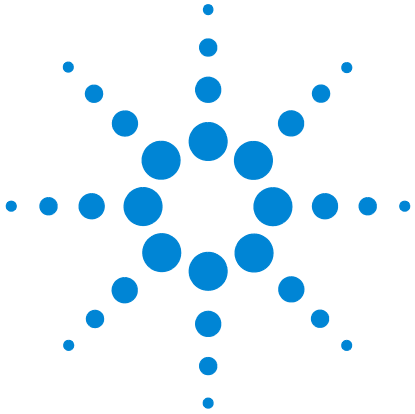


Agilent MassHunter Workstation Software

Quant-My-Way Flavors Setup Familiarization Guide

Agilent Technologies

Notices

Manual Part Number

G3335-90240

Edition

First edition, August 2017

Printed in USA

Agilent Technologies, Inc.
5301 Stevens Creek Boulevard
Santa Clara, CA 95051 USA

Warranty

The material contained in this document is provided "as is," and is subject to being changed, without notice, in future editions. Further, to the maximum extent permitted by applicable law, Agilent disclaims all warranties, either express or implied, with regard to this manual and any information contained herein, including but not limited to the implied warranties of merchantability and fitness for a particular purpose. Agilent shall not be liable for errors or for incidental or consequential damages in connection with the furnishing, use, or performance of this document or of any information contained herein. Should Agilent and the user have a separate written agreement with warranty terms covering the material in this document that conflict with these terms, the warranty terms in the separate agreement shall control.

Technology Licenses

The hardware and/or software described in this document are furnished under a license and may be used or copied only in accordance with the terms of such license.

Restricted Rights Legend

If software is for use in the performance of a U.S. Government prime contract or subcontract, Software is delivered and licensed as "Commercial computer software" as defined in DFAR 252.227-7014 (June 1995), or as a "commercial item" as defined in FAR 2.101(a) or as "Restricted computer software" as defined in FAR 52.227-19 (June 1987) or any equivalent agency regulation or contract clause. Use, duplication or disclosure of Software is subject to Agilent Technologies' standard commercial license terms, and non-DOD Departments and Agencies of the U.S. Government will receive no greater than Restricted Rights as defined in FAR 52.227-19(c)(1-2) (June 1987). U.S. Government users will receive no greater than Limited Rights as defined in FAR 52.227-14 (June 1987) or DFAR 252.227-7015 (b)(2) (November 1995), as applicable in any technical data.

Safety Notices

CAUTION

A **CAUTION** notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in damage to the product or loss of important data. Do not proceed beyond a **CAUTION** notice until the indicated conditions are fully understood and met.

WARNING

A WARNING notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in personal injury or death. Do not proceed beyond a WARNING notice until the indicated conditions are fully understood and met.

Contents

1 Introduction

The Agilent MassHunter Workstation Quantitative Analysis B.09.00 software provides tools to customize, save, and share a Quantitative Analysis flavor.

A MassHunter Quantitative Analysis flavor is a user interface with a specific set of tools and options. The Quantitative Analysis software provides a preset number of system flavors designed for several instruments and applications.

Use the Quant-My-Way Flavors Setup program to create customized Quantitative Analysis flavors that display the tools and menu options you need for your laboratory or function. Your custom flavors can then be saved, updated, and shared with others in your organization.

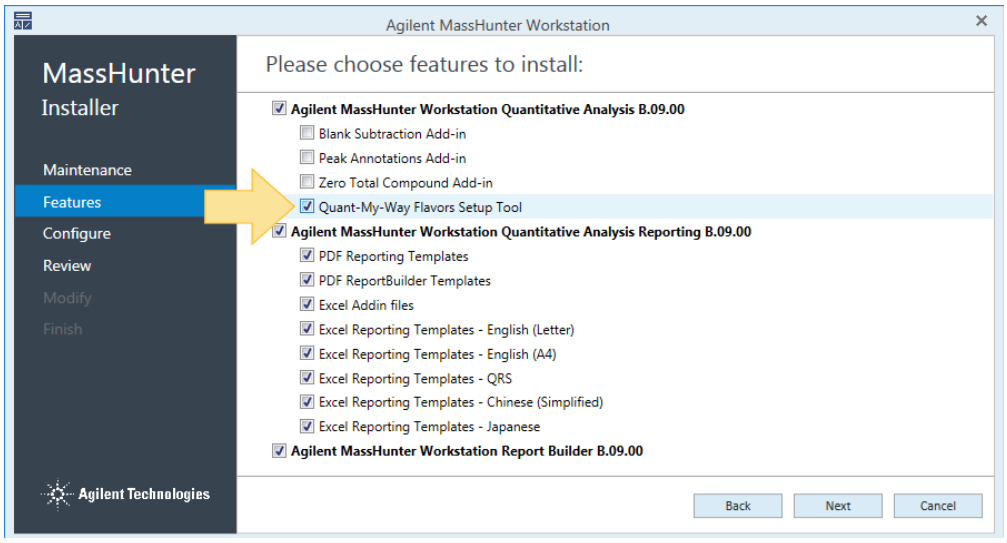
Install the Quant-My-Way Flavors Setup Program

The Quant-My-Way Flavors Setup program can be installed alone or with any other Quantitative Analysis feature during the MassHunter Workstation Quantitative Analysis B.09.00 installation. The Quant-My-Way Flavors Setup program should be installed on the workstation where a user will be creating and editing custom flavors.

You can install the Quant-My-Way Flavors Setup program during the MassHunter Workstation Quantitative Analysis installation ("Install Quant-My-Way Flavors Setup during installation), or it can be installed after Quantitative Analysis has already been installed ("Install Quant-My-Way Flavors Setup after installation" on page 7).

Install Quant-My-Way Flavors Setup during installation

1 During the MassHunter Workstation Quantitative Analysis B.09.00 installation, on the **Features** screen, select **Quant-My-Way Flavors Setup Tool**.

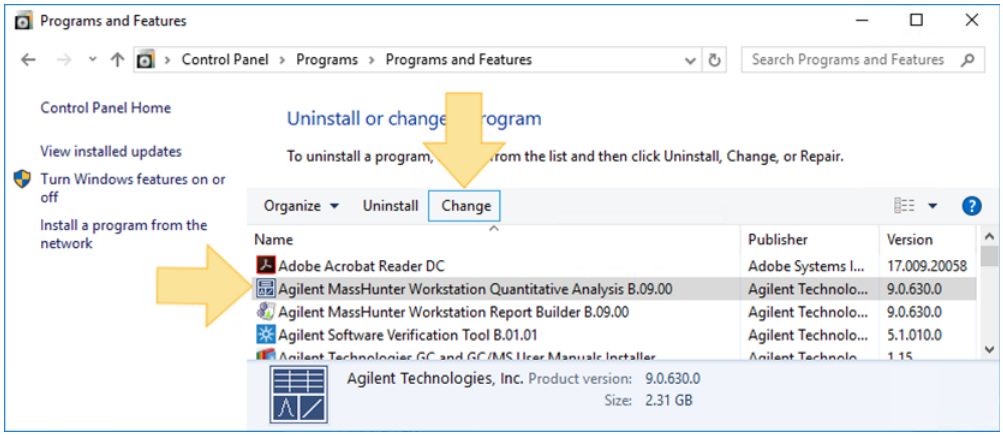


2 Click **Next**, and continue to complete the installation.

Install Quant-My-Way Flavors Setup after installation

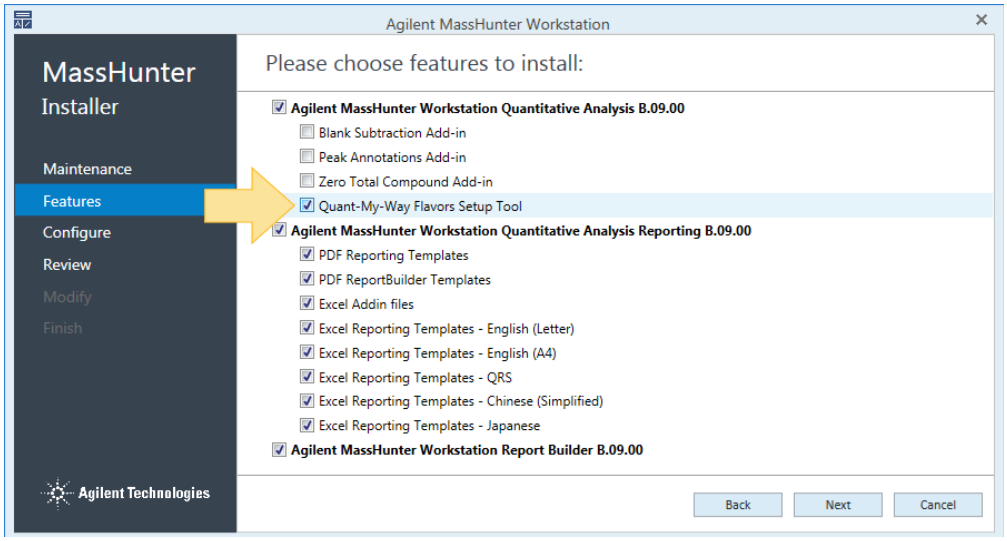
1 If the MassHunter Workstation Quantitative Analysis B.09.00 software has already been installed, from the **Windows Control Panel**, open **Programs and Features**.

2 Select **Agilent MassHunter Workstation Quantitative Analysis B.09.00**, and click **Change**.



3 On the Agilent MassHunter Workstation Installer **Maintenance** screen, click **Change**.

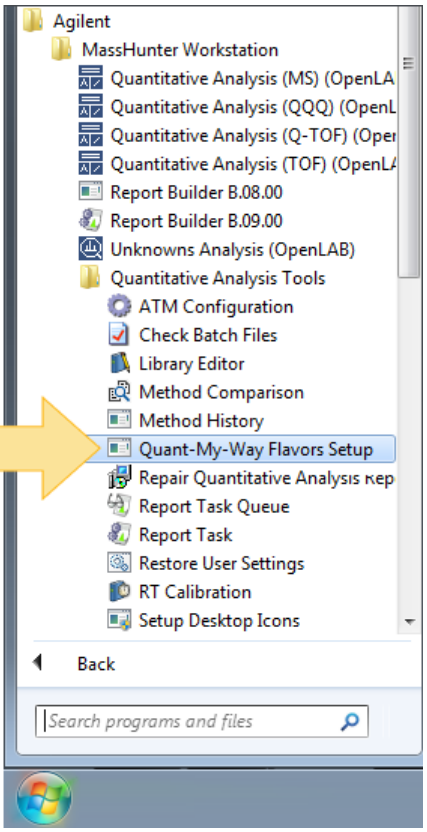
4 On the **Features** screen, select **Quant-My-Way Flavors Setup Tool**.



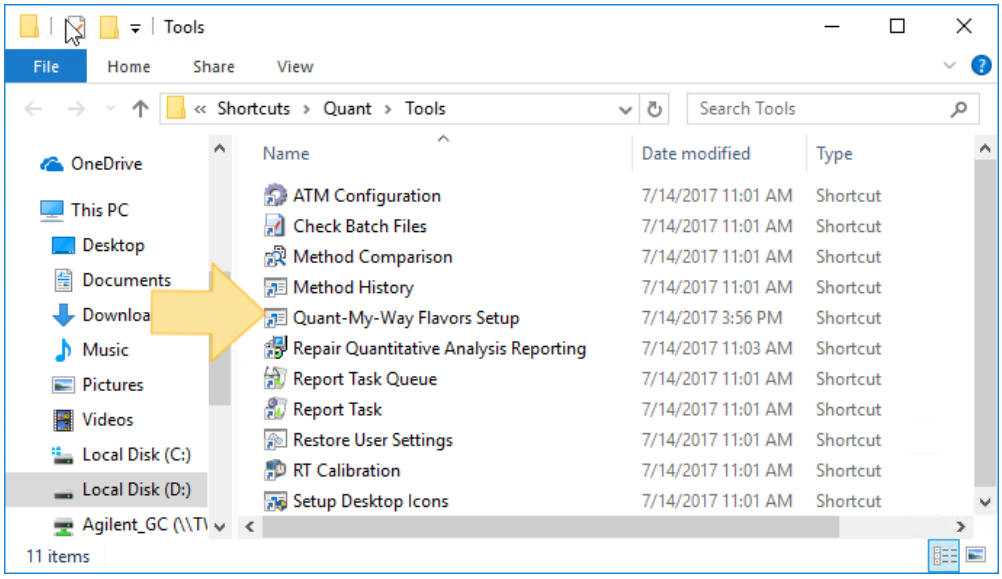
5 Click **Next**, and continue to complete the installation.

Open the Quant-My-Way Flavors Setup Program

Windows 7: Select **Windows Start > All Programs > Agilent MassHunter Quantitative Analysis Tools > Quant-My-Way Flavors Setup**.



Windows 10: Select **Windows Start > All Programs > Agilent MassHunter Quantitative Analysis Tools**, and open the **Quant-My-Way-Flavors Setup** program.



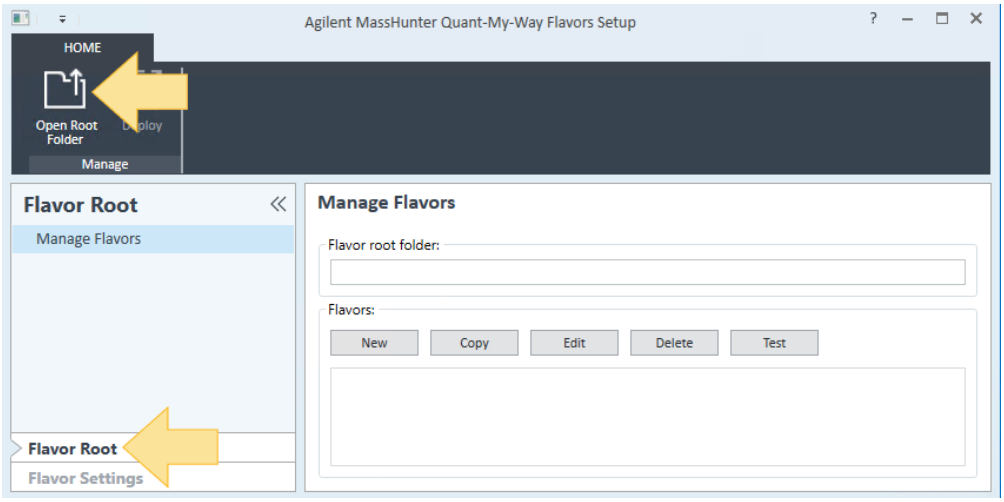
2
Create and Manage Flavors

Use the Quant-My-Way Flavors Setup program to create a custom flavor and manage your existing custom flavors and folders.

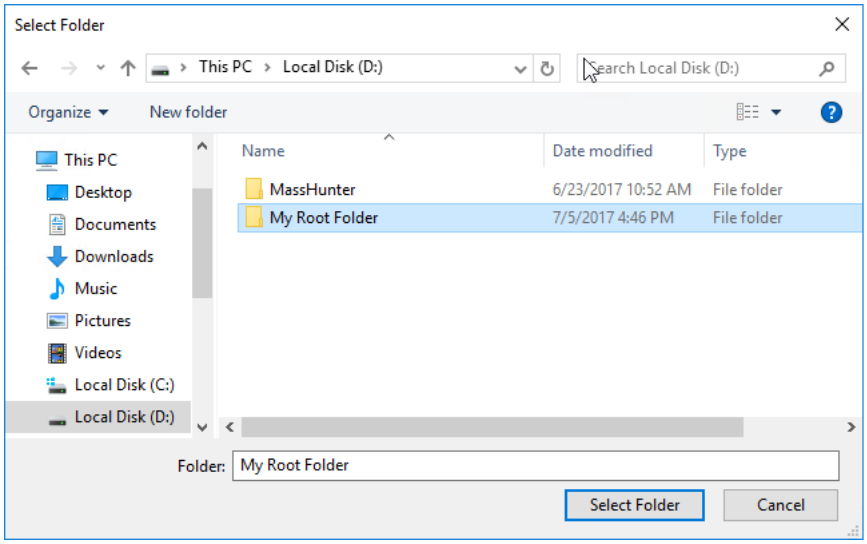
Create a Root Folder Location to Store Custom Flavors

The root folder is the directory folder where you will store your flavors. You can use any convenient location in your directory.

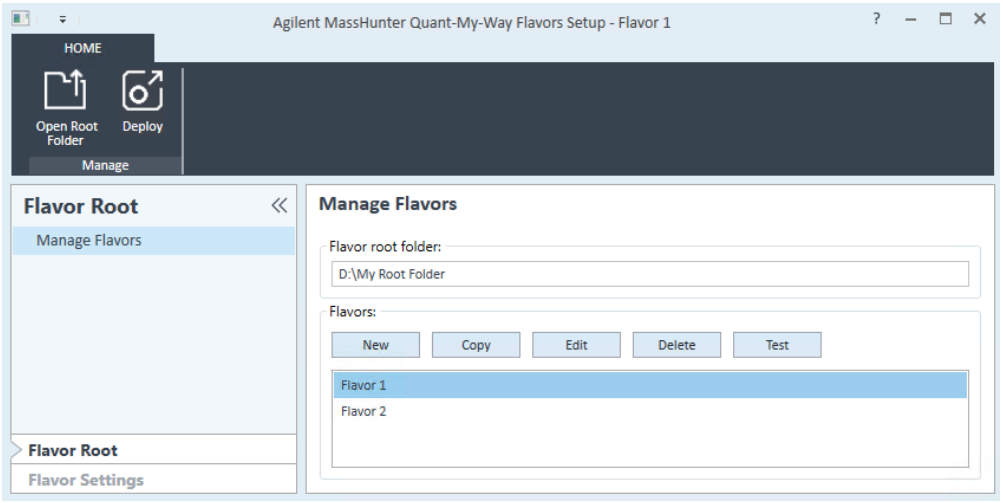
1 On the **Flavor Root** screen, click **Open Root Folder**.



2 Navigate to an existing folder, or create a **New Folder**, and click **Select Folder**.



The **Flavor root folder** path is displayed, and the existing **Flavors** are listed.

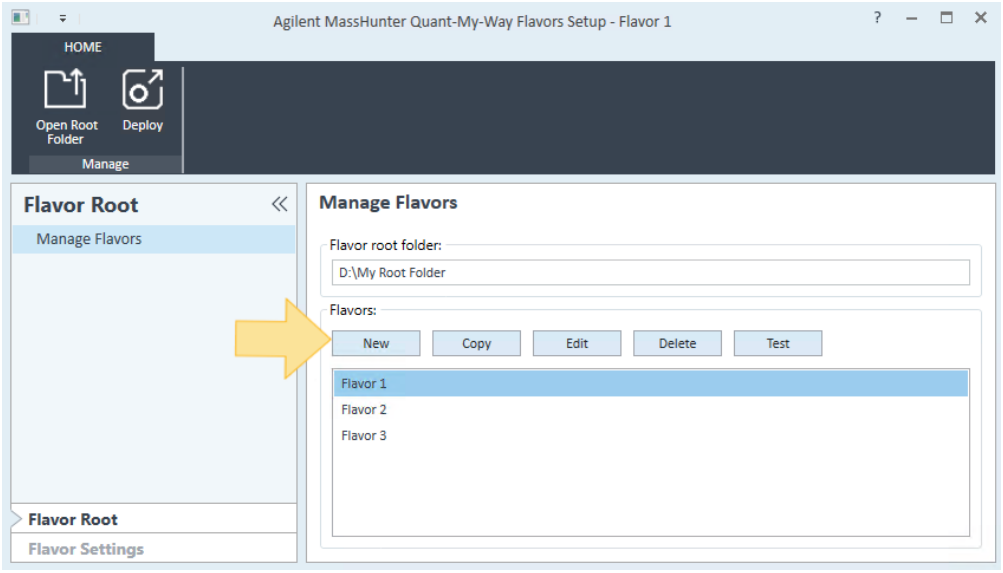


Create a Flavor

Create a flavor based on a standard system flavor, and then modify it as needed for display name, Batch Table, ribbon options, sample types, outliers, or by adding your own custom ribbon buttons and menus.

In this example, we will create a QQQ flavor that simplifies the user interface to include only the functions needed to perform routine data analysis. The method development functionality will be removed, as well as other non-essential data analysis tools.

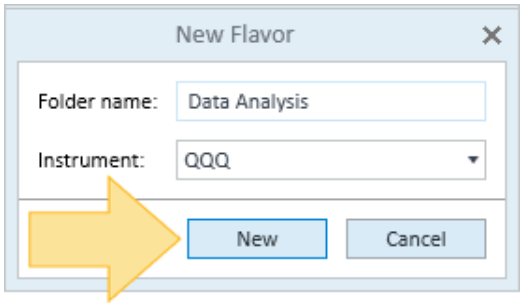
1 On the **Flavor Root** screen, click **New**.



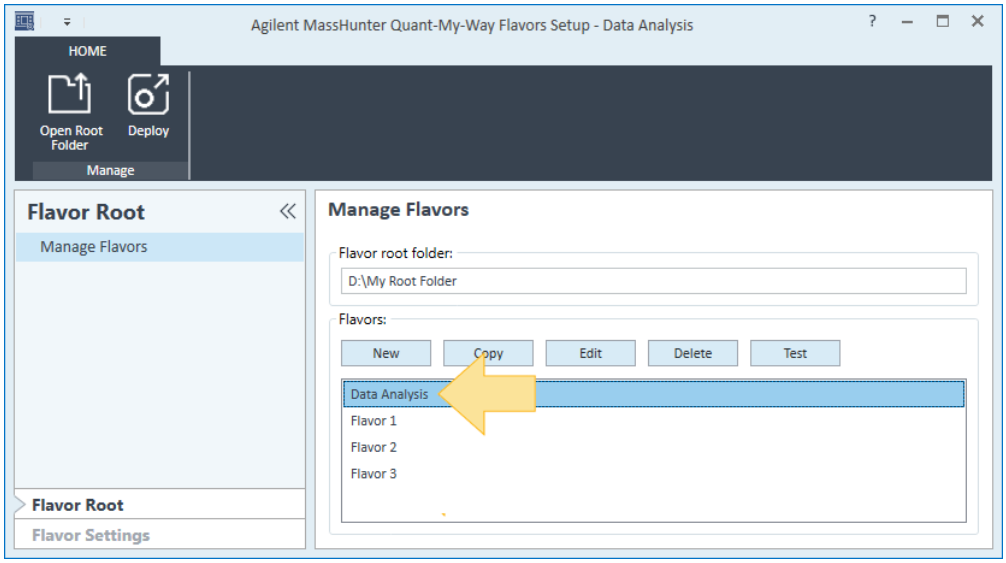
2 Enter a **Folder name**. This name will be used as the flavor name in the root folder. It will also be used as the default display name of the desktop icon and user interface of your flavor unless the display name is changed in the general settings. For this example, enter **Data Analysis**.

3 Select a standard system flavor **Instrument** on which to base your flavor.

4 Click **New**.



A folder is created in your root folder containing the configuration file (startup.xml) for your flavor.



Continue your customization by updating the Batch Table, ribbon options, sample types, outliers, or by adding your own custom ribbon buttons and menus. See "Customize a Flavor" on page 15.

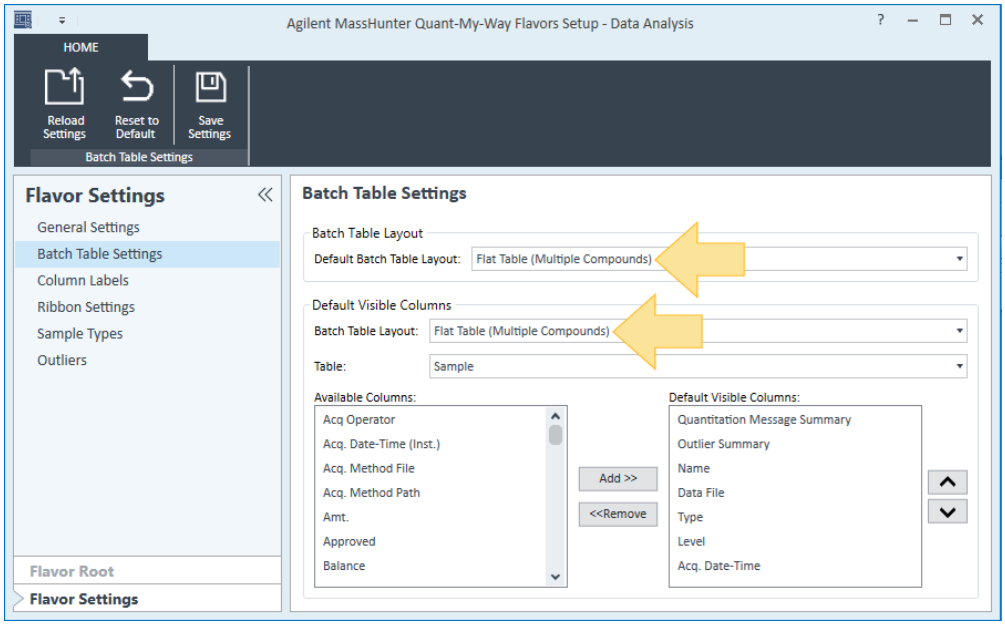
3 Customize a Flavor

Update your flavor with a new display name, Batch Table, ribbon, sample type, outliers, or with your own custom ribbon buttons and menus.

Remove Batch Table Columns

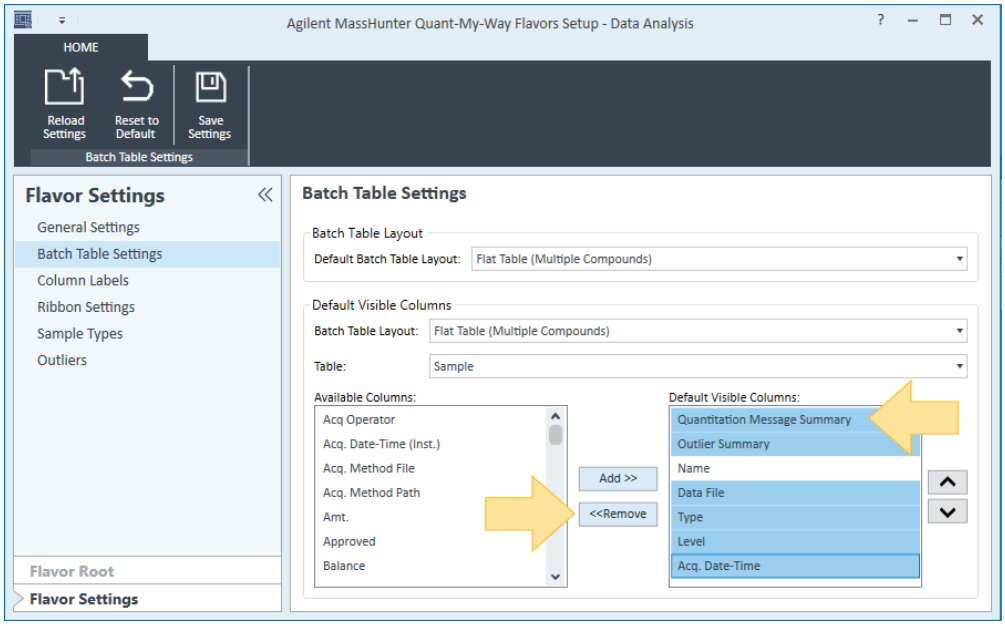
1 On the **Flavor Settings > Batch Table Settings** screen, select **Flat Table (Multiple Compounds)** from the **Default Batch Table Layout** list.

2 Select **Flat Table (Multiple Compounds)** from the **Batch Table Layout** list.

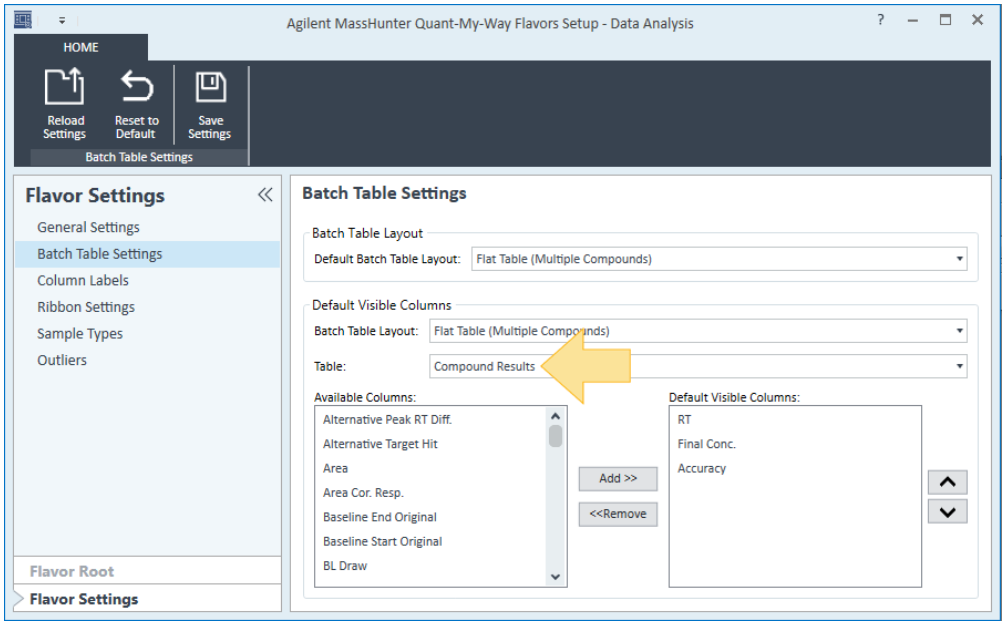


3 **Remove** the following **Default Visible Columns**:

- Quantitation Message Summary
- Outlier Summary
- Data File
- Type
- Level
- Acq. Date-Time

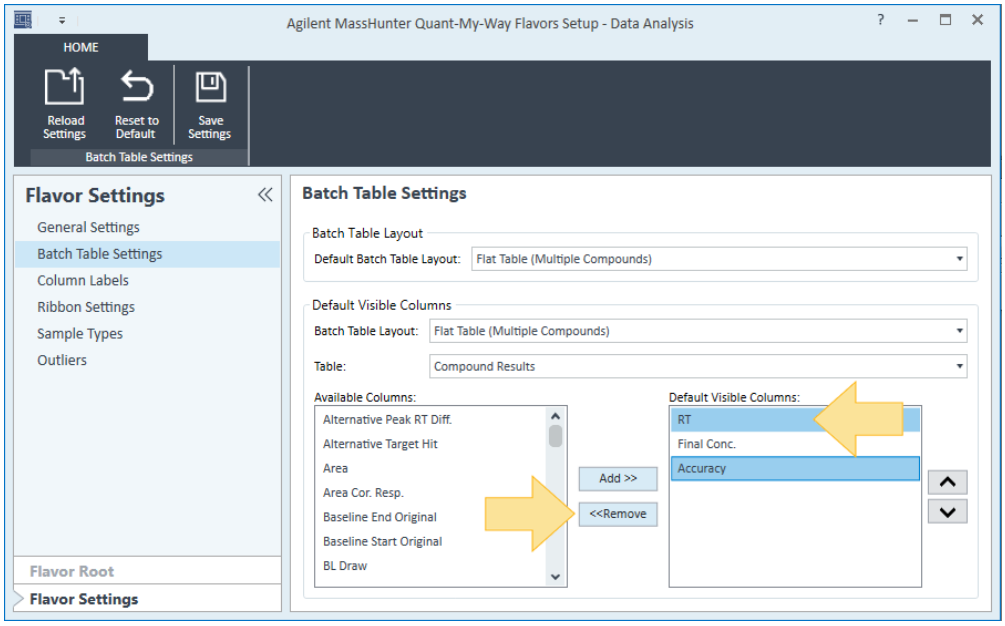


4 Select **Compound Results** from the **Table** list.

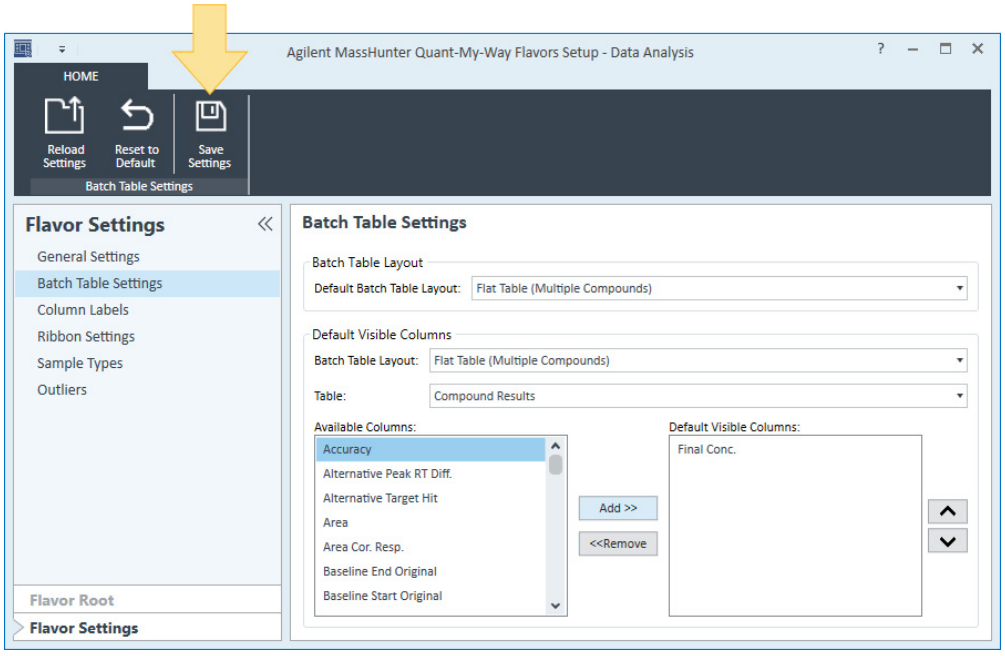


5 **Remove** the following **Default Visible Columns**:

- RT
- Accuracy



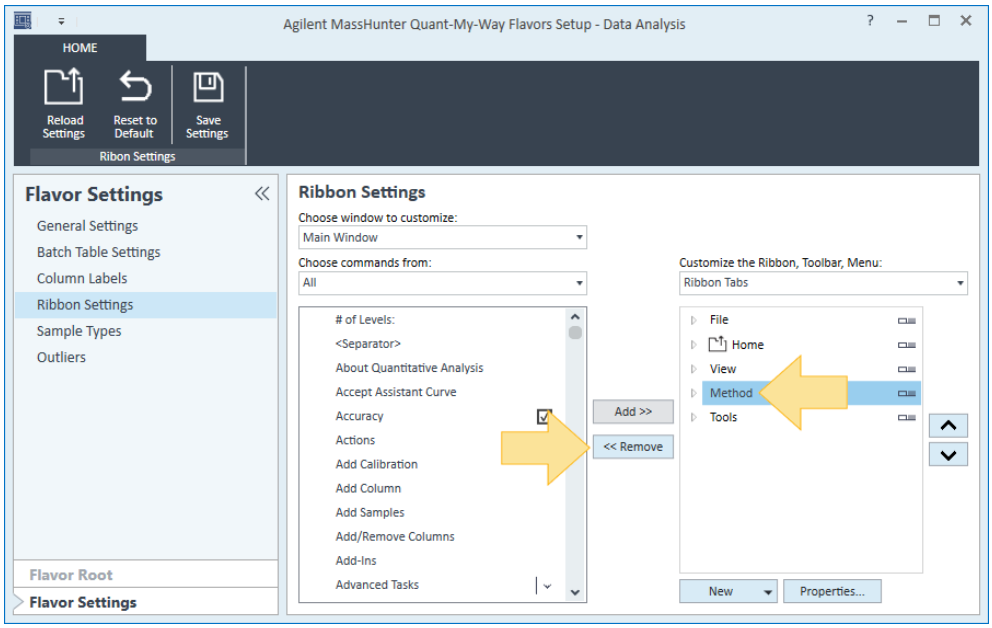
6 Click **Save Settings**.



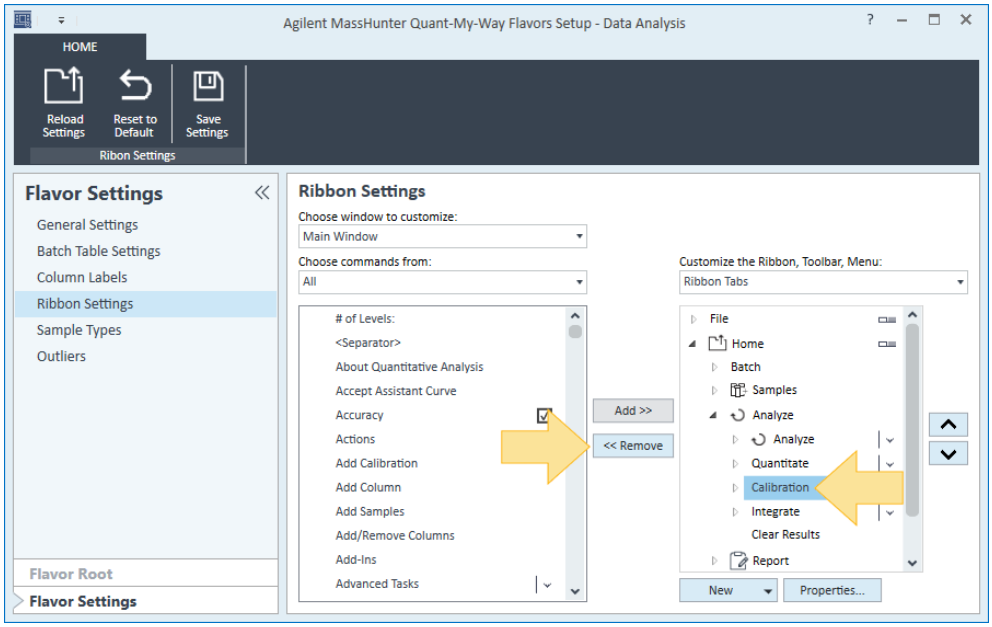
Customize the Quant-My-Way Ribbon

1 On the **Flavor Settings > Ribbon Settings** screen, remove the following:

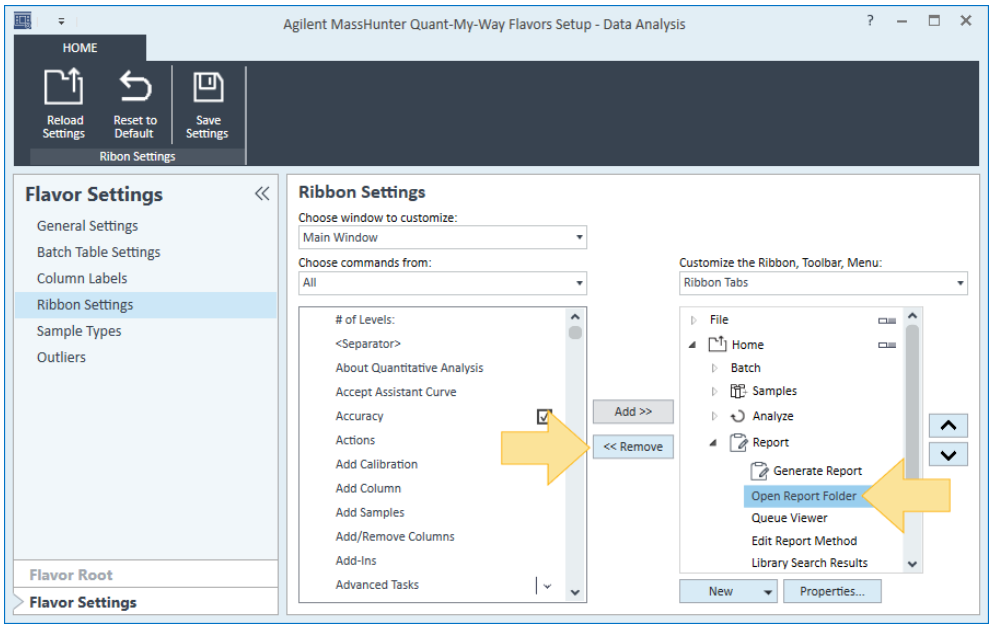
- **Method** tab



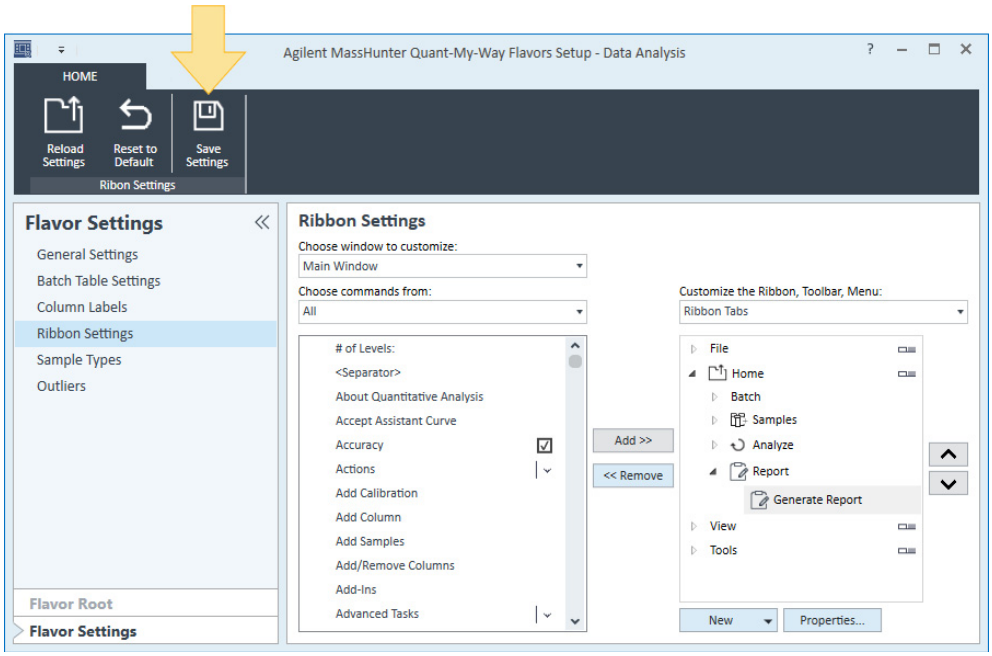
- **Calibration** menu (Home > Analyze)
- **Integrate** menu (Home > Analyze)
- **Clear Results** button (Home > Analyze)



- **Open Report Folder** button (Home > Report)
- **Queue Viewer** button (Home > Report)
- **Edit Report Method** button (Home > Report)
- **Library Search Results** button (Home > Report)
- **Library Search Reports** menu (Home > Report)



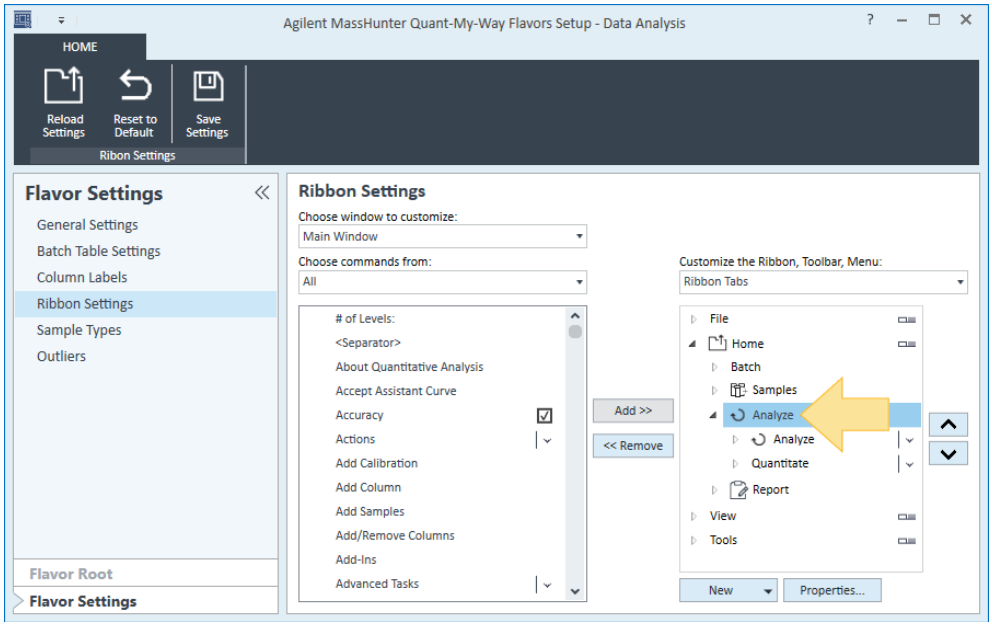
2 Click **Save Settings**.



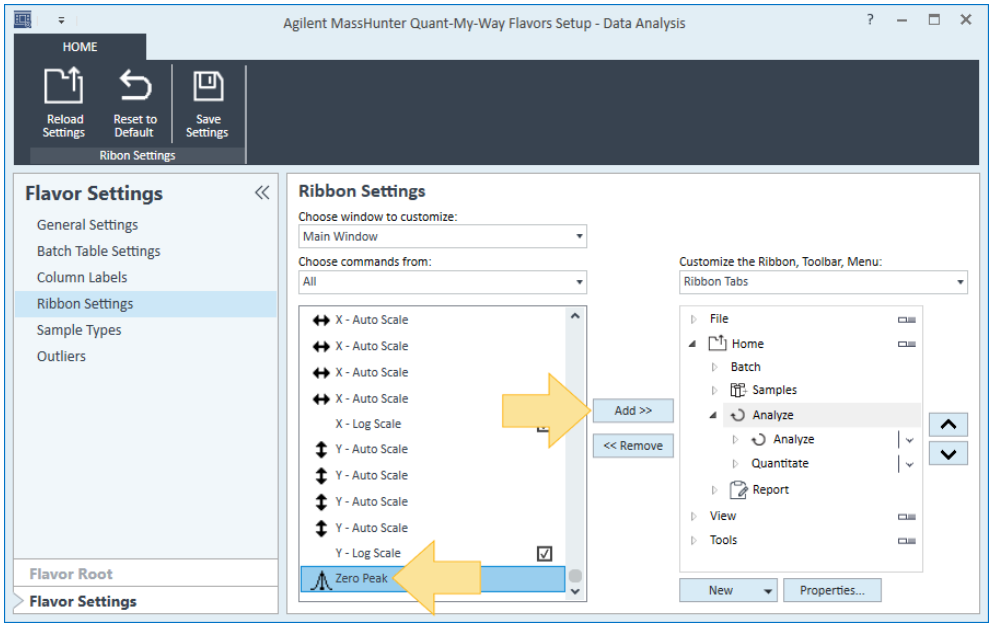
Create a Custom Ribbon Button

To create a custom ribbon button in the Quant-My-Way Flavors Setup program, you must create Python script for the button functionality. The script file (.py) must be saved in a **Tools** folder within your custom flavor folder. In this example, the script **ZeroExceptionPeaks.py** would be saved in **D:\My Root Folder\Data Analysis\Tools**.

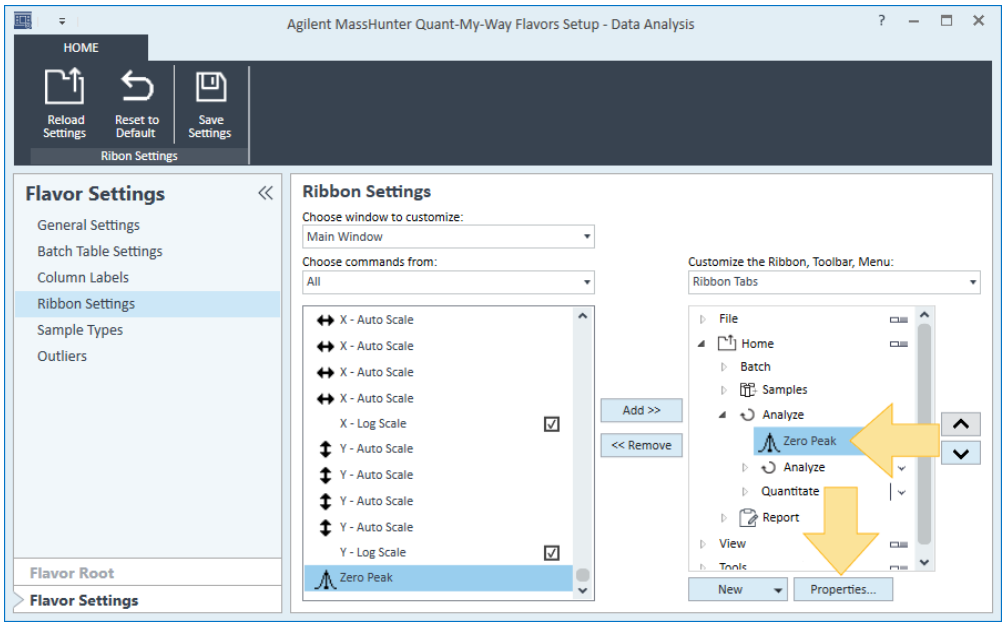
1 Select the **Analyze** menu in the right pane (**Home > Analyze**).



2 In the left pane, select **Zero Peak**, and click **Add** to add it to the **Analyze** menu.



3 Select the **Zero Peak** button in the right pane, and click **Properties**.



4 Select **Image only** from the **Minimum size** list.

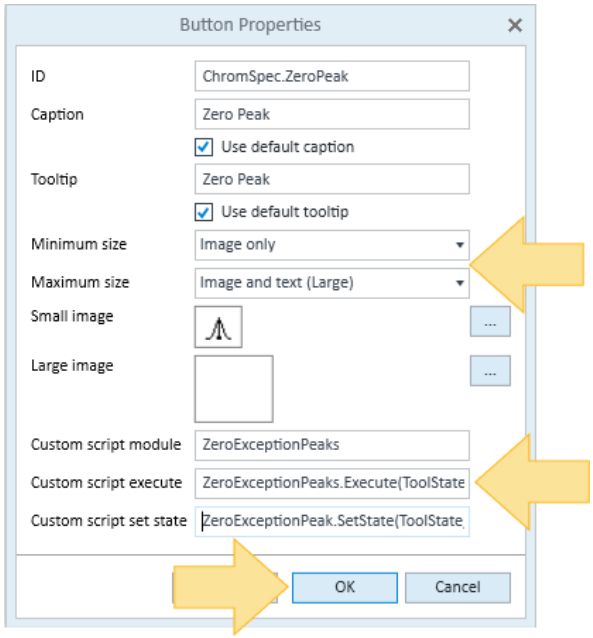
5 Select **Image and text (Large)** from the **Maximum size** list.

6 In the **Custom script module** field, enter **ZeroExceptionPeaks**.

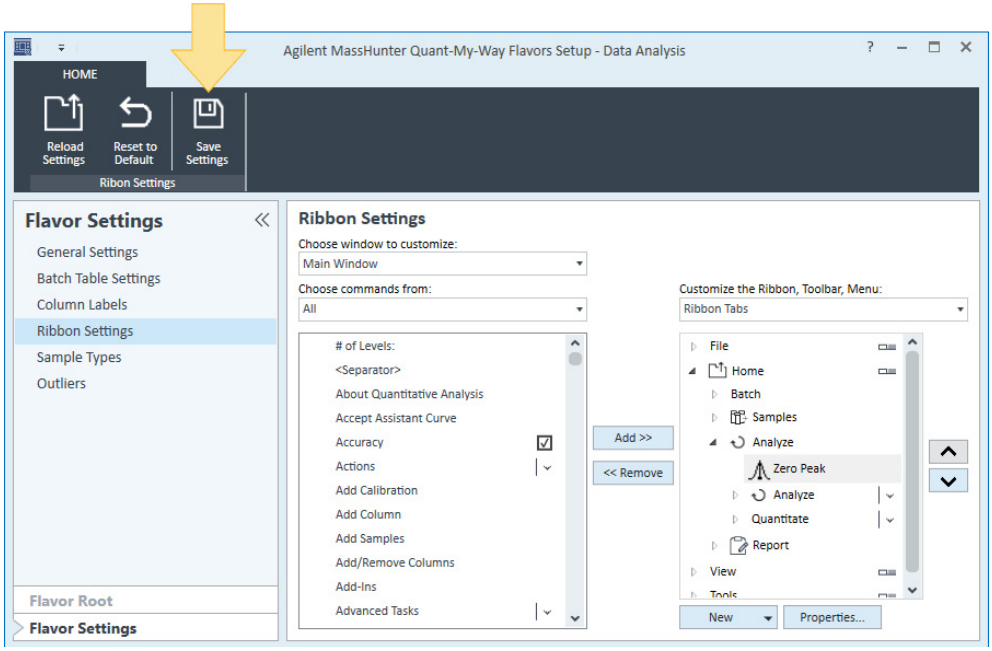
7 In the **Custom script execute** field, enter **ZeroExceptionPeaks.Execute(ToolState, UIState)**.

8 In the **Custom script set state** field, enter **ZeroExceptionPeaks.SetState(ToolState, UIState)**.

9 Click **OK**.



10 Click **Save Settings**.



4
Share and Install a Flavor

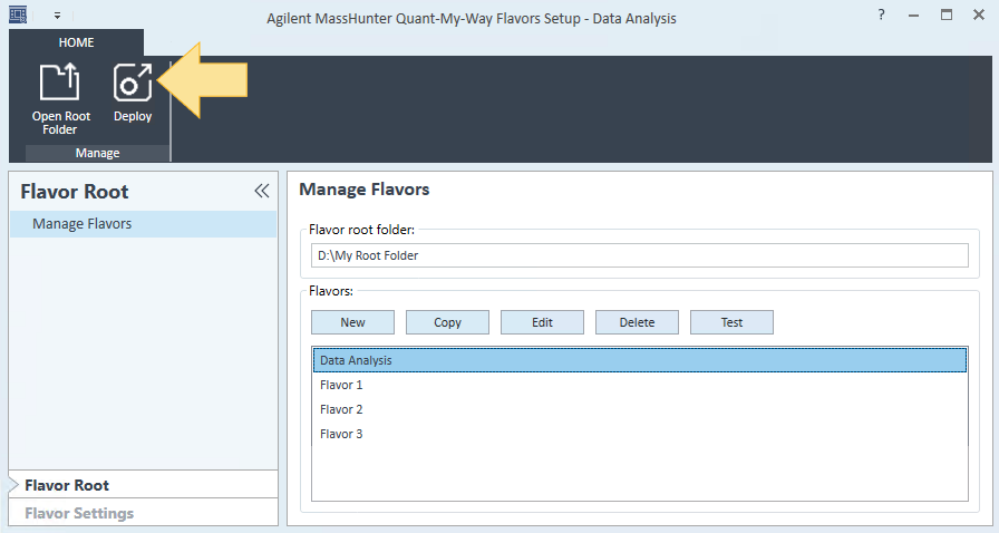
You can make custom flavors available to others in your organization to install and use in Quantitative Analysis.

Make a Flavor Available for Use

After you have created a custom flavor, you can make it available to others in your organization to use for data analysis by deploying it in the Quant-My-Way program.

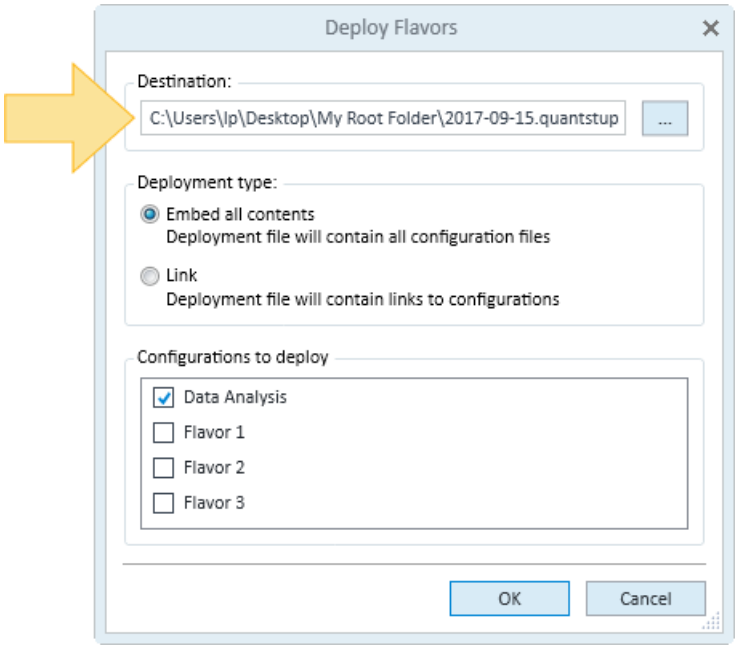
1 Open the root folder of the flavor you would like to make available for use.

2 Click **Deploy**.



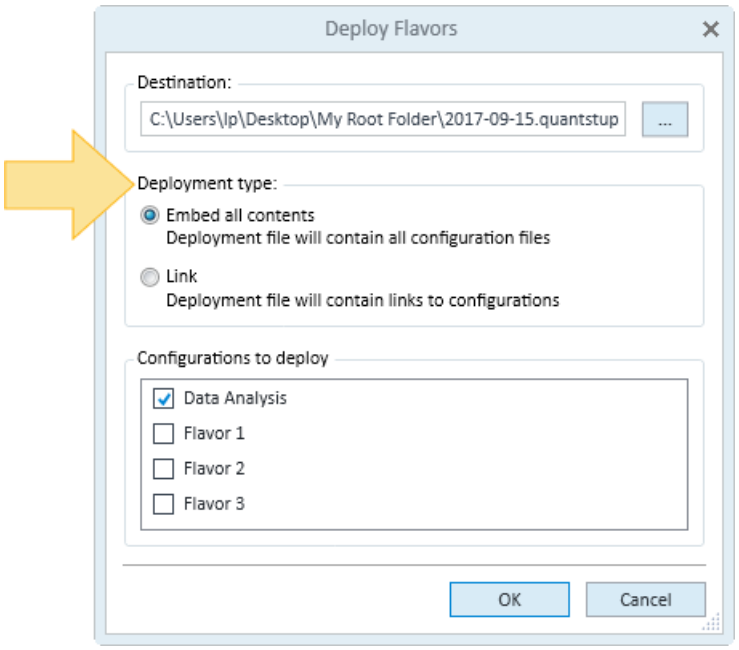
3 Use the default **Destination**, or enter the folder path where you want to save your deployment file.

4 Use the default installation file name, or enter a new name. The date is used for the default name.

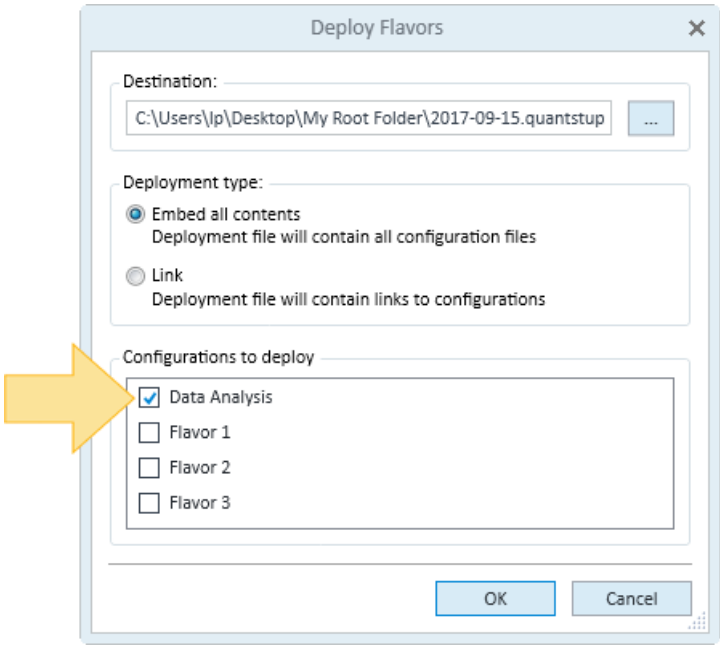


5 **Embed** or **Link** the flavor configuration to the installation file that will be created for this deployment.

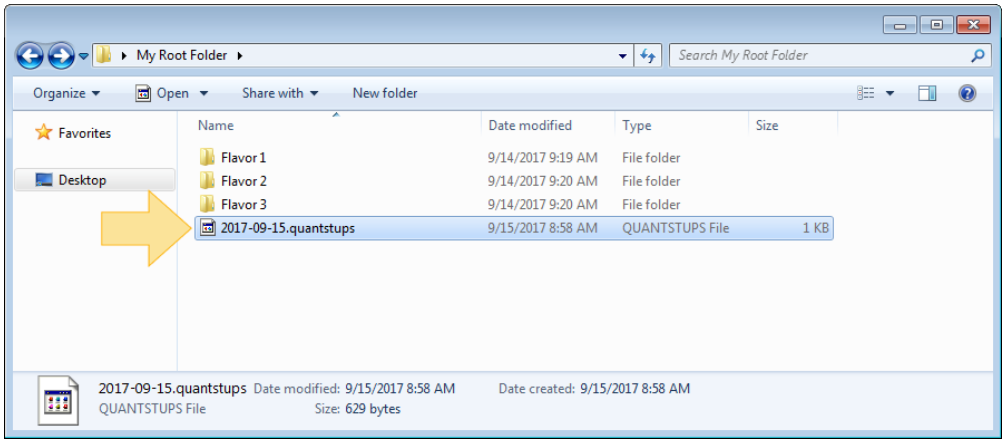
- In an embedded deployment, a flavor will remain as it was configured when it was installed on a workstation.
- In a linked deployment, a flavor will update whenever it is updated in the Quant-My-Way Flavors Setup program.



6 Select the **Configurations to deploy**. Multiple flavors in a root folder may be deployed as a group. Installing this deployment file will install all the flavors selected.



7 Click **OK**. A deployment file (QUANTSTUPS File) is created. The deployment file is used to install the flavors included in this deployment onto the workstation where you want to use them for data analysis.



Install a Flavor

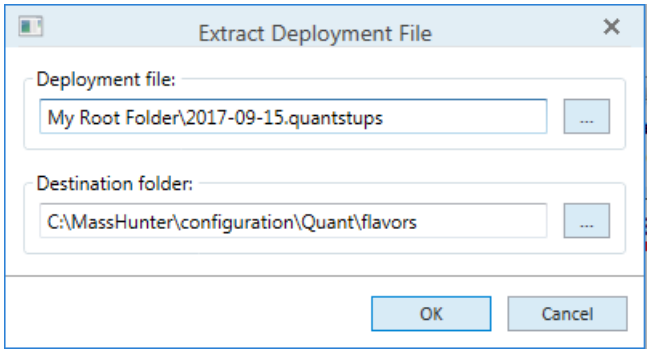
After the custom flavor is deployed, it is available to you or others in your organization to install on a workstation for quantitative analysis.

1 Install MassHunter Workstation Quantitative Analysis B.09.00 on the workstation where you want to install the custom flavor. The Quant-My-Way Flavors Setup program is not required to install a flavor.

2 From the Windows directory on the workstation where you want to install the flavor, navigate to and open the deployment file (QUANTSTUPS file) containing the flavor you want to install.

3 Use the selected **Deployment file**, or browse to the QUANTSTUPS file you want to install.

4 Use the default **Destination folder**, or enter the folder path where you want to save your flavor files.



5 Click **OK**. The flavor is installed on the workstation, and a shortcut icon to the flavor is added to the desktop.

When the flavor is launched for use, the Quantitative Analysis user interface will be displayed in the Windows operating system language of the workstation where it is launched.

4 Share and Install a Flavor

Agilent Technologies

Printed in USA, August 2017

G3335-90240