you have to reorder your samples. • The sample order shown in this step is used in subsequent views where the results are organized by sample.

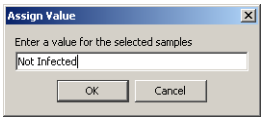
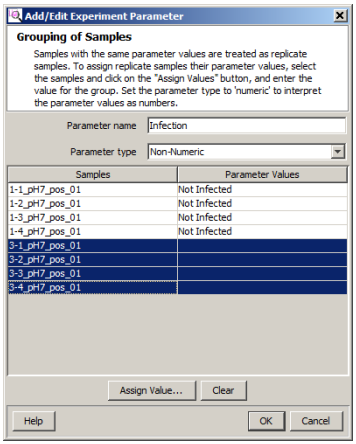
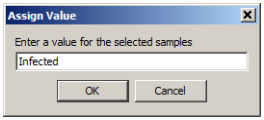
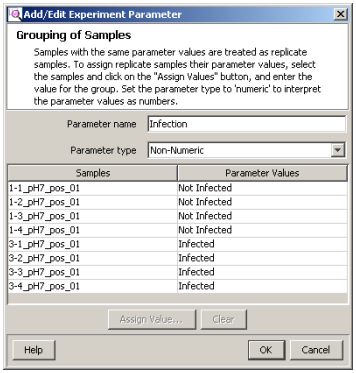


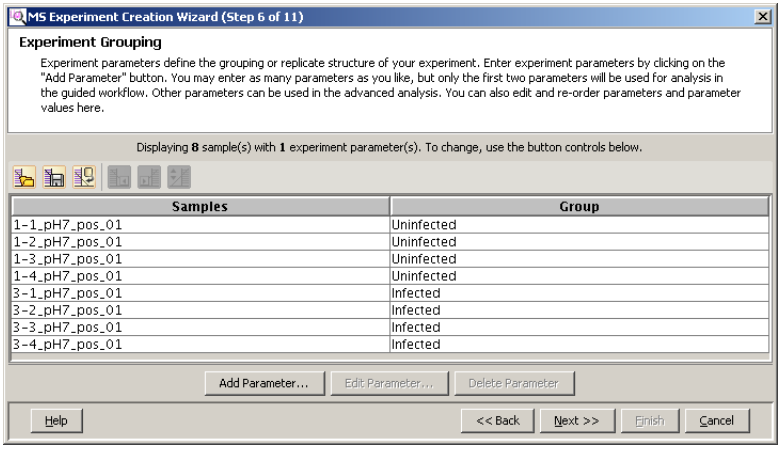


Steps	Detailed Instructions	Comments
4 Define the sample grouping with respect to the independent variables and the replicate structure of your experiment in the **MS Experiment Creation Wizard (Step 6 of 11)**.	**a** Click **Add Parameter**.	• In **Experiment Grouping**, samples with the same parameter values are treated as replicates. • For the *Malaria Demo* samples you specify which files contain data from infected samples and which contain data from uninfected samples. • An independent variable is an essential element, constituent, attribute, or quality in a data set that is deliberately controlled in your experiment. An independent variable is referred to as a parameter and is assigned a parameter name. • The attribute values within an independent variable are referred to as parameter values. Samples with the same parameter value.

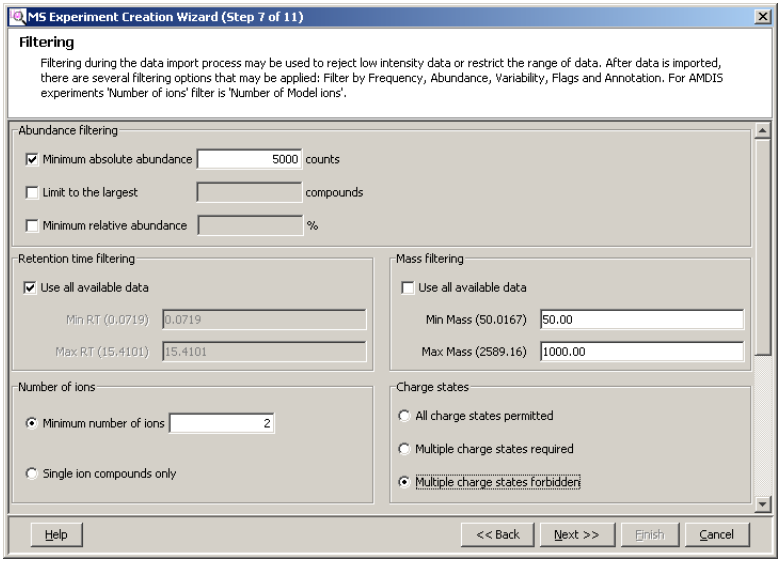
	**b** Type a name for your **Parameter name** in the **Add/Edit Experiment Parameter** dialog box. Type `Infection` for the *Malaria Demo*.
	c Click your replicate **Samples** that share the same first parameter value in your data. For example:
	• 1-1_pH7_pos_01
	• 1-2_pH7_pos_01
	• 1-3_pH7_pos_01
	• 1-4_pH7_pos_01
	d Select the **Parameter type** for your grouping. **Non-Numeric** is selected for the *Malaria Demo*.
	e Click **Assign Value**.
		• Parameter Type options:
		  • Select **Non-Numeric** if the grouping is not a quantitative value.
		  • Select **Numeric** if the grouping value is quantitative or a value that reflects a degree of proportionality among the samples with respect to an independent variable. A numeric parameter type allows some data plots to be scaled by the parameter values.

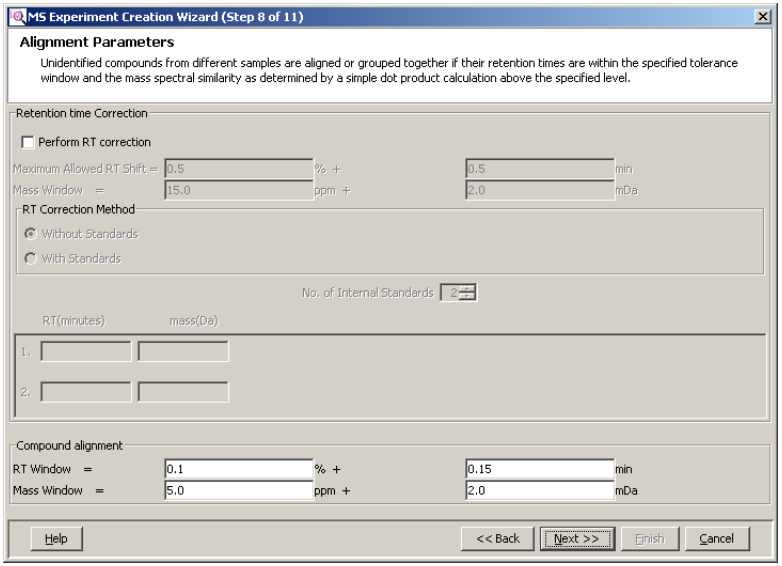
Steps	Detailed Instructions	Comments
	**f** Type the value for your first grouping in the **Assign Value** dialog box. For the *Malaria Demo* type `Not Infected`. **g** Click **OK**.	• In the *Malaria Demo* example the samples are assigned parameter values representing the Infection parameter name. • The highlighted samples are assigned the value typed in the **Assign Value** dialog box. • You may change the value of any sample, or group of samples; highlight the sample and click **Assign Value** or **Clear**.
	**h** Click your replicate **Samples** that share the same second parameter value in your data. For example: • 3-1_pH7_pos_01 • 3-2_pH7_pos_01 • 3-3_pH7_pos_01 • 3-4_pH7_pos_01 **i** Click **Assign Value**.	
	**j** Type the value for your second grouping in the **Assign Value** dialog box. For the Malaria data type `Infected`. **k** Click **OK**.	
	**l** Review your entries and grouping assignment accuracy in the **Add/Edit Experiment Parameter** dialog box. **m** Click **OK** when the grouping for this parameter name is complete.	

Steps	Detailed Instructions	Comments
	n Click **Next** when you have completed your experiment grouping.	• You can save your experiment grouping in a tab separated value (TSV) file by using the **Save experiment parameters to file** button .
		• You can view, edit, and create TSV files using Microsoft Excel or Windows Notepad. • By using the **Load experiment parameters from file** button you can quickly apply a previously created or saved experiment grouping. • ***Note:*** You may also add grouping or change your grouping during the **Analysis: Significance Testing and Fold Change Wizard** and at any time thereafter.

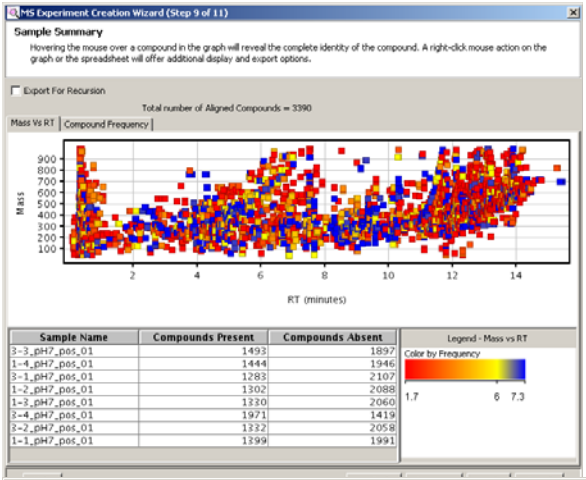
Steps	Detailed Instructions	Comments
5 Select and enter the data filter parameters in the **MS Experiment Creation Wizard (Step 7 of 11)**.	**a** Mark the **Minimum absolute abundance** check box under Abundance filtering. **b** Type a value of `5000` **counts**. **c** Clear the **Limit to the largest** and **Minimum relative abundance** check boxes. **d** Mark the **Use all available data** check box under Retention time filtering. **e** Clear the **Use all available data** check box and type `50` for **Min Mass**, and type `1000` for **Max Mass** under Mass filtering. **f** Click **Minimum number of ions** and type `2` for **Minimum number of ions** under Number of ions. **g** Click **Multiple charge states forbidden** under Charge states. **h** Click **Next**.	• Filtering during the data import process may be used to reject low-intensity data or restrict the mass spectral range of your data. • In Find Compounds by Formula (FbF) generated data files the term abundance actually refers to the feature volume. Whereas, in Find Compounds by Molecular Feature (MFE) generated data files the term abundance actually refers to the feature chromatographic area. • Filtering by mass may improve your statistical analysis by rejecting masses that are not significant to the experiment. • Filtering works with both GC/MS and LC/MS data.

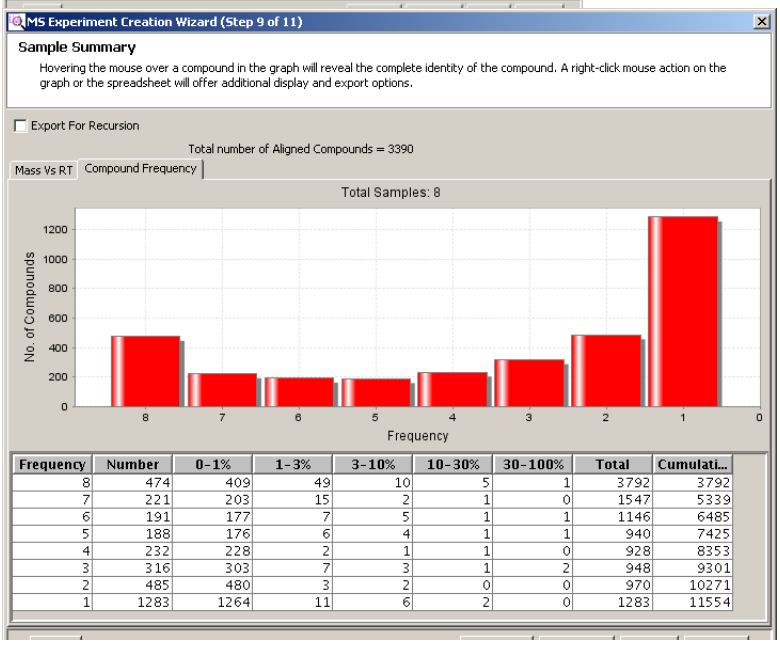


Steps	Detailed Instructions	Comments
6 Select and enter the retention time and mass alignment parameters in the **MS Experiment Creation Wizard (Step 8 of 11)**.	**a** Clear the **Perform RT Correction** check box under Retention time Correction. **b** Type `0.1` **%** and `0.15` **min** for **RT Window** under Compound alignment. **c** Type `5.0` **ppm** and `2.0` **mDa** for **Mass Window**. **d** Click **Next**.	• Alignment parameters are used by MPP to align and group compounds by similar mass and retention time across multiple sample files. The values you enter depend on your experimental conditions and the resolution of your MS instrument. • In general, a larger retention time shift may be used to compensate for less than ideal chromatography and a smaller mass window may be used for higher resolution mass spectrometers. • It is recommended to inspect the quality of your sample data to determine the best values for your alignment parameters.



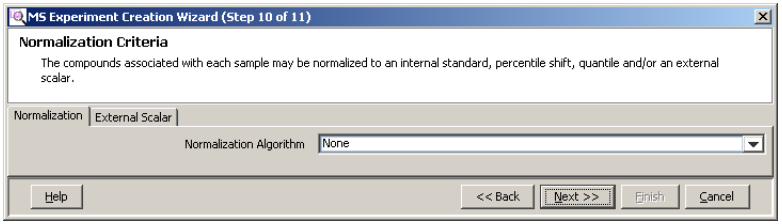
Steps	Detailed Instructions	Comments
7 View and review the compounds present and absent in each sample in the **MS Experiment Creation Wizard (Step 9 of 11)**.	**a** Clear the **Export For Recursion** check box. **b** Click **Next**.	• The unidentified compounds are aligned, and MPP displays summary data from the alignment. • The Compound Frequency chart and table report the number of *common* entities that appear in your samples (i.e., there are 474 entities that appear in all 8 samples, and 1283 entities that appear in only 1 sample - "one-hit wonders"). The percent columns show you abundance distribution of the *identical* entities normalized to the most abundant *common* entity. • If most of the "one-hit wonders" have a low relative abundance your sample data alignment is likely good. If the "one-hit wonders" have a high relative abundance (i.e., in the 30-100% column) then you may need to improve your sample data alignment. • In the Mass vs. RT table, replicate samples are expected to have a similar number of compounds present and absent. • Any part of the sample summary may be exported; **right-click** on that part of the summary. Click **Export As**, and click the image type. The option **Image** allows you to enter the image file location, file name, image size, and resolution to meet your publication requirements.

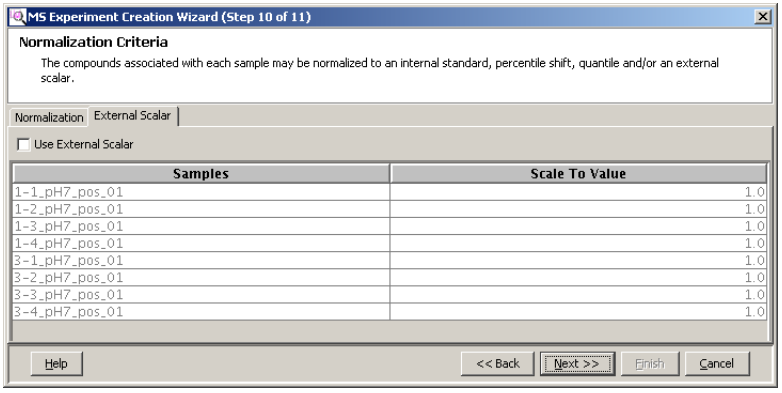




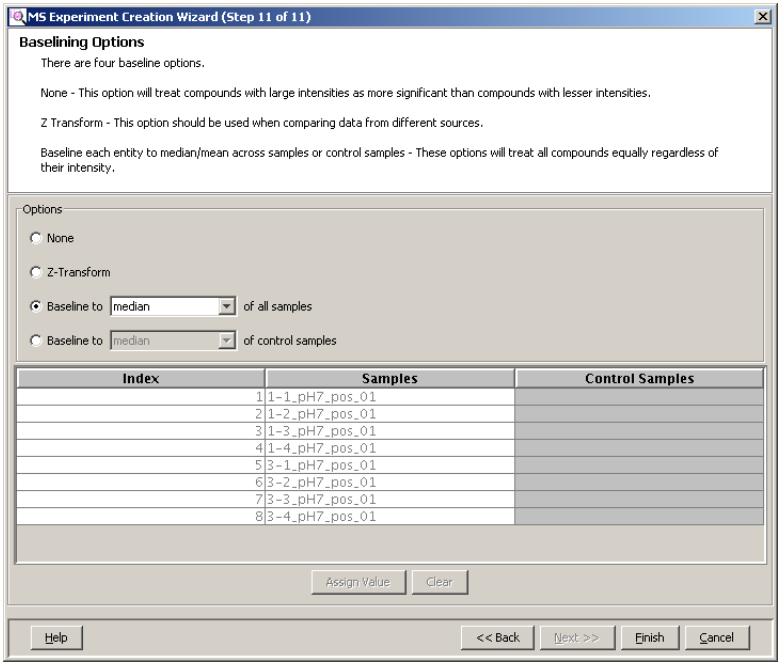
Frequency	Number	0-1%	1-3%	3-10%	10-30%	30-100%	Total	Cumulati...
8	474	409	49	10	5	1	3792	3792
7	221	203	15	2	1	0	1547	5339
6	191	177	7	5	1	1	1146	6485
5	188	176	6	4	1	1	940	7425
4	232	228	2	1	1	0	928	8353
3	316	303	7	3	1	2	948	9301
2	485	480	3	2	0	0	970	10271
1	1283	1264	11	6	2	0	1283	11554

Steps	Detailed Instructions	Comments
8 Select whether to normalize the data to reduce the variability caused by sample preparation and instrument response in the **MS Experiment Creation Wizard (Step 10 of 11)**.	**a** Select **None** for the **Normalization Algorithm** in the Normalization tab. **b** Clear the **Use External Scalar** check box in the External Scalar tab. **c** Click **Next**.	• You may use normalization and external scalar techniques to reduce the variability caused by sample preparation and instrument response in your data.





Steps	Detailed Instructions	Comments
9 Select whether to compare features in each sample to the response of the features across multiple samples in the **MS Experiment Creation Wizard (Step 11 of 11)**.	**a** Click **Baseline to ____ of all samples**. **b** Select **median** for the **Baseline to ____ of all samples**. **a** Click **Finish**.	• There are four baselining options: • **None:** Recommended if only a few features in the samples exist. • **Z-Transform:** Recommended if the data sets are very dense, i.e., with data where very few instances of compounds are absent from any sample, such as a quantitation data set from recursion. • **Baseline to ____ of all samples:** The abundance for each compound is normalized to its selected statistical abundance across all of the samples. This has the effect of reducing the weight of very large and very small compound features on later statistical analyses. • **Baseline to ____ of control samples:** The abundance for each compound is normalized to its selected statistical abundance across just the samples selected as the control samples. This has the effect of weighting the compound features to a known value that is considered to be normal in the population while reducing the effect of large and small compound features.
10 Continue to improve the quality of your results and produce an initial differential expression for your analysis.	Because you chose **Analysis: Significance Testing and Fold Change** for **Workflow type** in the **New Experiment** dialog box you are immediately directed to the next exercise.	• If you chose **Data Import Wizard** for **Workflow type** in the **New Experiment** dialog box you are done creating your experiment and can use the operations available in the Workflow Browser.



Exercise 3. Perform your initial differential analysis

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 2.

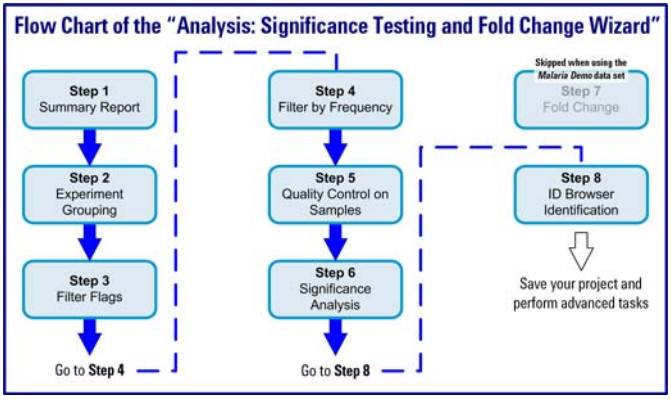
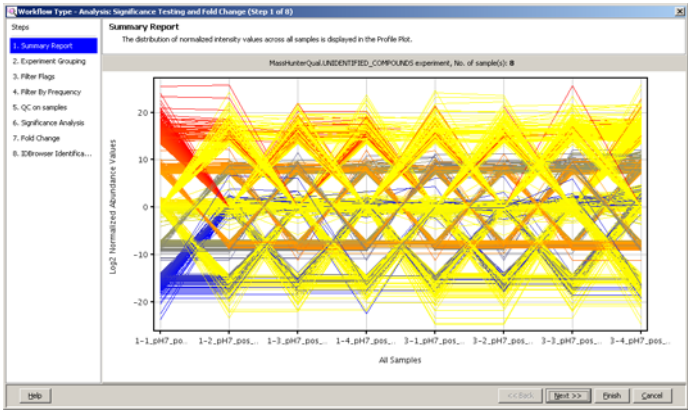
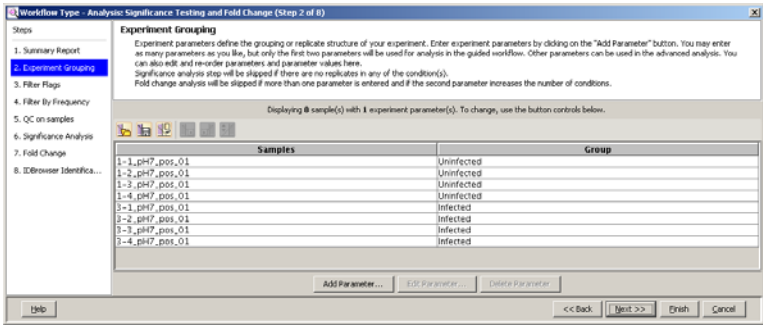
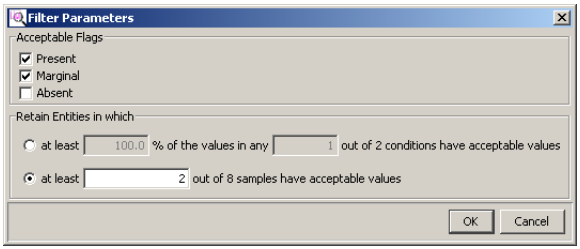


Figure 2 Analysis: Significance Testing and Fold Change Wizard

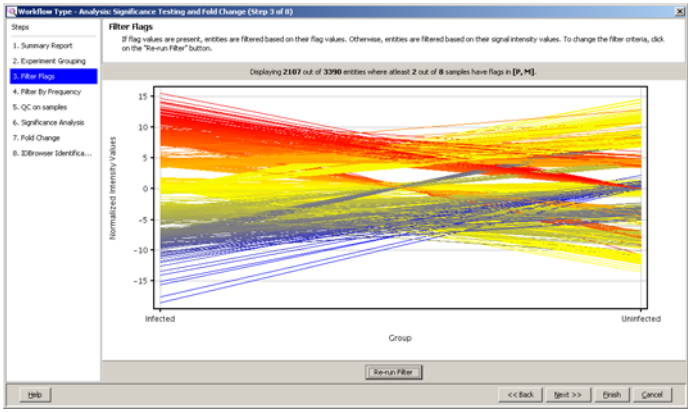
Steps	Detailed Instructions	Comments
1 Summary Report (Step 1 of 8): Review your data in the **Summary Report** workflow step. 	**a** Verify that you see the **Analysis: Significance Testing and Fold Change Wizard** as shown below. **b** Click **Next**.	• The **Analysis: Significance Testing and Fold Change Wizard** shows a profile plot and a series of steps to finish the experiment setup and your initial analysis. The current step is highlighted. • You do not enter analysis parameters at this time. You may review the data, change the plot view, export selected data, or export the plot to a file by a **click** or **right-click** at desired features available on the plot.

Steps	Detailed Instructions	Comments
2 Experiment Grouping (Step 2 of 8): Enter the sample grouping with respect to the independent variables and the replicate structure of your experiment in the **Experiment Grouping** workflow step.	**a** Verify that your **Experiment Grouping** looks like the example below. **b** Click **Next.**	• In **Experiment Grouping**, samples with the same parameter values are treated as replicates. • In the *Malaria Demo* samples you specify which files contain data from infected samples and which contain data from uninfected samples. • If you are using your own data set, click **Add Parameter** and set up a parameter and enter the parameter values for each data file and return to this display.
3 Filter Flags (Step 3 of 8): Enter values that filter entities in your samples based on the quality of their presence in specified samples and conditions in the **Filter Flags** workflow step.	**a** Review your data, change the plot view, export selected data, or export the plot to a file. **b** Click **Re-run Filter** to enter parameters in the **Filter Parameters** dialog box. **c** Mark the **Present** and **Marginal** check boxes. **d** Clear the **Absent** check box. **e** Click **at least ___ out of X samples have acceptable values** and type 2 in the entry box. By setting this parameter to a value of two or more, "one-hit wonders" are filtered. **f** Click **OK**.	• A flag is used to denote the quality of an entity within a sample. A flag indicates if the entity was detected in each sample as follows: Present means the entity was detected, Absent means the entity was not detected, and Marginal means the signal for the entity was saturated. • This filter removes irreproducible entities from further consideration as you continue your analysis. • A major objective of Filter Flags is to remove "one-hit wonders" from further consideration. A "one-hit wonder" is an entity that appears in only one sample, is absent from the replicate samples, and does not provide any utility for statistical analysis.

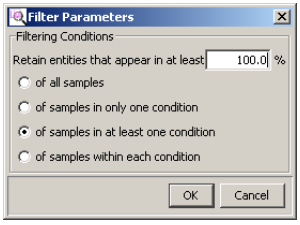




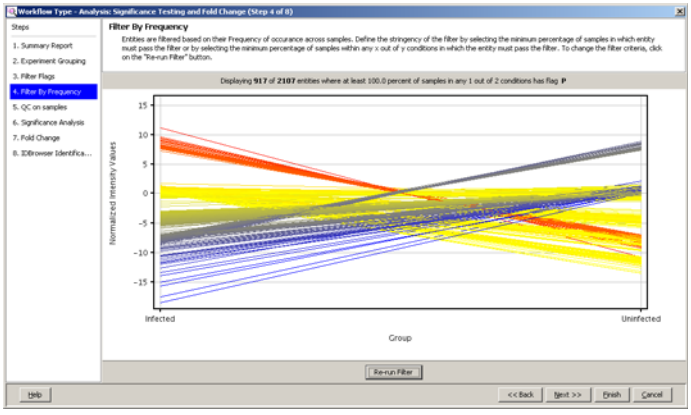
Steps	Detailed Instructions	Comments
	g Review the profile plot and repeat the **Re-run Filter** until you obtain the best results for your experiment. **h** Click **Next.**	



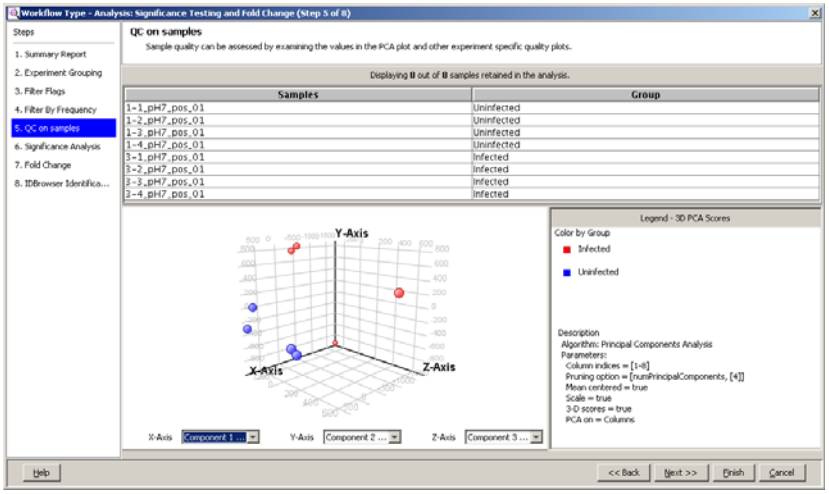
4 Filter by Frequency (Step 4 of 8): Enter values that filter the remaining entities in your samples based on their frequency of occurrence among the samples and conditions in the **Filter by Frequency** workflow step.	**a** Review your data, change the plot view, export selected data, or export the plot to a file. **b** Click **Re-run Filter** to enter parameters in the **Filter Parameters** dialog box. **c** Type `100` in the **Retain entities that appear in at least** box. **d** Click **of samples in at least one condition**. **e** Click **OK**.	• Filter Frequency allows you to filter the input data based upon the frequency with which any compound appears in each sample in the experiment. The filter is specified by typing the minimum percentage and selecting the applicable condition.



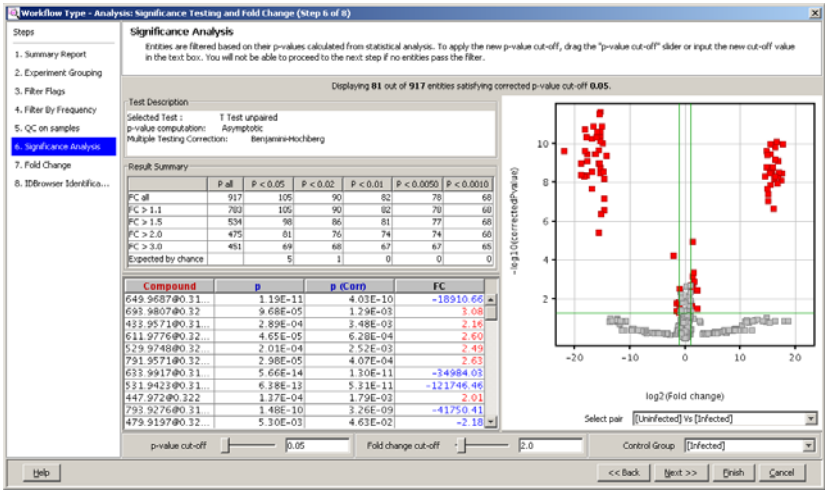
Steps	Detailed Instructions	Comments
	f Review the profile plot and repeat the **Re-run Filter** until you obtain the best results for your experiment. **g** Click **Next.**	



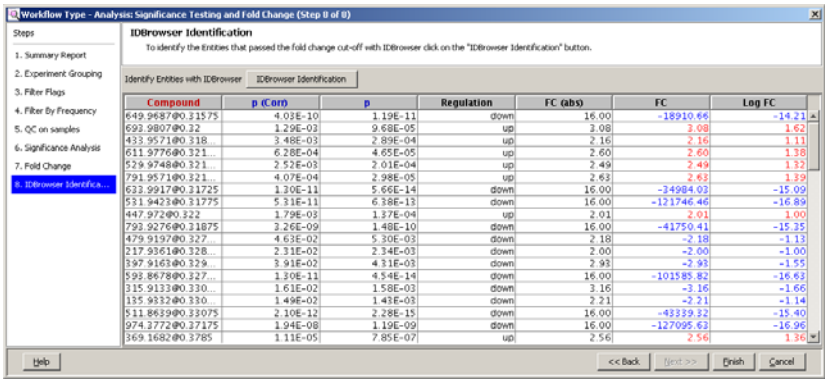
5 QC on samples (Step 5 of 8): Assess the sample quality of your experiment using the **QC on samples** workflow step.	**a** Review your data, change the plot view, export selected data, or export the plot to a file. **b** Click **Next**.	



Steps	Detailed Instructions	Comments
6 Significance Analysis (Step 6 of 8): Assess the differential significance and fold change of your samples using the **Significance Analysis** workflow step.	**a** Review your data, change the plot view, export selected data, or export the plot to a file. **b** Move the **p-value cut-off** slider or type a value to make adjustments. The default value is 0.05. **c** Move the **Fold change cut-off** slider or type a value to make adjustments. The default value is 2.0. **d** Click **Next**.	• In Significance Analysis, entities are filtered based on their p-values calculated from statistical analysis. • The entities that satisfy the Significance Analysis are passed on for the Fold Change Analysis. • MPP shows the fold change of the abundance value for each compound across the various samples in the experiment. • Set the fold change filter so that you focus on the compounds that have intensity values that are most significant among the samples in the experiment. • The Significance Analysis wizard page allows you to adjust the cutoff values for either the p-value or fold change.
7 Significance Analysis (Step 7 of 8): Because Fold Change was included in the prior step (Step 6 of 8), this separate Fold Change step is skipped.		• Fold Change is included in Step 6 of 11 because the significance analysis is a t-test due to the data consisting of one parameter with two conditions (parameter values).

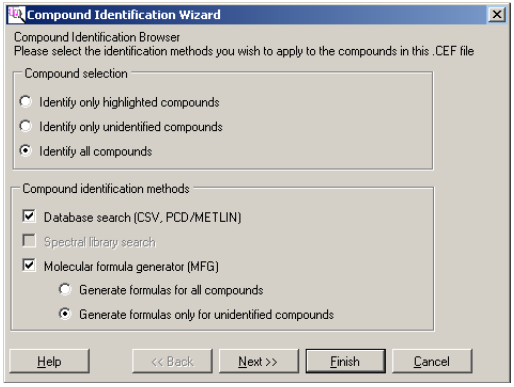
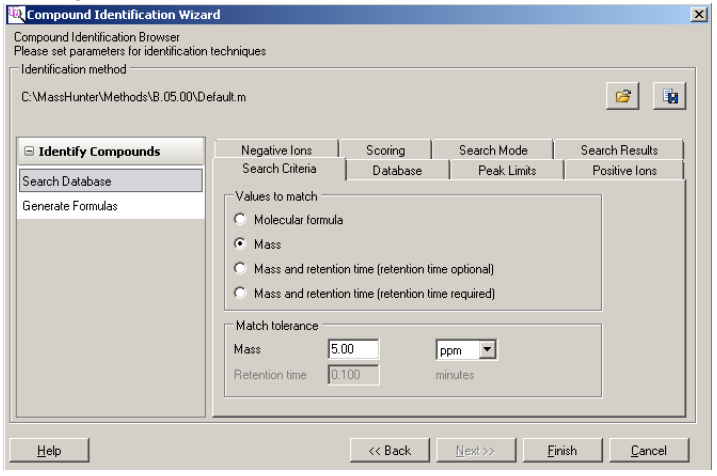


Steps	Detailed Instructions	Comments
8 Significance Analysis (Step 8 of 8): Identify the entities in your experiment using the **IDBrowser Identification** workflow step.	**a** Review the table of compounds that remain after all of the previous filtering steps. **b** Click **IDBrowser Identification**. **c** Continue with the next exercise.	• The compounds remaining are also referred to as entities. • The compounds are identified only by their mass and retention time in the *Compound* column of the table. • ID Browser helps you identify the compounds in the table.

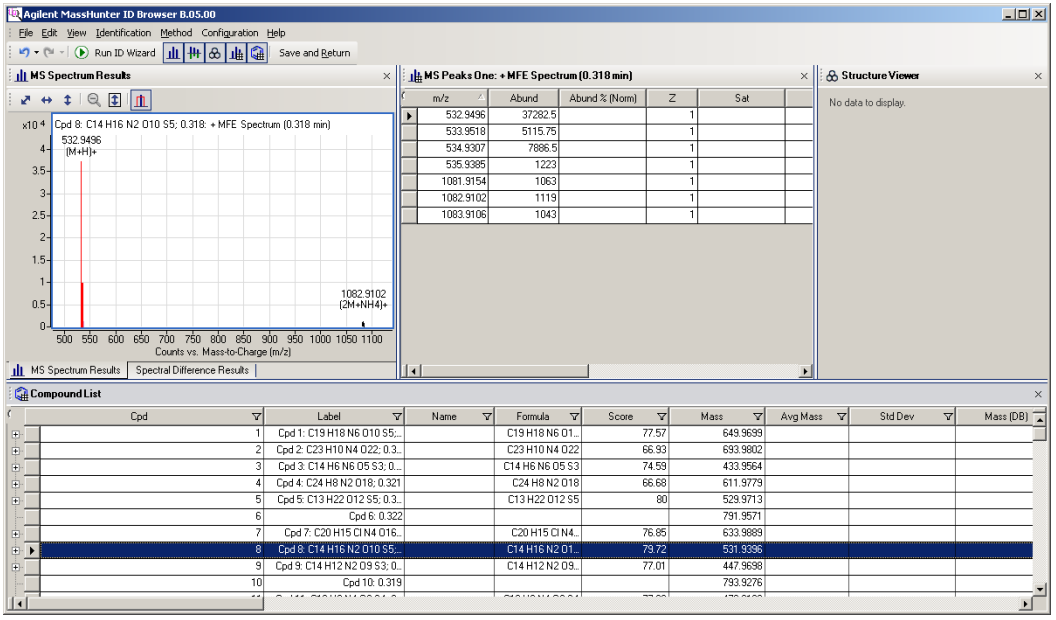


Exercise 4. Use MassHunter ID Browser to identify your compounds

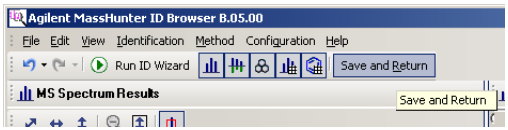
Identify the compounds that remain after applying the filtering steps of the **Significance Testing and Fold Change Wizard**.

Steps	Detailed Instructions	Comments
1 Set up your identification method in the first dialog box of the **Compound Identification Wizard**. 	**a** Review the identification method. **b** Click **Next**.	• When you launch ID Browser it receives the list of entities (also referred to as compounds) from the last step of the previous exercise. • If you started ID Browser from the Workflow Browser, click **Run ID Browser** on the ID Browser toolbar.
2 Set the parameters for your identification technique in the second dialog box of the **Compound Identification Wizard**. 	**a** Review the identification techniques. **b** Click **Finish**.	• ID Browser provides you with many ways to adjust the identification algorithm. • Click **Help** to get a full description of the options and features available to set up your identification technique.

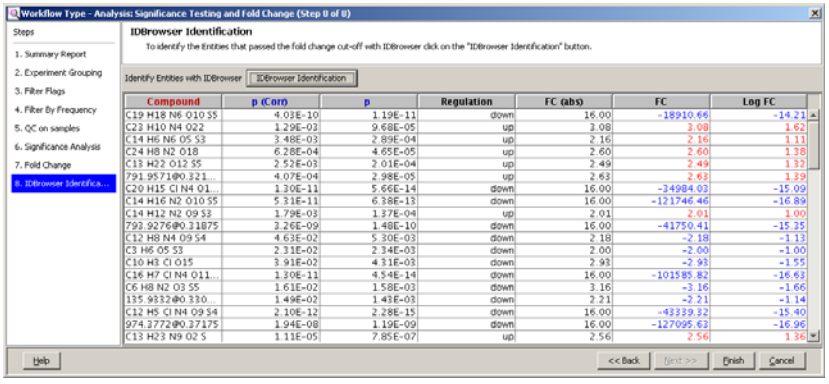
Steps	Detailed Instructions	Comments
3 Review and adjust your identifications.	**a** Review the identification technique. **b** Click **Finish**.	• ID Browser shows you information about each identified entity and gives you the ability to make adjustments to the identifications.



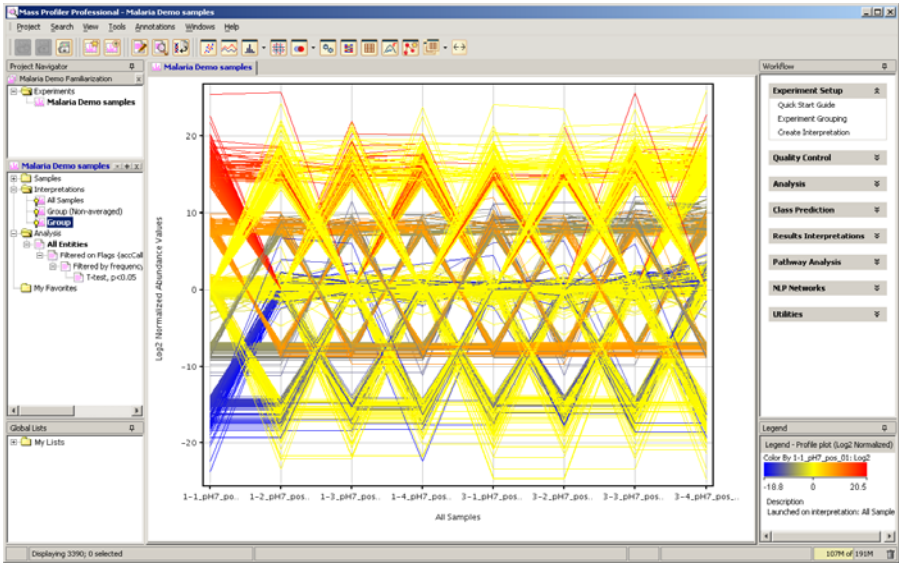
4 Accept the current identifications and return to Mass Profiler Professional.	**a** Click **Save and Return** on the ID Browser toolbar.	• ID Browser sends all of the information it has generated back to your entity list in Mass Profiler Professional.



Steps	Detailed Instructions	Comments
5 Examine the results in Mass Profiler Professional.	**a** Study the compounds that are now identified in the compound table. **b** Click **Finish**.	• The compound column in the table shown in **Significance Analysis (Step 8 of 8)** is updated with your identifications from ID Browser.



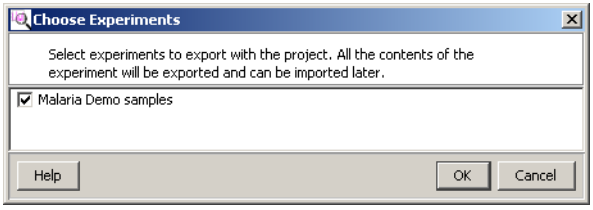
6 Review the profile plot, the **Analysis: Significance Testing and Fold Change Wizard** is now complete.	**a** Review the profile plot. **b** Click on any entity list in the Experiment Navigator to review the results.	• You can follow the results from your analysis in the hierarchical presentation in the Experiment Navigator on the left sidebar.



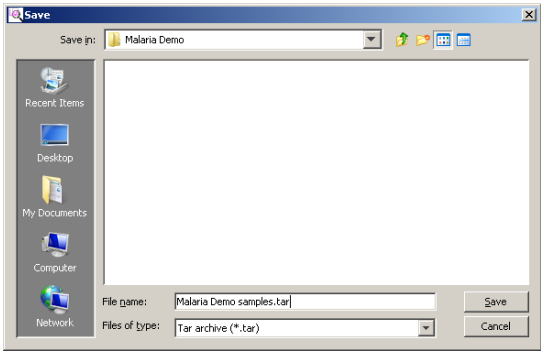
Exercise 5. Save your project

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.

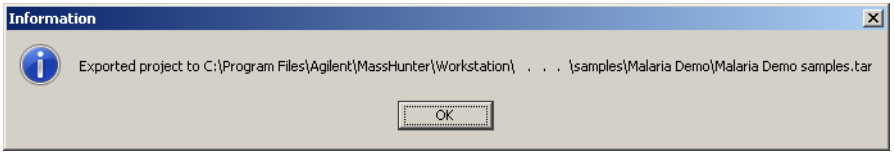
Steps	Detailed Instructions	Comments
1 Export your project to a TAR file.	**a** Click **Project > Export Project**. **b** Mark the check box next to the experiment you wish to save **c** Click **OK**.	• You have completed creating your project and analyzing an experiment. It is recommended to archive your progress by exporting your project.



d Select or create the file folder.
e Type your file name in **File name**.
f Click **Save**.



g Click **OK**.



Advanced Tasks

The operations available in the Workflow Browser 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.

It is recommended that you follow the procedures in the *Mass Profiler Professional Software - Application Guide* for an additional level of detailed information to help you use MPP with your data.

The *Metabolomics Discovery Workflow* and *Mass Profiler Professional User Manual* provide you with techniques and explanations to perform advanced analysis tasks.

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

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.

In some cases, BioCyc Pathway/Genome databases are described by other specific publications that can be found by selecting the database and then going to the Summary Statistics pages under the Tools menu. The resulting page sometimes contains a citation for that database.

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In this book

The *Agilent G3835AA MassHunter Mass Profiler Professional Software - Familiarization Guide* presents the functionality of Mass Profiler Professional using a “Malaria” project containing an experiment called “Malaria LCMS ESI+ pH 7.”

Revision A, November 2012

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