Technical Overview

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Method Manager for Streamlined Statistical Analysis and Model Building

Introduction

Advancements in data analysis techniques for analyzing mass spectrometry data pose new challenges for the customization of analysis workflows. The ability to automate workflows capable of analyzing samples faster with newer algorithms, minimal manual intervention and record the entire workflow in a concise manner is crucial to the efficient operation of laboratories. Agilent is therefore offering simplified workflows for data transformation, normalization, quality control, statistical analysis, and model building in Agilent Mass Profiler Professional (MPP) software. The new Method Manager in the software allows the user to easily build a method for repeated use. A method is a set of tasks required for analyzing a dataset. This Technical Overview describes the development of an MPP method for mass spectrometry data analysis.

Workflow overview

MPP enables the data analysis workflow for many instruments including LC/Q-TOF, LC/TOF, GC/Q-TOF, LC/TQ, GC/TQ, ICP/MS, etc. The acquired data is processed in Agilent MassHunter software suite for feature extraction and the results are imported into MPP for statistical analysis. The analysis workflow in MPP is streamlined using the Method Manager.

Method Manager in Mass Profiler Professional

Method Manager automates experiment creation, data filtering, statistical analysis as well as model building in MPP. It allows the creation, execution, and monitoring of a method. The user can drag and drop the tasks of choice in the drawing area to create a method. Advanced features like normalization and missing value imputation can also be configured from the same interface. The tool allows method creation with any number of tasks in any operational order. For example, a method starting with experiment creation can go to data filtering and statistical analysis, as well as to fold change analysis. It can even be edited to add additional tasks like clustering, correlation, and model building. Figure 1 shows the user interface for creating and running a method in Method Manager.

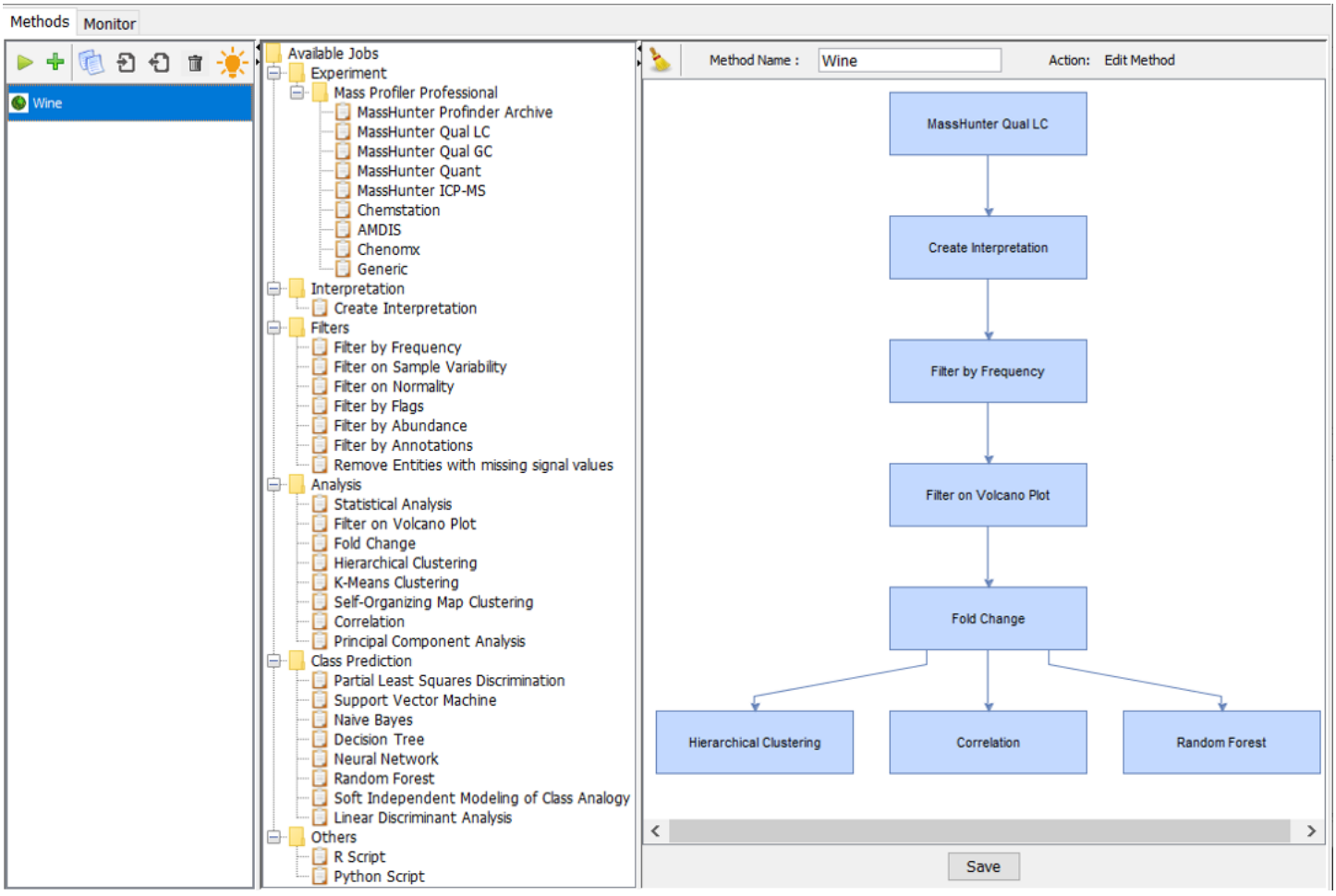

Figure 1. Method Manager in Mass Profiler Professional. The left panel shows the list of already created methods. The right panel shows the tasks in the selected method created by drag and drop of tasks from the central panel.

Method Manager in MPP enables different combinations of tasks to be run in an automated manner. For example, two different workflows can be created for model building as shown in Figure 2. The results of these workflows are saved in MPP after method completion. The ability to run several workflows in parallel significantly saves time and minimizes the possibility of error without operator intervention.

The parameters used in automated analysis at each step can be saved in a report. This significantly improves the simplicity of the entire workflow and enhances the user's capability to record information accurately. The method can also be shared to ensure repeatability of results.

Automated classification analysis using MassHunter Software Suite

Building a classification model in MPP includes steps such as data transformations, normalizations, filtering, statistical analysis, and selection of an appropriate class prediction algorithm. These can be automated using Method Manager as demonstrated earlier. In specific applications such as food authenticity where the workflow includes classifying unknown samples, further routine analysis can be performed by Agilent MassHunter Classifier software. The complete workflow is illustrated in Figure 3.

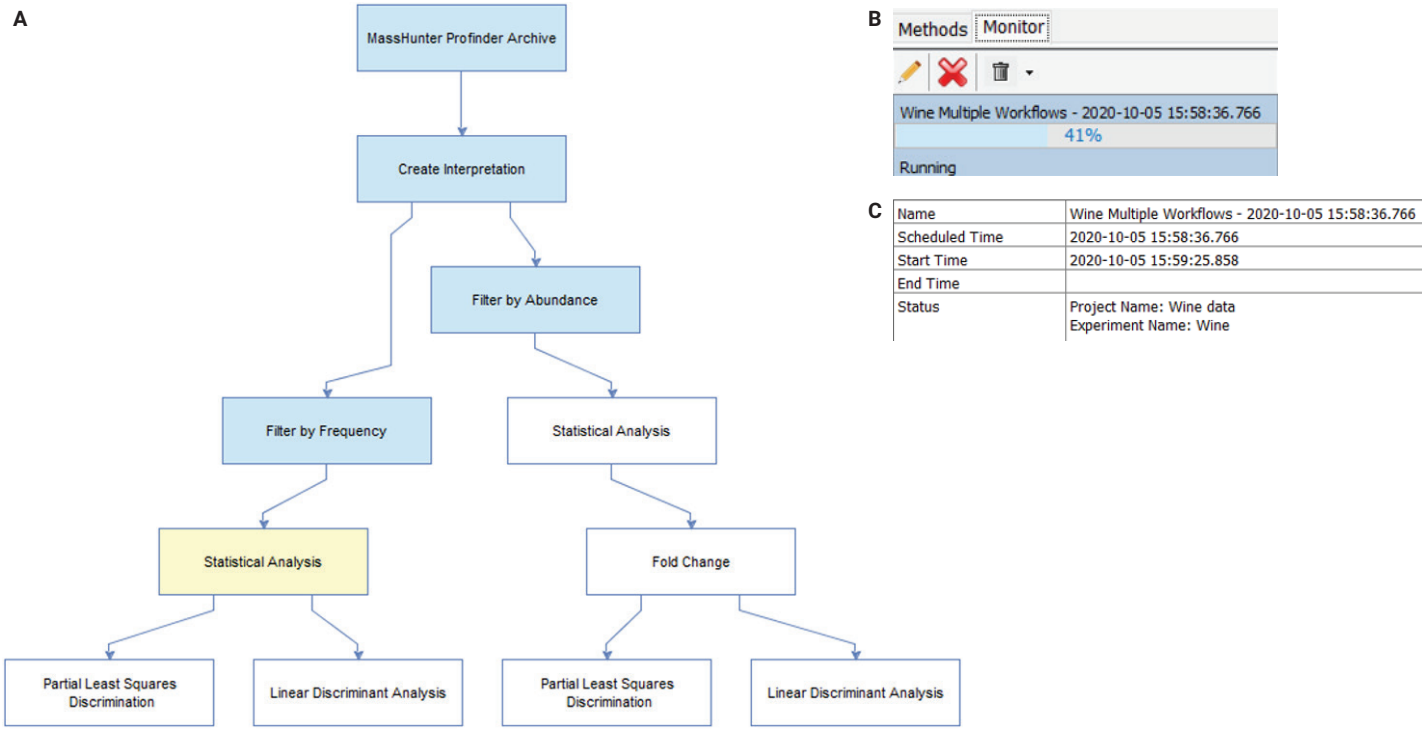

Figure 2. Monitor tab of Method Manager. (A) Multiple workflows in Method Manager. Two workflows are created using different sets of tasks. The color in the boxes indicates the progress of a method. Blue indicates finished tasks, yellow indicates tasks in progress, and white indicates tasks yet to be completed in the queue. (B) The progress bar shows the percentage completion of the method. (C) The table provides details on method scheduled, start, and end time along with project information.

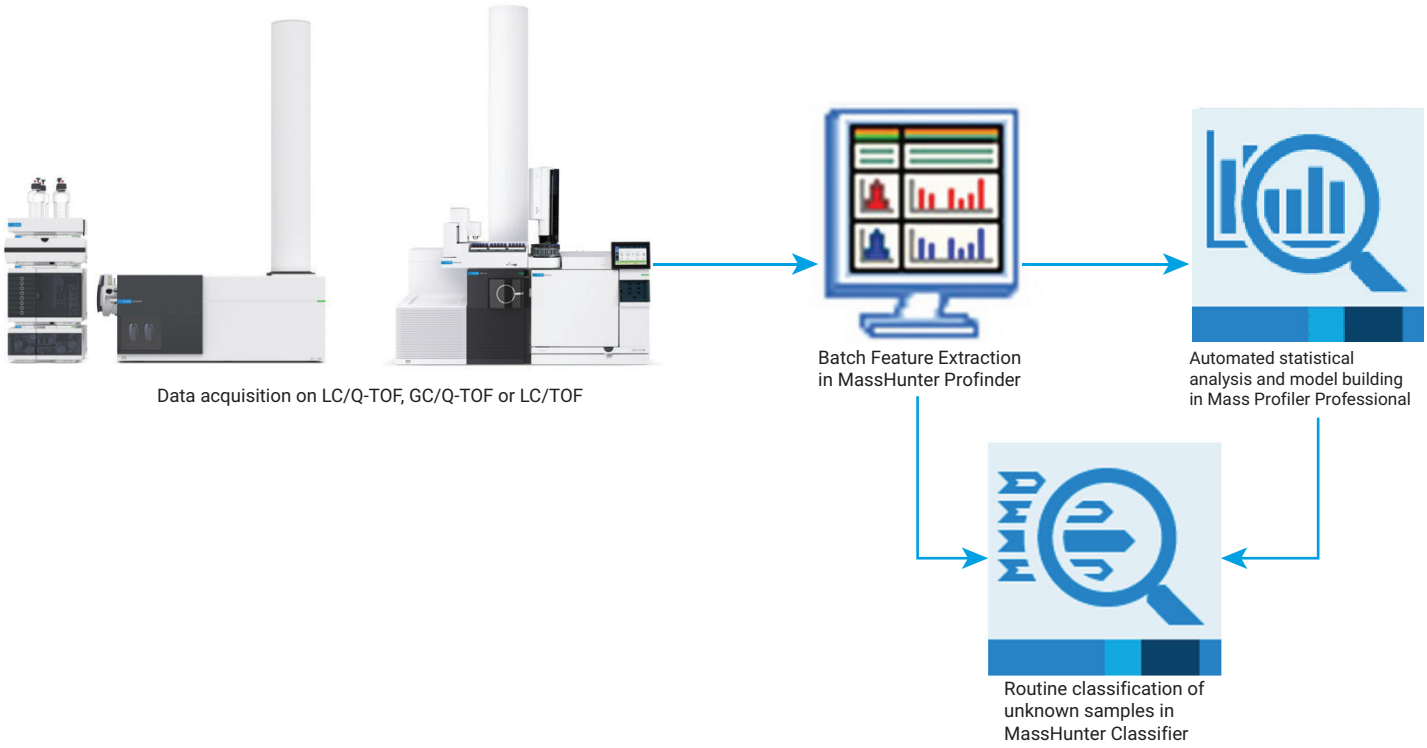

Figure 3. Method development workflow with classification data.

Conclusion

The simplified configuration of a method, its repeatability, and the ability to easily share the method ensures consistent results. Users can create custom workflows by selecting appropriate algorithms based on their interest. The one-click solution to capturing all the analysis parameters in a single report further enables quick referencing for any future need. Thus, the newly introduced method development significantly improves the turnaround time required for a fast and reliable solution to differential analysis.

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