Agilent MassHunter Workstation Software Reporting

Familiarization Guide

Agilent Technologies

Notices

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In This Guide...

This guide contains information to learn to use your Agilent MassHunter Workstation Software Reporting Excel Add-In.

Exercise 1 Creating Reports

In this exercise, you produce reports using the Qualitative Analysis program and the Quantitative Analysis program.

Exercise 2 Customizing a template

In this exercise, you learn how to customize both a Qualitative Analysis template and a Quantitative Analysis template. You make a copy of the template, open it in Excel, change the footer of the template, test the template, save the template and use the template in the Qualitative Analysis and the Quantitative Analysis programs.

Exercise 3 Customizing a table

In this exercise, you customize a table. You learn how to rename a column, delete a column, change the width of a column, and move a column. You also learn how to add a column to a table and how to add a mapped column to a table. In addition, you learn how to add a filter to a table using Excel features and using the Advanced Properties dialog box. Lastly, you learn how to move or delete a column in a table that has been filtered.

Exercise 4 Additional ways to customize a table

In this exercise, you learn how to do the following tasks:

- Add a table
- Format a table (transpose and hide headers)
- Add a formula column
- Add an ISTD column to a Quantitative Analysis template
- Add a column that is already mapped

Exercise 5 Graphics

In this exercise, you use the **Add Graphics** commands to add graphics to a template. You also learn how to display multiple graphics in the same row.

Exercise 6 Advanced topics

In this exercise, you do a variety of advanced tasks including:

- Adding a page break and a sheet break
- Setting up and using Test mode
- Adding repeating sections
- Changing values in the Options worksheet
- Adding a formula using the **IF** function
- Using the **VLOOKUP** function

Contents

Exercise 1
Creating Reports

In this exercise, you explore how reports are generated in different programs.

The first exercise shows you the steps to create a report in the Qualitative Analysis program.

- In Task 1, you open the Qualitative Analysis program with multiple data files.
- In Task 2, you print an analysis report.
- In Task 3, you print a compound report.
- In Task 4, you print a graphics report.

The second section shows you the steps to create a report in the Quantitative Analysis program.

- In Task 5, you open the Quantitative Analysis program and load a batch.
- In Task 6 you create a report method.
- In Task 7 you generate a Quantitative report using the report method.

Each exercise is presented in a table with three columns:

- **Steps** – Use these general instructions to proceed on your own to explore the program.
- **Detailed Instructions** – Use these if you need help or prefer to use a step-by-step learning process.
- **Comments** – Read these to learn tips and additional information about each step in the exercise.

Creating Reports in the Qualitative Analysis Program

Increasing Speed of Qualitative Analysis Report Generation

One of the easiest ways to increase the speed of report generation is by limiting the number of graphics in the template. You can change which graphics are included in a report using either the Analysis Report section in the Method Editor or the Compound Report section in the Method Editor.

You can also try any of the following options to improve reporting speed:

- Filter for only the samples or compounds that you need to report. See "Task 7. Add a filter to a table" on page 73.
- Turn off any unneeded formatting options. See "Task 5. Change values on the Options worksheet" on page 133.
- Delete unused XML maps. See "Task 1. Add a table to a template" on page 86.
- Limit VLOOKUP ranges to the minimum. See "Task 7. Use the VLOOKUP function" on page 140.
- Print on a standalone system, if possible.
- Set the Microsoft Image Writer as the default printer if you are printing to a networked printer.

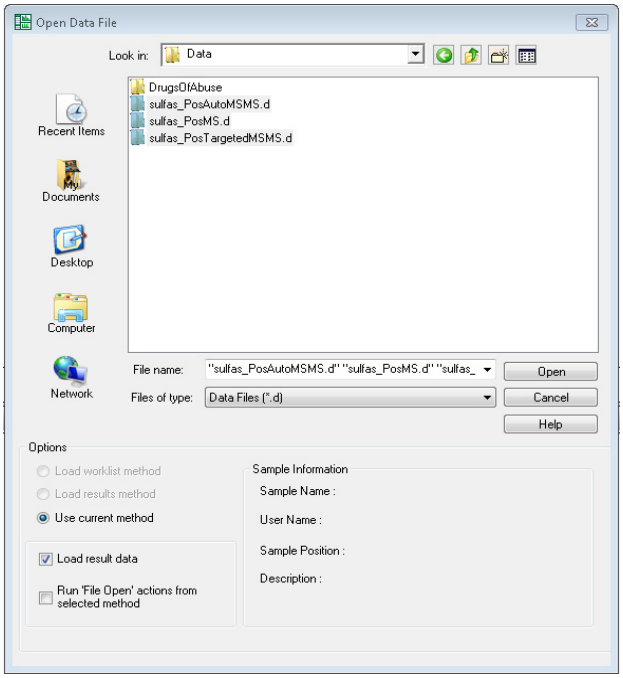
Task 1. Open the Qualitative Analysis program

In this task you open multiple data files using the current method.

Task 1. Open the Qualitative Analysis program with multiple data files

Steps	Detailed instructions	Comments
1 Open the **Qualitative Analysis** program and open the data files, **sulfas-PosAutoMSMS**, **sulfas-PosMS.d** and **sulfas-PosTargetedMSMS.d** in the folder **\MassHunter\Data**, or in the folder where you copied them.	**a** Double-click the **Agilent MassHunter Qualitative Analysis** icon,  . The system displays the **Open Data Files** dialog box. **b** Go to the folder **\MassHunter\Data**, or the folder where the example files are located.	• The sulfas-PosMS.d file contains MS (TOF or Q-TOF) data. The sulfas-PosAutoMSMS.d and sulfas-PosTargetedMSMS.d files contain both MS and MS/MS (Q-TOF) data. • You can get help for any window, dialog box, or tab by pressing the **F1** key when that window is active.

Task 1. Open the Qualitative Analysis program with multiple data files (continued)

Steps	Detailed instructions	Comments
	 **Figure 1** The Open Data File dialog box is automatically opened	
	• Ensure **Use current method** is clicked. • Ensure the check box for **Run 'File Open' actions from selected method** is clear.	
	c Press and hold the **Shift** key while you click **sulfas_PosAutoMSMS**, **sulfas_PosMS.d** and **sulfas-PosTargetedMSMS.d**. **d** Click **Open**. All three data files are displayed in Data Navigator, and three chromatograms are displayed in the Chromatogram Results window.	• If you press the **Ctrl** key instead, you can pick files which are not directly next to each other in the list. • What you see in the main window at this point depends on the method, layout, display, and plot settings used before you opened these files.

Task 1. Open the Qualitative Analysis program with multiple data files (continued)

Steps	Detailed instructions	Comments

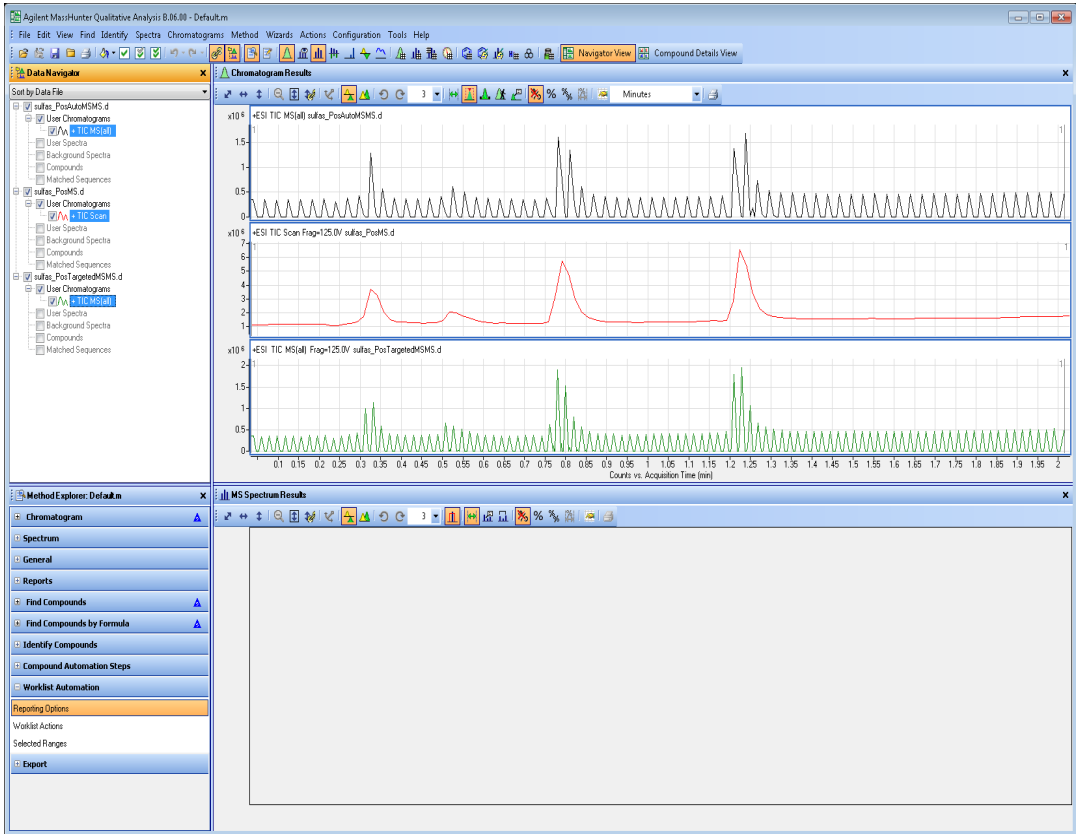


Figure 2 Qualitative Analysis main window

2 Return the main window to its default workflow, **General**. The default method and layout are loaded.

- Make sure you can see all three chromatograms.

a If necessary, click **Configuration > Configure for Workflow > General**.

b In the **Workflow Configuration** dialog box, mark:

- **Load workflow's default method**
- **Load workflow's default layout**

c Click the down arrow next to the **Maximum number of list panes** list in the **Chromatogram Results** toolbar, and select **3**.

- The display and plot settings will remain the same even after you switch to the General workflow. These settings differ depending on your specific situation.
- You can change the layout by clicking **Configuration > Window Layouts > Load Layout**.

Task 1. Open the Qualitative Analysis program with multiple data files (continued)

Steps	Detailed instructions	Comments
		Lists maximum number of panes. The default method and layout are loaded. To load the default display and plot settings, click **Configuration > Plot Line Definitions**.

Figure 3 Qualitative Analysis main window with the General Workflow selected

Task 2. Print an analysis report

When you want to print an analysis report after performing any of the tasks in this exercise or the next one, use these instructions.

An analysis report can contain the results from extracting and integrating chromatograms, extracting spectra, finding compounds, searching the database for peak spectra, or generating formulas from peak spectra.

Task 2. Print an analysis report

Steps	Detailed instructions	Comments
1 Save the intermediate report files.	**a** Click **Configuration > Intermediate Report Files**. **b** Mark the **Keep intermediate report directories** check box. **c** Click **OK**.	• Normally, intermediate report directories are not kept. However, when you are customizing a report, you use these files to verify any changes that you make to the templates. • After you have finished customizing your report templates, remember to clear the **Keep intermediate report directories** check box.
2 Change the analysis report selections. ◦ Mark the check boxes for the chromatograms, spectra or tables you want to print. ◦ Clear the check boxes for the chromatograms, spectra or tables you do not want to print.	**a** In **Method Explorer**, click **Reports > Analysis Report**. **b** Mark the check boxes for any additional sections you want to print. **c** Clear any chromatogram and spectra choices you do not want to print.	• A section in a report is only included if: ◦ You mark the check box in this section. ◦ The results are available in the Qualitative Analysis program. For example, if you have not integrated the chromatogram, the peak table cannot be included. • If you are keeping the intermediate report directories to customize a template, mark all of these check boxes. You also need to generate all of these results. Then, all results are available when you are customizing a template.

Task 2. Print an analysis report (continued)

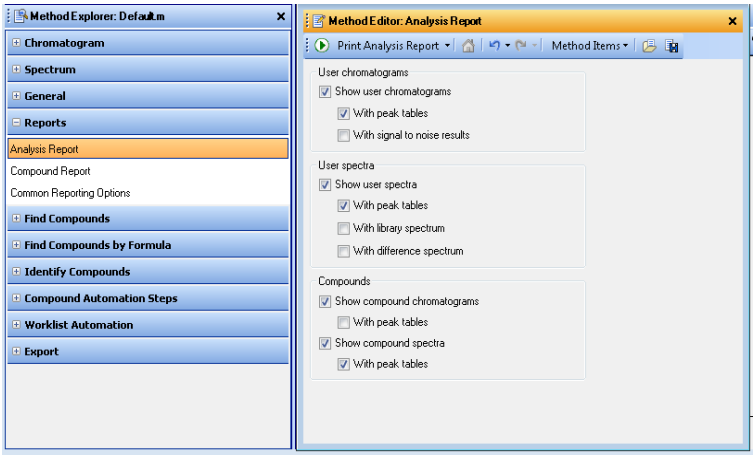
Steps	Detailed instructions	Comments
		Before printing the analysis report, you generate the results that you want to include. For example, if you want to include compound chromatograms, you need to run one of the **Find Compounds** algorithms. If you want to increase the speed of printing a report, remove any unnecessary graphics. Including graphics in a report slows down report generation.

Figure 4 Analysis Report section in the Method Editor

3 Select the template to use when printing this report.	**a** In **Method Explorer**, click **Reports > Common Reporting Options**. **b** Verify that the correct **Report template folder** is selected. **c** Verify that the correct **Analysis report template** is being used. **d** Click the **Options** tab. **e** Verify the settings on this tab.	• The report templates shipped with the software are separated into two folders. One folder contains reports formatted to print on Letter size paper. The other folder contains reports that print on A4 size paper. • Three different analysis report templates are available in each folder.

Task 2. Print an analysis report (continued)

Steps	Detailed instructions	Comments

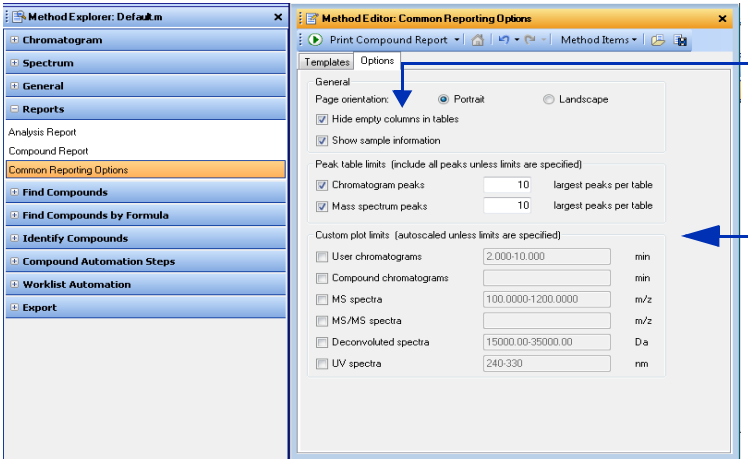


Figure 5 Common Reporting Options > Options tab in the Method Editor window

4 Print the report.	• You can interactively print the report in multiple ways:
	  • From the main menu, click **File > Print > Analysis Report.**
	  • From the main toolbar, click the **Printer** icon.
	  • Click the **Print Analysis Report** icon,  in the Method Editor toolbar.
	  • Right-click the **Analysis Report** section in the **Method Editor**, and click **Print Analysis Report**.
	  • Right-click the data file in the **Data Navigator**, and click **Print Analysis Report**.
	  • Click **Generate Analysis Report** in the **Actions** menu.
		The Run icon  in the **Method Editor** toolbar sometimes allows you to choose an action from a set of possible actions. For example, if you switch to the **Reports > Common Reporting Options** section, four different actions are possible when you click the **Run** icon. If you click the **arrow**, a list of possible actions is shown, and you can choose which action to do. Choosing a different action from the list changes the default action. If you simply click the **Run** button, the default action is performed.

Task 3. Print a compound report

In this task, you generate a compound report. Refer to the *Familiarization Guide for Qualitative Analysis* or the online Help for the Qualitative Analysis program for information on finding compounds.

Task 3. Print a compound report

Step	Detailed instructions	Comments
1 Save the intermediate report files.	**a** Click **Configuration > Intermediate Report Files**. **b** Mark the **Keep intermediate report directories** check box. **c** Click **OK**.	• Normally, intermediate report directories are not kept. However, when you are customizing a report, you use these files to verify any changes that you made to the templates. • After you have finished customizing your report templates, remember to clear the **Keep intermediate report directories** check box.
2 Change the compound report selections: ◦ Run one of the **Find Compounds** algorithms ◦ Mark the check boxes for the chromatograms, spectra or tables you want to print. ◦ Clear the check boxes for the chromatograms, spectra or tables you do not want to print.	**a** Click **File > Open Data File** to load a data file. **b** Click one of the commands in the **Find** menu to find compounds. **c** In **Method Explorer**, click **Reports > Compound Report**. **d** Mark the check boxes for any additional sections you want to print. **e** Clear any chromatogram and spectra choices you do not want to print.	• Only sections that are marked in the **Compound Report** tab are included in the report. • A section in a report is only included if: ◦ You mark the check box in this section. ◦ The results are available in the Qualitative Analysis program. For example, if you have not found compounds, then the compound table cannot be included. • If you are keeping the intermediate report directories to customize a template, you mark all of these check boxes. You also need to generate all of these results. Then, all results are available when you are customizing a template.

Task 3. Print a compound report (continued)

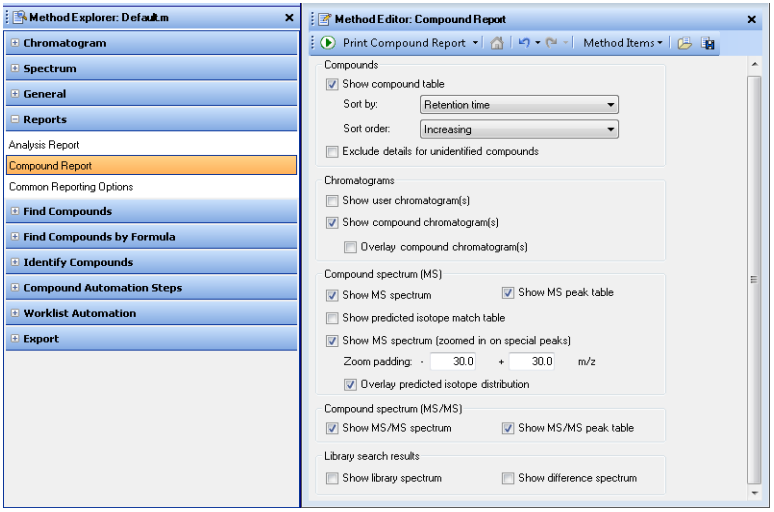
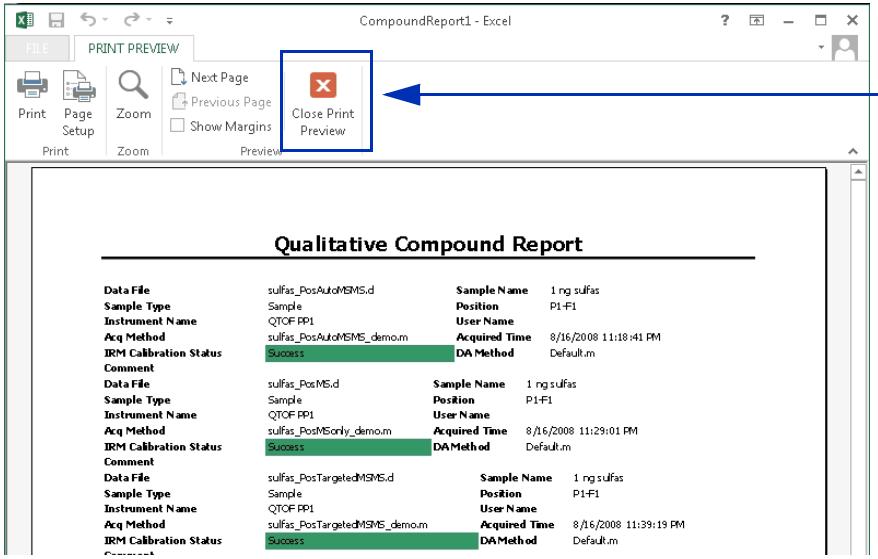
Step	Detailed instructions	Comments
			To increase the speed of creating a report, remove any unnecessary graphics. Including graphics in a report slows down the creation of reports.

Figure 6 Compound Report tab in the Method Editor

3 Select the template to use when printing this report.	**a** In **Method Explorer**, click **Reports > Common Reporting Options**. **b** Verify the correct **Report template folder** is selected. **c** Verify the correct **Compound report template** is being used **d** Click the **Options** tab. **e** Verify the settings on this tab.	• The report templates shipped with the software are separated into two folders. One folder contains reports formatted to print on Letter size paper. The other folder contains reports that print on A4 size paper. • Several different compound report templates are available in each folder.

Task 3. Print a compound report (continued)

Step	Detailed instructions	Comments
4 Print the report. • Preview the report.	**a** Click the **arrow** in the icon and select **Print Compound Report** to print the report. **b** In the **Print Compound Report** dialog box, click **All results**. **c** Mark **Print report**. **d** Mark **Print preview**. **e** (optional) Select the **Printer name** to use. If you want to print the report to a printer, select the printer in this dialog box. **f** Click **OK**.	• You also can print a compound report by doing any of the following: ◦ Right-click the **Compound Report** section in the **Method Editor**, and click **Print Compound Report**. ◦ Click **File > Print > Compound Report**. ◦ Click **Generate Compound Report** in the **Actions** menu. • You can create a PDF file by marking the **Save report as PDF file** check box. This option only works if you installed the Microsoft Excel PDF add-in after installing Excel.



This button closes the **Print Preview** window without sending the report to the printer.

Figure 7 The Print Preview window showing the Compound Report

5 Close the Print Preview window.	Click **Close Print Preview** in the toolbar.	• If you want to print the report, click the **Print** button. The report prints on the printer selected in the Print Compound Report dialog box.

Task 4. Generate a graphics report

In this task, you generate a graphics report. This report is generated when you click **Print** in the shortcut menu in one of the graphics windows.

Task 3. Print a graphics report

Step	Detailed instructions	Comments
1 Save the intermediate report files.	**a** Click **Configuration > Intermediate Report Files**. **b** Mark the **Keep intermediate report directories** check box. **c** Click **OK**.	• Normally, intermediate report directories are not kept. However, when you are customizing a report, you use these files to verify any changes that you made to the templates. • After you have finished customizing your report templates, remember to clear the **Keep intermediate report directories** check box.
2 Select the folder to use when printing this report. ◦ You can select the folder to use. ◦ A graphic report always uses either the template graphic or graphicfullpage.	**a** In **Method Explorer**, click **Reports > Common Reporting Options**. **b** Verify that the correct **Report template folder** is selected.	• The report templates shipped with the software are separated into two folders. One folder contains reports formatted to print on Letter size paper. The other folder contains reports that print on A4 size paper.
3 Print a graphics report.	**a** Right-click the **Chromatogram Results** window and click **Print**. **b** In the **Print** dialog box, click **All chromatograms**. **c** Clear the **One chromatogram per page** check box. **d** Select the **Printer name**. **e** Mark the **Print Preview** check box. **f** Click the **Options** tab. **g** Review the settings. **h** Click **OK**.	• You can only print a graphic if a graphic is currently showing in the Qualitative Analysis program. • You can print a graphics report from any of the graphics windows including: ◦ Chromatogram Results window ◦ Spectrum Preview window ◦ MS Spectrum Results window ◦ Deconvolution Results window ◦ UV Spectrum Results window • If the **One chromatogram per page** check box is marked, then the **graphicfullpage** template is used.

Task 3. Print a graphics report (continued)

Step	Detailed instructions	Comments

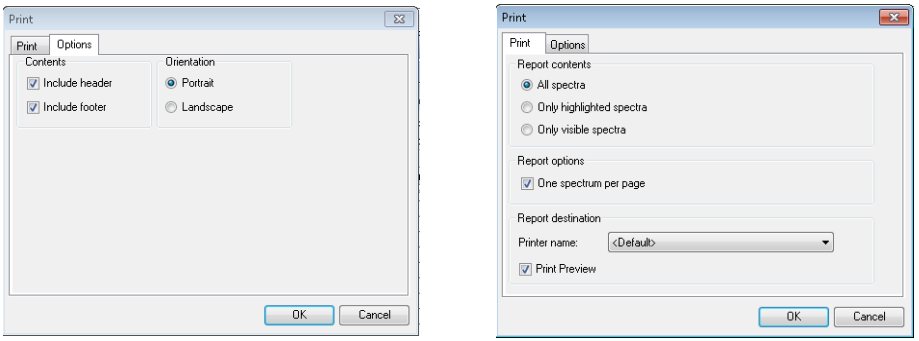
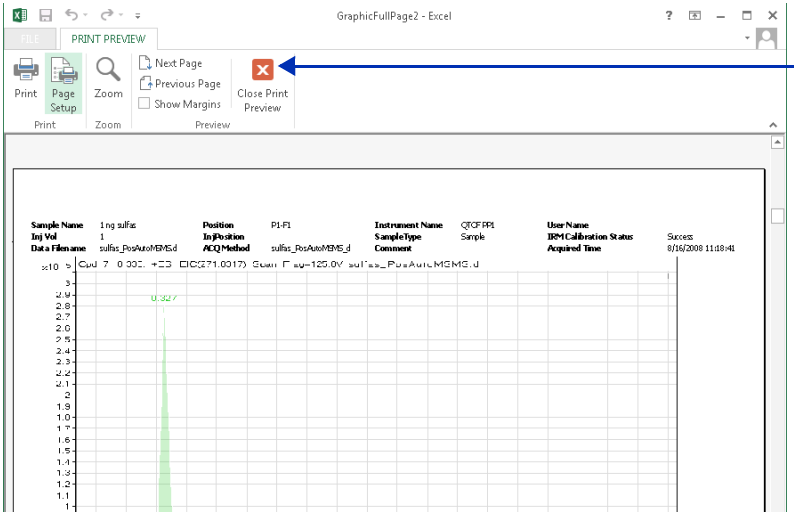


Figure 8 The Options and Print tab in the Print dialog box



This button closes the **Print Preview** window without sending the report to the printer.

Figure 9 The Print Preview window showing the Graphics Report

4 Close the Print Preview window.	Click **Close Print Preview** in the toolbar.	• If you want to print the report, click **Print**. The report is printed on the printer selected in the **Print Compound Report** dialog box.

Creating Reports in the Quantitative Analysis Program

Increasing Speed of Quantitative Analysis Report Generation

One of the easiest ways to increase the speed of report generation is by selecting a PDF template provided in the program.

If you can't find an existing template in PDF format that serves your needs, then you can increase the speed of your report generation by using one of the numerous Excel templates that does not include many, or any, graphics. Reports that do not include graphics print more quickly. Many of the templates that do not include graphics are in the **ESTD/Results** folder, the **ISTD/Results** folder, and the **LIMs** folder.

You can also try any of the following options to improve reporting speed:

- Filter for only the samples or compounds that you need to report. See "Task 7. Add a filter to a table" on page 73.
- Turn off any unneeded formatting options. See "Task 5. Change values on the Options worksheet" on page 133.
- Delete unused XML maps. See "Task 1. Add a table to a template" on page 86.
- Limit VLOOKUP ranges to the minimum. See "Task 7. Use the VLOOKUP function" on page 140.
- Print on a standalone system, if possible.
- Set the Microsoft Image Writer as the default printer if you are printing to a networked printer.

Task 5. Open a batch in the Quantitative Analysis program

In this task you open a batch file that you created previously.

Task 5. Open the Quantitative Analysis program

Steps	Detailed instructions	Comments
1 Open the **Quantitative Analysis** program and then open a batch file. • Select either the default batch or the batch you created, if you did the exercises in the Quantitative Analysis Familiarization Guide.	**a** Double-click the **Agilent MassHunter Quantitative Analysis** (QQQ) icon  . **b** Click **File > Open Batch**. **c** Move to the folder ***Your Directory*\DrugsOfAbuse\.** **d** Select a batch. You can select either **DrugsOfAbuseDemo.batch.bin** or ***iii*_Test_01**. **e** Click **Open**.	• You can also start the program by clicking **Programs > Agilent > MassHunter Workstation > Quantitative Analysis (QQQ)** from the Start menu. • Several different **Quantitative Analysis** icons are shown on the desktop. You select the one that matches your data type. For these examples, select the **QQQ** icon. • You can get help for any window, dialog box, or tab by pressing the **F1** key when that window is active.

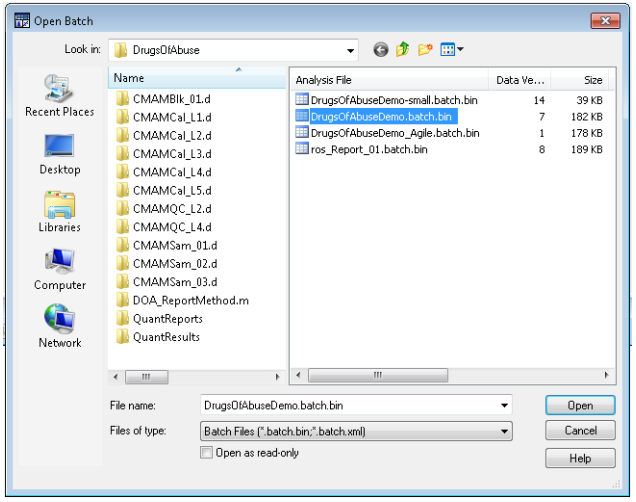


Figure 10 Open a batch file

Task 5. Open the Quantitative Analysis program (continued)

Steps	Detailed instructions	Comments
2 Analyze the batch, and inspect the results for each compound. • Examine the Quantitation Message(s), which identify samples with no quantitated signals. • Save the batch to the file ***iii*_Report_01**, where "**iii**" are your initials.	**a** Click Analyze Batch in the toolbar to start batch analysis. **b** Pass the mouse cursor over the quantitation message for Sample 1. **c** Pass the mouse cursor over the flags for the first two calibration standards. **d** Click **File > Save Batch As**. **e** Type `iii_Report_01`. **f** Click **Save**.	• Note that two calibration standards contain outlier data. Outlier data is data that is not in the range that you set as acceptable.

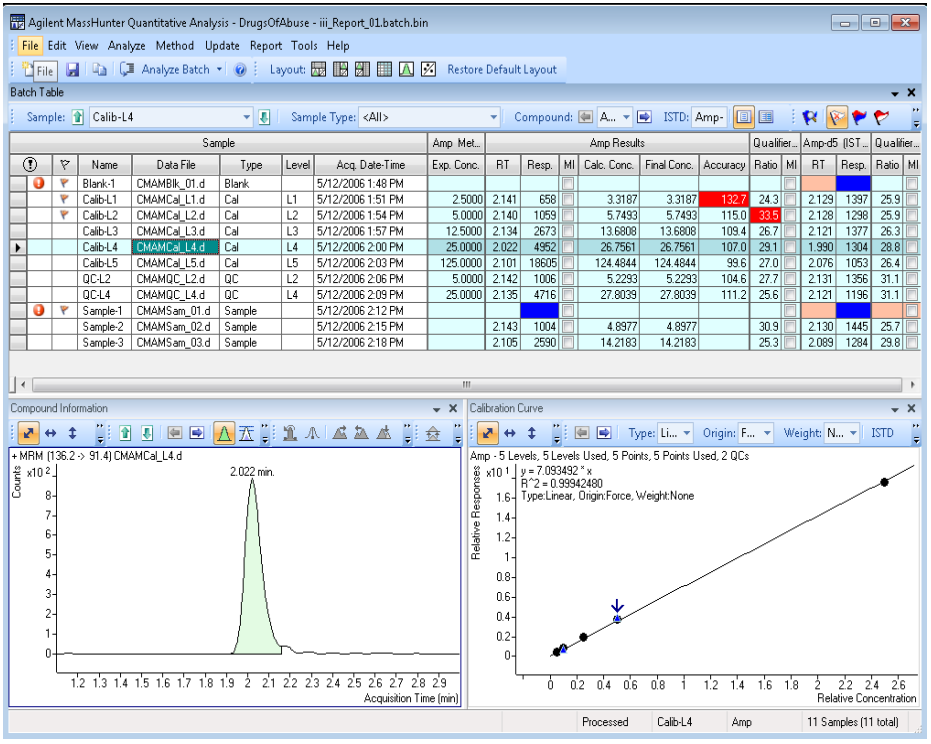
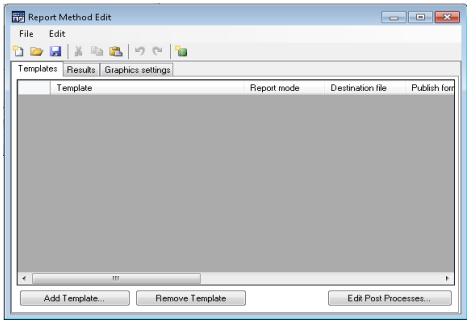


Figure 11 Quantitative Analysis program after analyzing batch

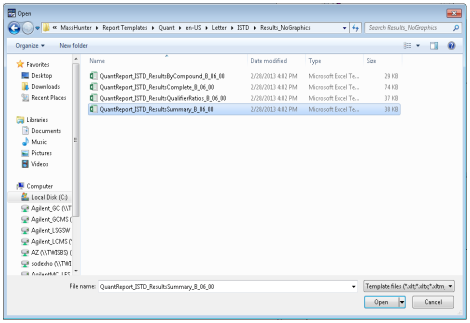
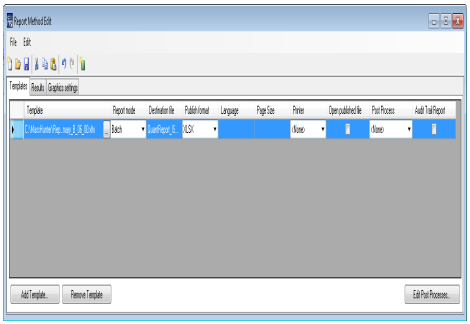
Task 6. Create a quantitation report method

In this task, you generate ISTD report using the one of the provided ISTD templates.

Task 6. Create a quantitation report method

Steps	Detailed instructions	Comments
1 If necessary, open the batch file ***iii*_Report_01.batch.xml**. • If the batch is already open, skip to step 2.	**a** To start the Quantitative Analysis program, click the **Quantitative Analysis (QQQ)** icon on your desktop. **b** Click **Open Batch** on the toolbar to display the Open Batch dialog box. **c** Move to ***Your Directory*\DrugsOfAbuse** and select ***iii*_Test_01.batch.bin.** **d** Click **Open**.	• You can also start the program by clicking **Programs > Agilent > MassHunter Workstation > Quantitative Analysis (QQQ)** from the Start menu. • If the default layout is not shown, click **Restore Default Layout** on the toolbar before opening the batch. Restore Default Layout
2 Select report template.	**a** Click **Report > Generate**. The system displays the **Generate Report** dialog box. **b** Select **New...**. The **Report Method Edit** window opens.	The Batch folder and file from your batch is displayed under Batch file. For faster report generation, choose a PDF template at **\MassHunter\Report Templates\Quant\PDF-Reporting** See the Quant DA online help for more details on configuring reports.
		

Task 6. Create a quantitation report method (continued)

Steps	Detailed instructions	Comments
	c From the **Template** tab, select **Add Template...**. The Open dialog box opens. **d** Navigate to and select **\MassHunter\ Report Templates\Quant\en-US\ Letter\ISTD\Results_NoGraphics\ QuantReport_ISTD_ResultsSummary**.	
		
	e Select **Open**. The template is added to the **Report Method Edit** window.	
		

Task 7. Generate quantitation reports using a report method

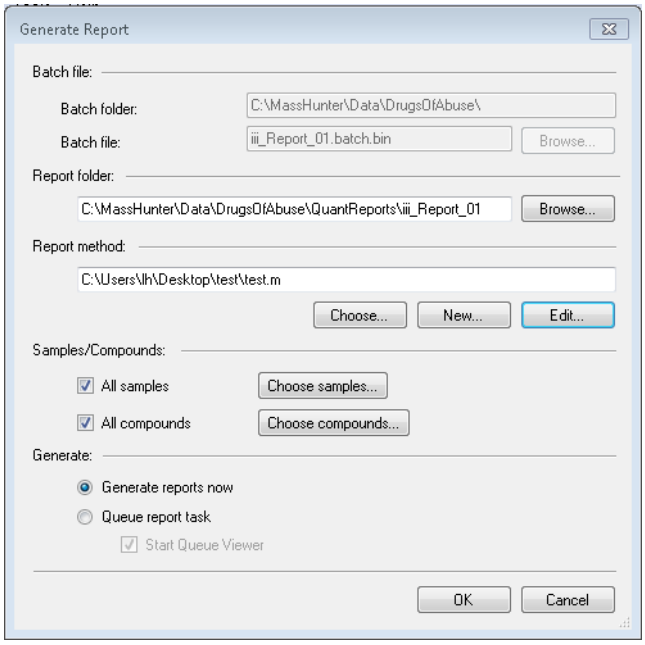
In this task, you generate ISTD and compound reports using the corresponding templates.

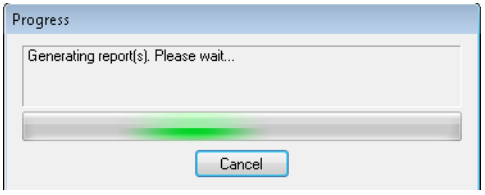
Task 7. Generate quantitation reports using a report method

Steps	Detailed instructions	Comments
1 If necessary, open the batch file ***iii*_Report_01.batch.bin**. • If the batch is already open, skip to step 2.	**a** To start the Quantitative Analysis program, click the **Quantitative Analysis (QQQ)** icon on your desktop. **b** Click **Open Batch** on the toolbar to display the Open Batch dialog box. **c** Move to \ ***Your Directory*** \ **DrugsOfAbuse** and select ***iii*_Test_01.batch.bin.** **d** Click **Open**.	• You can also start the program by clicking **Programs > Agilent > MassHunter Workstation > Quantitative Analysis (QQQ)** from the Start menu. • If the default layout is not shown, click **Restore Default Layout** on the toolbar before opening the batch. Restore Default Layout
2 Select options for your report.	**a** Select **Report > Generate...**. **b** Under **Report folder** use the default location or select **Browse...** to use another location. **c** Under **Report method**, select **Choose...**. **d** In the Open window, navigate to and select the method you created in "Task 6. Create a quantitation report method" on page 25. The method is displayed under **Report method**. **e** Select **All samples** and **All compounds** or use **Choose samples...** or **Choose compounds...** to select the items you want in your report. **f** Under **Generate**, select **Generate reports now**.	• Under **Generate**, you may choose **Queue report task** and **Start Queue Viewer** to view the report status as it is generated.

Task 7. Generate quantitation reports using a report method (continued)

Steps	Detailed instructions	Comments





Exercise 2
Customizing a template

In this exercise, you open a template and change the header and footer. You also verify the changes that you made. You modify both a Qualitative Analysis template and a Quantitative Analysis template.

- In Task 1, you open a Qualitative Analysis template in Excel.
- In Task 2, you customize the footer of the Qualitative Analysis template.
- In Task 3, you use this new template in the Qualitative Analysis program.
- In Task 4, you open a Quantitative Analysis template in Excel.
- In Task 5, you customize the footer of the Quantitative Analysis template.
- In Task 6, you use this new template in the Quantitative Analysis program.

Each exercise is presented in a table with three columns:

- Steps – Use these general instructions to proceed on your own to explore the program.
- Detailed instructions – Use these if you need help or prefer to use a step-by-step learning process.
- Comments – Read these to learn tips and additional information about each step in the exercise.

Task 1. Open a Qualitative Analysis template

In this task, you prepare and open a Qualitative Analysis template.

Task 1. Open a Qualitative Analysis template

Step	Detailed instructions	Comments
1 Make a copy of the AnalysisReport Microsoft Excel Template file and rename the file **iii_CustomAnalysisReport**	**a** Open the **Windows Explorer** program. **b** Move to the **Report Templates\Qual** folder in the folder where you installed the data. **c** Move to the **Letter** or **A4** folder **d** Right-click the **AnalysisReport** Microsoft Excel Template file and click **Copy**. **e** Click **Edit > Paste** to add a copy of the report template to the current folder. **f** Right-click the new file, **AnalysisReport-Copy** and click **Rename**. **g** Type *iii_CustomAnalysisReport*	• You do the same steps to open a **Quantitative Analysis** template.

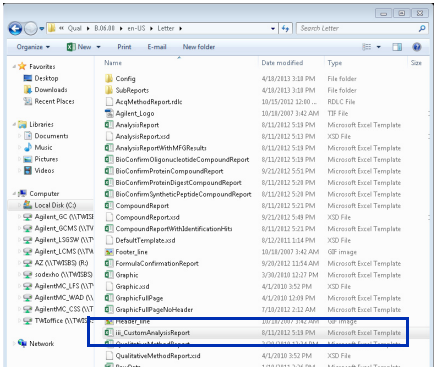
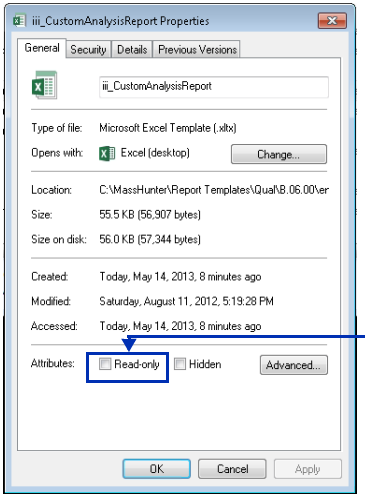


Figure 12 Report Templates\Qual\Letter folder

Task 1. Open a Qualitative Analysis template (continued)

Step	Detailed instructions	Comments
2 If needed, remove the **Read-only** attribute from the new template.	**a** Right-click the new file and click **Properties**. **b** Clear the **Read-only** check box in the Attributes section. **c** Click **OK**.	• If a template is read-only, you cannot save any changes to the template.
	 **Figure 13** Properties dialog box	Clear the **Read-only** check box.
3 Open the template.	• Right-click the new file and click **Open**.	

Task 2. Customize the footer of the Qualitative Analysis template

In this task, you change the footer of the Qualitative Analysis template that you opened in "Task 1. Open a Qualitative Analysis template" on page 30.

Task 2. Customize the footer of the Qualitative Analysis template

Step	Detailed instructions	Comments
1 Switch to the **Page Layout** view: • Switch to the **Design** worksheet if necessary.	Click **Page Layout** in the Workbook Views group in the **View** tab in the Ribbon. You can also click the **Page Layout** icon ( ) at the bottom of the Excel program to switch to the Page Layout view.	• In the Page Layout view, the header and footer are visible. • The header is printed at the top of each page and the footer is printed at the bottom of each page. • The header and the footer each have three different parts: left, center and right. Click any of these sections to edit that part.

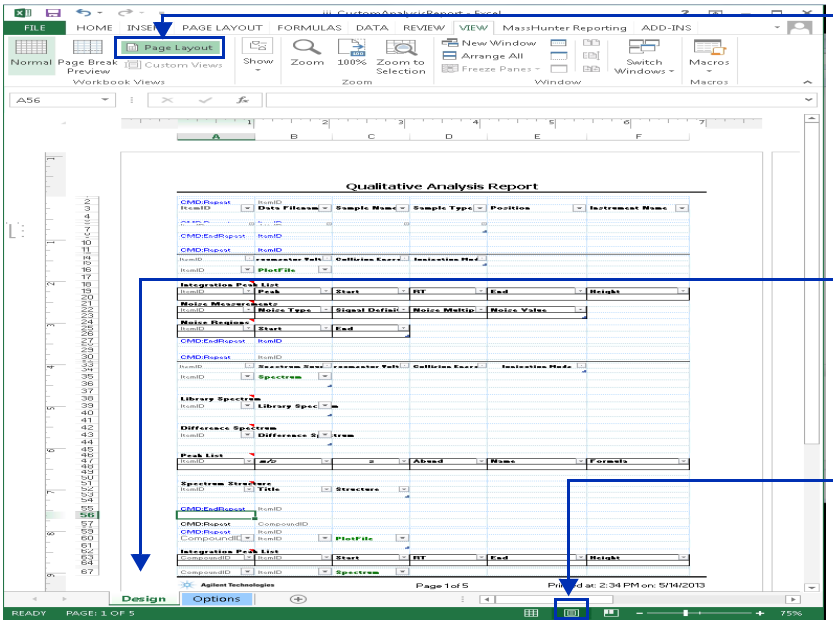
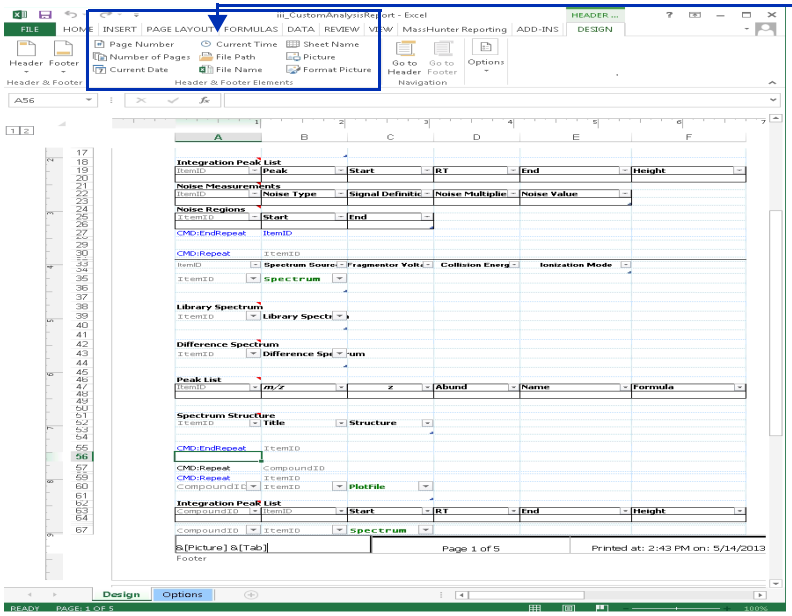


Figure 14 Switching to the Page Layout view in Excel

Task 2. Customize the footer of the Qualitative Analysis template (continued)

Step	Detailed instructions	Comments
2 Change the footer. • Add the worksheet name to the left section of the footer.	**a** Scroll to the bottom of the design page in Excel. **b** Click the left section of the footer. A text section appears containing the text **&[Picture]**. **c** Insert a space. **d** Click **Sheet Name** in the **Header & Footer Elements** group in the **Design** tab. The text **&[Tab]** is added. **&[Tab]** is the name of the tab or worksheet.	• Excel has different keywords in the header or footer that refer to different pieces of information: • &[Page] = the page number • &[Pages] = the total number of pages • &[Date] = the date the report was created • &[Time] = the time the report was created • &[File] = the name of the Excel template file • &[Picture] = the picture that you selected



The **Header & Footer Tools** are shown in the Design tab when you click one of the sections in the header or footer. You can click these buttons to quickly add these items to the header or footer.

By default, the sheet name is Design. See "Task 1. Add a page break and a sheet break" **on page 116**, to learn how to change the sheet name.

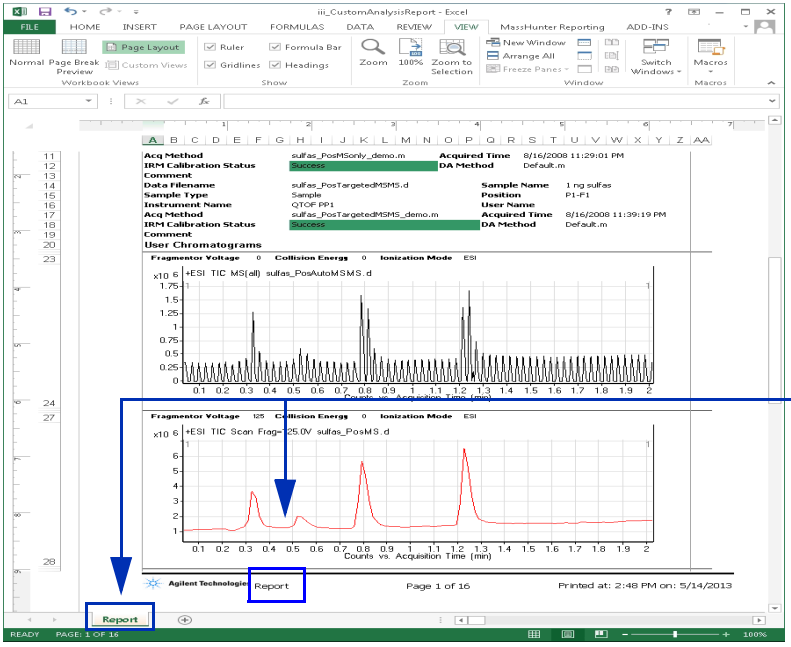
Figure 15 The Header and Footer Design Tab in Excel

Task 2. Customize the footer of the Qualitative Analysis template (continued)

Step	Detailed instructions	Comments
3 Finish editing the footer.	**a** Click in any of the cells in the spreadsheet to stop editing the footer. **b** Click **Normal** in the **Workbook Views** group in the **View** tab in the **Ribbon**.	
4 Test the changes to the template.	**a** Click the **MassHunter Reporting** tab. **b** Click **Process Report**. **c** Click **Browse.** **d** Move to the **\MassHunter\reports\temp** folder. **e** Double-click one of the folders that contains analysis results. **f** Select **Report.** **g** Click **Open**. **h** Click **OK**. **i** After the report is processed, click **Page Layout** in the Workbook Views group in the **View** tab in the Ribbon. **j** Scroll to the bottom of the page to see the change. The name of the tab is added after the Agilent logo.	• The Process Report command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon. • You can only see the header and the footer in the Page Layout view.

Task 2. Customize the footer of the Qualitative Analysis template (continued)

Step	Detailed instructions	Comments



The name of the tab is Report. This word is also added to the footer on each page.

Figure 16 Verifying changes in the footer after using the Process Report command

5 Save the changes to the template.

- You have to clear the results first.
- You can either save the template to the same name or to a new name.

a Click **Clear Results** in the **MassHunter Reporting** tab in the **Ribbon**.

b Click **File > Save**.

- You can click **Save As** if you want to change the name of the template.
- The **Save as type** is **Excel Template**.

Task 2. Customize the footer of the Qualitative Analysis template (continued)

Step	Detailed instructions	Comments

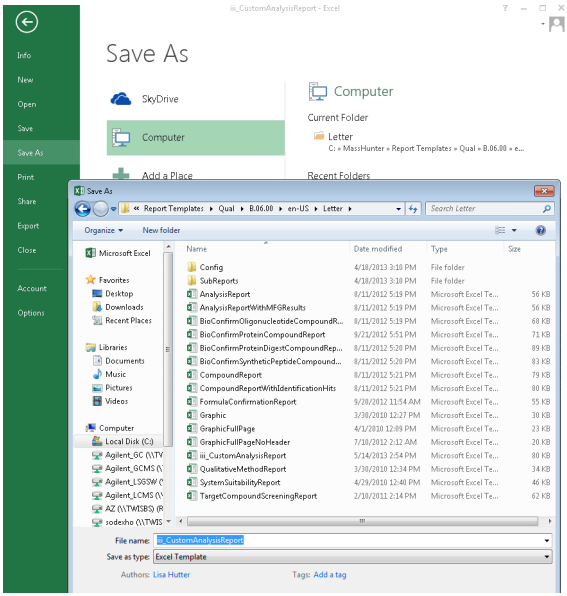


Figure 17 The Save As menu

Task 3. Use the new template in the Qualitative Analysis program

To use the new template in the Qualitative Analysis program you change the template that is used for an analysis report.

An analysis report can contain the results from extracting and integrating chromatograms, extracting spectra, finding compounds, searching the database for peak spectra, or generating formulas from peak spectra.

Task 3. Use the new template in the Qualitative Analysis program

Steps	Detailed instructions	Comments
1 Open the **Qualitative Analysis** program and open the data files, **sulfas-PosAutoMSMS**, **sulfas-PosMS.d** and **sulfas-PosTargetedMSMS.d** in the folder **\MassHunter\Data**, or in the folder where you copied them.	• Follow the instructions in "Task 1. Open the Qualitative Analysis program" on page 10.	
2 Change the template that is used for the analysis report.	**a** In **Method Explorer,** click **Reports > Common Reporting Options**. **b** Select the template ***iii*_CustomAnalysisReport** as the **Analysis report template**, where *iii* are your initials. **c** Clear any chromatogram and spectra choices you do not want to print.	• The new report template is automatically found and included in the list of possible analysis report templates when the Qualitative Analysis program is started. • If the Qualitative Analysis program is already running, the new template is not included in the list. The program will search for new templates if you do the following: **a** Click the  button next to the Report template folder. **b** Click **OK**. Do not change the folder that is selected.

Task 3. Use the new template in the Qualitative Analysis program (continued)

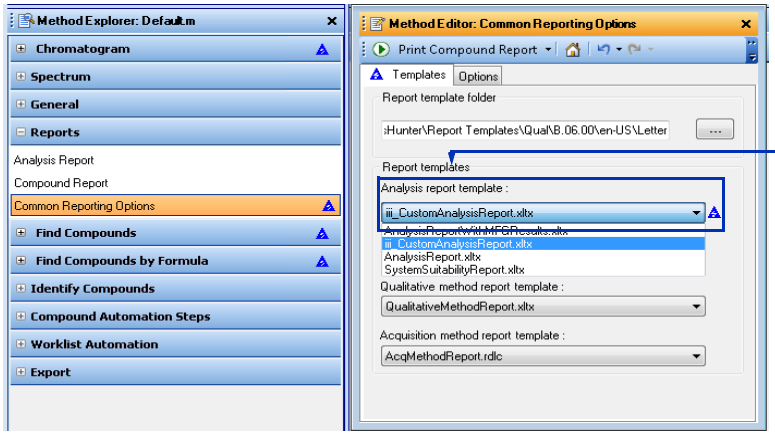
Steps	Detailed instructions	Comments
		You select the new report template for the Analysis report here.

Figure 18 Analysis Report section in the Method Editor

3 Select the template to use when printing this report.	**a** In **Method Explorer**, click **Reports > Common Reporting Options**. **b** Verify that the correct **Report template folder** is selected. **c** Verify that the correct **Analysis report template** is being used. **d** Click **Options**. **e** Verify the settings on this tab.	• The report templates shipped with the software are separated into two folders. One folder contains reports that are formatted to print on Letter size paper. The other folder contains reports that print on A4 size paper. • Three different analysis report templates are available in each folder.

Task 3. Use the new template in the Qualitative Analysis program (continued)

Steps	Detailed instructions	Comments
4 Print the report.	• You can interactively print the report in multiple ways: ◦ From the main menu, click **File > Print > Analysis Report.** ◦ From the main toolbar, click the **Printer** icon. ◦ Select **Print Analysis Report** from the list,  in the **Method Edit**or toolbar. ◦ Right-click the **Analysis Report** section in the **Method Editor**, and click **Print Analysis Report**. ◦ Select the data file in the **Data Navigator**, and click **Print Analysis Report**. ◦ Click **Generate Analysis Report** in the **Actions** menu.	The **Run** icon  in the **Method Editor** toolbar sometimes allows you to choose an action from a set of possible actions. For example, if you switch to the **Reports > Common Reporting Options** section, four different actions are possible when you click **Run**. If you click the arrow, a list of possible actions is shown, and you can choose which action to do. Choosing a different action from the list changes the default action. If you simply click **Run**, the default action is performed.

Task 4. Open a Quantitative Analysis Excel template

In this task, you prepare and open an Excel Quantitative Analysis template.

Task 4. Open a Quantitative Analysis Excel template

Steps	Detailed instructions	Comments
1 Make a copy of the QuantReport_ISTD_Summary_*B_04_00* Microsoft Excel Template file and rename the file **iii_Custom_ISTD_Summary.**	**a** Open the **Windows Explorer** program **b** Open the **Report Templates\Quant\en-US** folder in the folder where you installed the data. **c** Move to the **Letter** or **A4** folder. **d** Move to the **ISTD/Results_NoGraphics** folder. **e** Right-click the **QuantReport_ISTD_ResultsSummary_B_06_00** file and click **Copy**. **f** Click **Edit > Paste** to add a copy of the report template to the current folder. **g** Right-click the new file, **QuantReport_ISTD_ResultsSummary_B_06_00 - Copy,** and click **Rename**. **h** Type `iii_Custom_ISTD_Summary`.	• You do the same steps to open a Qualitative Analysis template. • In the **Report Templates\Quant\en-US\Letter or A4** folder, the templates are separated into additional folders, including **ESTD** and **ISTD**.

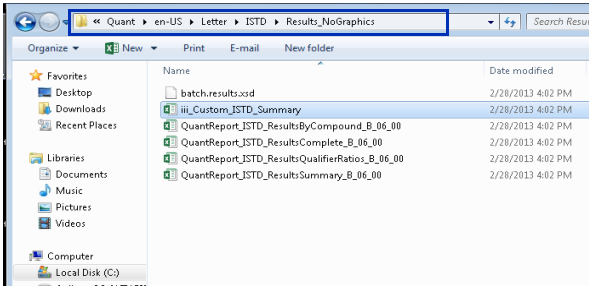
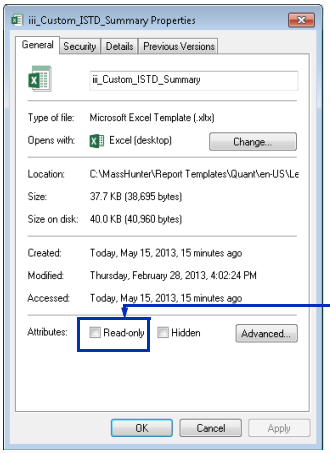


Figure 19 MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Results_NoGraphics folder

Task 4. Open a Quantitative Analysis Excel template (continued)

Steps	Detailed instructions	Comments
2 Remove the **Read-only** attribute from the new template.	**a** Right-click the new file and click **Properties**. **b** Clear the **Read-only** check box in the Attributes section. **c** Click **OK**.	• If a template is read-only, you cannot save any changes to the template.
	 Clear the **Read-only** check box. This check box may already be clear.	
	Figure 20 Properties dialog box	
3 Open the template.	• Right-click the **new file** and click **Open**.	

Task 5. Customize the footer of the Quantitative Analysis Excel template

In this task, you change the footer of the Quantitative Analysis Excel template that you opened in "Task 4. Open a Quantitative Analysis Excel template" on page 40.

Task 5. Change the footer of the Quantitative Analysis Excel template

Steps	Detailed instructions	Comments
1 Switch to the **Page Layout** view.	Click **Page Layout** in the Workbook Views group in the **View** tab in the Ribbon. You can also click the **Page Layout** icon ( ) at the bottom of the Excel program to switch to the Page Layout view.	• In the Page Layout view, the header and footer are visible. • The header is printed at the top of each page and the footer is printed at the bottom of each page. • The header and the footer each have three different parts: left, center and right. You can click any of these sections to edit that part.

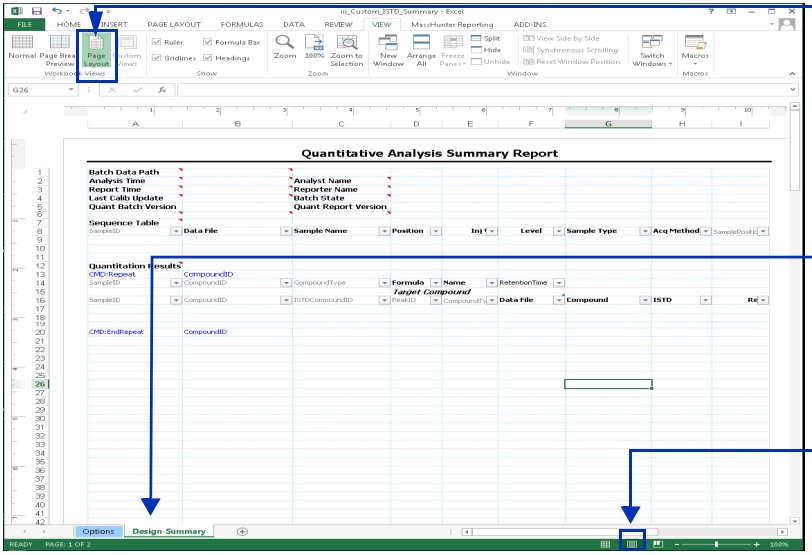
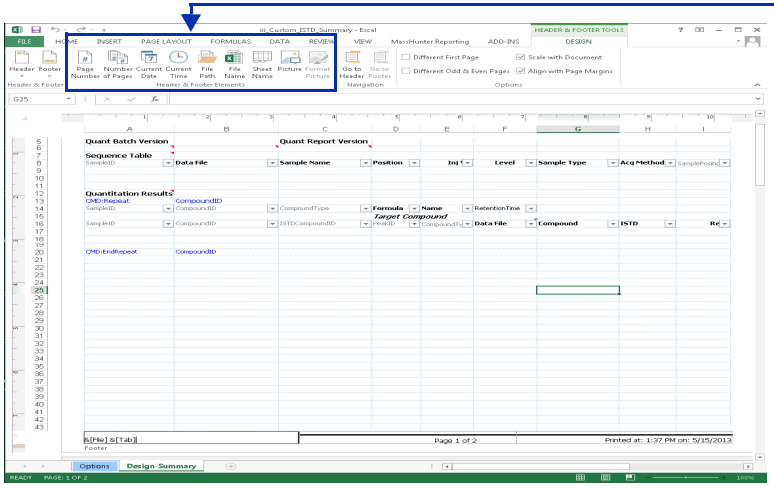


Figure 21 Switching to the Page Layout view in Excel

Task 5. Change the footer of the Quantitative Analysis Excel template (continued)

Steps	Detailed instructions	Comments
2 Change the footer. • Add the worksheet name to the left section of the footer.	**a** Scroll to the bottom of the design page in Excel. **b** Click the left section of the footer. A text section appears containing the text **&[File]**. **c** Insert a space. **d** Click **Sheet Name** in the **Header & Footer Elements** group in the Design tab. The text **&[Tab]** is added. **&[Tab]** is the name of the tab or worksheet.	• Excel has different keywords in the header or footer that refer to different pieces of information: • &[Page] = the page number • &[Pages] = the total number of pages • &[Date] = the date the report was created • &[Time] = the time the report was created • &[File] = the name of the Excel template file • &[Picture] = the picture that you selected when



The **Header & Footer Elements** are shown in the Design tab when you click one of the sections in the header or footer. You can click these buttons to quickly add these items to the header or footer.

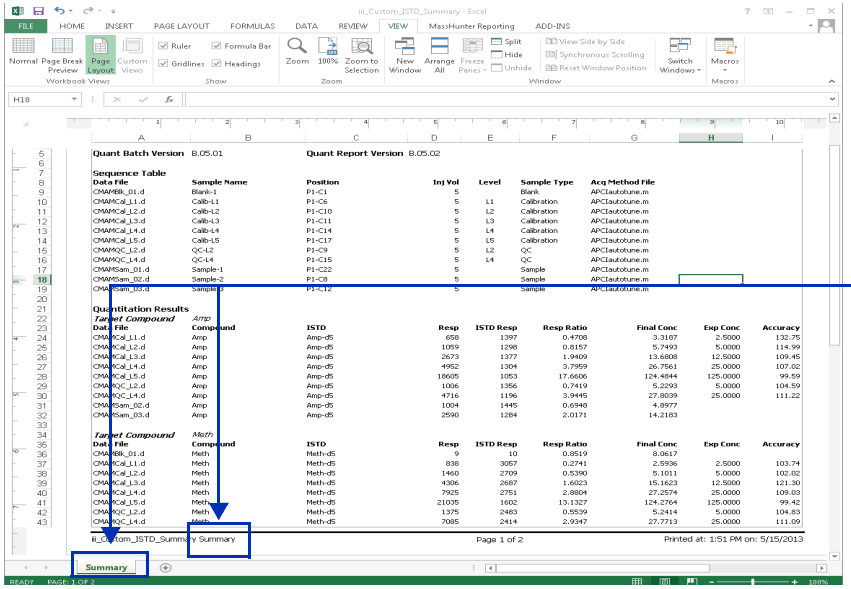
By default, the worksheet name in the template is **Design-Summary**. The worksheet name in the report is **Summary**. In Step 5, you will learn how to change the worksheet name.

Figure 22 The Header and Footer Design Tab in Excel

3 Finish editing the footer.	**a** Click in any of the cells in the spreadsheet to stop editing the footer. **b** Click **Normal** in the **Workbook** Views group in the **View** tab in the **Ribbon**.	

Task 5. Change the footer of the Quantitative Analysis Excel template (continued)

Steps	Detailed instructions	Comments
4 Test the changes to the template.	**a** Click **Process Report**. **b** Click **Browse**. **c** Move to the **\MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuseDemo** folder. **d** Select **report.results**. **e** Click **Open**. **f** Click **OK**. **g** After the report is processed, click **Page Layout** in the **Workbook** Views group in the **View** tab in the **Ribbon**. **h** Scroll to the bottom of the page to see the change. The name of the tab is added after the Agilent logo.	• The Process Report command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon. • You can only see the header and the footer in the Page Layout view.



The name of the tab is Summary. This word is also added to the footer on each page.

Figure 23 Verifying changes in the footer after using the Process Report command

Task 5. Change the footer of the Quantitative Analysis Excel template (continued)

Steps	Detailed instructions	Comments
5 Save the changes to the template. • You have to clear the results first. • You can either save the template to the same name, or to a new name.	**a** Click **Clear Results** in the **MassHunter Reporting** tab in the **Ribbon**.	• Click **Save As > Other Formats** if you want to change the name of the template. • The **Save as type** is **Excel Template** for most reports.

Task 6. Use the new Excel template in the Quantitative Analysis program

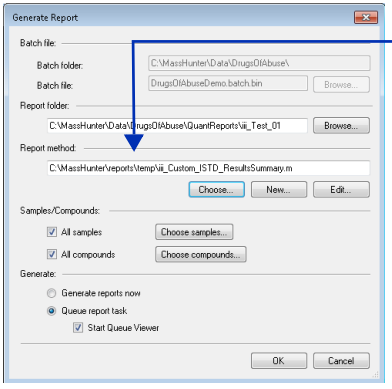
To use the new Excel template in the Quantitative Analysis program you need to select the new template in the Report dialog box.

Task 6. Use the new Excel template in the Quantitative Analysis program

Steps	Detailed instructions	Comments
1 Open the **Quantitative Analysis** program and open a batch file. • Select either the default batch or the batch you created if you did the exercises in the Quantitative Analysis Familiarization Guide. • Analyze the batch, and inspect the results for each compound.	• Follow the instructions in "Task 5. Open a batch in the Quantitative Analysis program" on page 23.	• If the **Quantitative Analysis** program is already running, you do not need to restart the program.
2 Open the **Generate Report** dialog box. • Verify the default destination directory for reports is ***Your Directory*\DrugsofAbuse\QuantReports**. • The default file name is ***iii*_Test_01**, where "**iii**" are your initials.	**a** Click **Report > Generate**. The system displays the Generate Report dialog box. **b** Click ... . **c** Specify the **Report folder** for example, ***Your Directory*\DrugsOfAbuse\QuantReports*iii*_Test_01**.	

Task 6. Use the new Excel template in the Quantitative Analysis program (continued)

Steps	Detailed instructions	Comments
3 Create a new Report method that uses the template. **iii_Custom_ISTD_Summary.**	**a** Select **New...**. The Report Method Edit window opens. **b** From the **Template** tab, select **Add Template...**. The Open dialog box opens. **c** Navigate to and select **\MassHunter\ Report Templates\Quant\en-US\ Letter\ISTD\Results_NoGraphics\ iii_Custom_ISTD_ResultsSummary**. **d** Select **Open**. The template is added to the Report Method Edit window. **e** Select **File > Save Method As...**. **f** In the **Save As** dialog box, navigate to **\MassHunter\reports\temp** and create a folder **iii_Custom_ISTD_ResultsSummary**. **g** Select **Save**. **h** From the **Report Method Edit** window, select **File > Exit**. The method using your template is now displayed under **Report method**.	



The new template is shown here.

Task 6. Use the new Excel template in the Quantitative Analysis program (continued)

Steps	Detailed instructions	Comments
4 Generate the report. • View the status of the report generation in the Task Queue Viewer.	**a** Click **OK** in the **Generate Report** dialog box to generate the report. Select **All samples** and **All compounds** or use **Choose samples** or **Choose compounds** to select the items you want in your report. **b** Under **Generate**, select **Queue report task** and **Start Queue Viewer** to view the report status as it is generated. **c** Watch the progress of the report in the **Status** column.	• If you add multiple templates to the Reports section, only one job is added to the queue which will print all of the reports. The reports are printed in the order requested. You can see the status of the reports in the Task Queue Viewer program.

Exercise 3
Customizing a table

In this exercise, you customize a table in a Quantitative Analysis template. After each change, you verify the changes and save the template to a new name. An example method is available for each of these tasks

- In Task 1, you rename a column header in a table.
- In Task 2, you delete a column from a table.
- In Task 3, you change the width of a column in a table.
- In Task 4, you move a column in a table.
- In Task 5, you add a column to a table.
- In Task 6, you add a mapped column to a table.
- In Task 7, you add a filter to two different tables using the Report Designer add-in and using features in Excel.
- In Task 8, you delete a column and move a column in each of those filtered tables.

Each exercise is presented in a table with three columns:

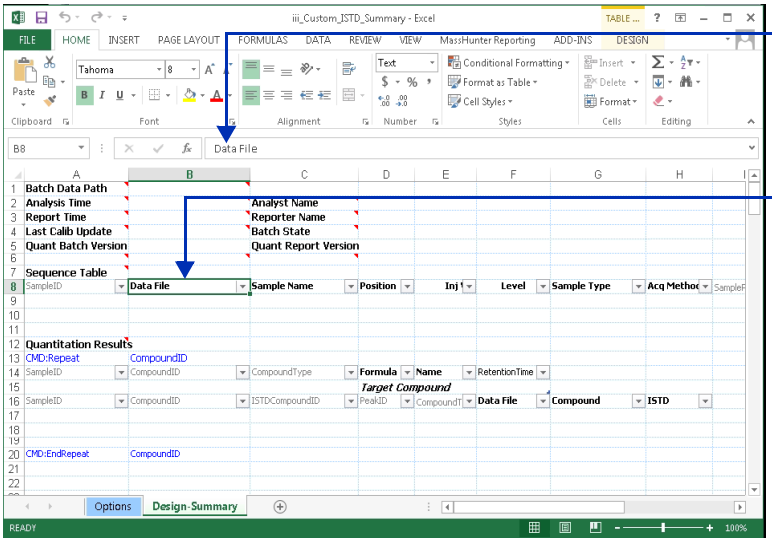
- **Steps** – Use these general instructions to proceed on your own to explore the program.
- **Detailed instructions** – Use these if you need help or prefer to use a step-by-step learning process.
- **Comments** – Read these to learn tips and additional information about each step in the exercise.

Task 1. Rename a column header in a table

In this task, you rename a column header in a table in a Quantitative Analysis template.

Task 1. Change the column header in a Quantitative Analysis table

Step	Detailed instructions	Comments
1 Open the **Quantitative Analysis** template **\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Results_NoGraphics*iii*_Custom_ISTD_Summary** template, where "***iii***" are your initials.	• Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, **iii_Custom_ISTD_Summary**, where "*iii*" are your initials.	• If you did not do the previous task, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Change the name of the **Data File** column to **Acquisition File**.	**a** Find the table labeled **Sequence Table**. **b** Click the cell containing the words **Data File**. This column is the second column in the table.	



The contents of the current cell are shown here in the Formula bar.

Click this cell in the **Sequence Table**.

One of the column headers in a table in the **Quantitation Results** section also is called **Data File**. Columns in different tables can have the same name.

Figure 24 Selecting the **Data File** cell in Excel

Task 1. Change the column header in a Quantitative Analysis table (continued)

Step	Detailed instructions	Comments
	c Type *Acquisition File*. You can also click in the **Formula Bar** to overwrite only part of the name.	• Two columns in the same table cannot have the same name. Excel automatically changes the name of the column that appears second in the table if two column names are the same.

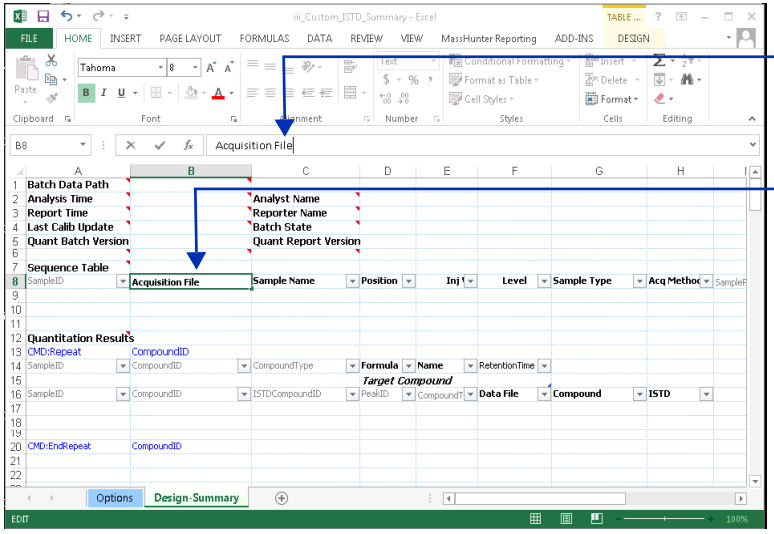


Figure 25 Changing the header of the column to **Acquisition File**

3 Test the changes to the template.	**a** Click **Process Report**. **b** Click **Browse**. **c** Move to the **MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuseDemo** folder. **d** Select **report.results.** **e** Click **Open**. **f** Click **OK**. **g** Find the **Sequence Table.** The first column is now called **Acquisition File**.	• The Process Report command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon. • If you do not click in another field after changing the name to Acquisition File, the Process Report command does not start.

Task 1. Change the column header in a Quantitative Analysis table (continued)

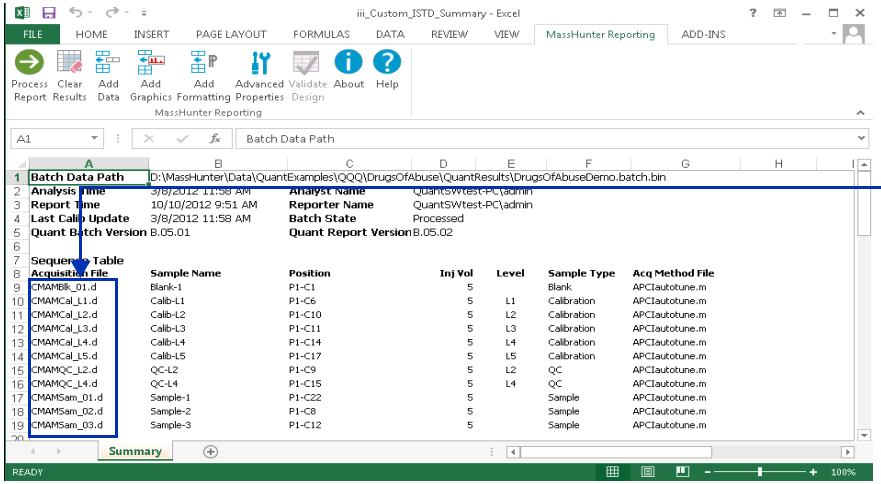
Step	Detailed instructions	Comments
		The column header is now Acquisition File.

Figure 26 Verifying changes in the column header after using the Process Report command

4 Save the changes to the template.

- You have to clear the results first.
- You save the template to the new name, **iii_1_Custom_ISTD_Summary**.

a Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon.

b Click **File > Save As**.

c In the **Save As** dialog box, type `iii_1_Custom_ISTD_Summary`.

d Verify the folder selected in **Save in** is correct.

e Click **Save**.

- The **Save as** type is **Excel Template**.

Task 2. Delete a column from a table

In this task, you delete a column from a table in a Quantitative Analysis template.

Task 2. Delete a column from a Quantitative Analysis table

Step	Detailed instructions	Comments
1 Open the **Quantitative Analysis** template **\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Results_NoGraphics\iii_1_Custom_ISTD_Summary.**	• Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, **iii_1_Custom_ISTD_Summary**, where "**iii**" are your initials.	• If you did not do the previous task, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Delete the column **Position** in the **Sequence Table**.	**a** Find the table labeled **Sequence Table**. **b** Click the cell containing the words **Position**. This column is the fourth column in the table.	

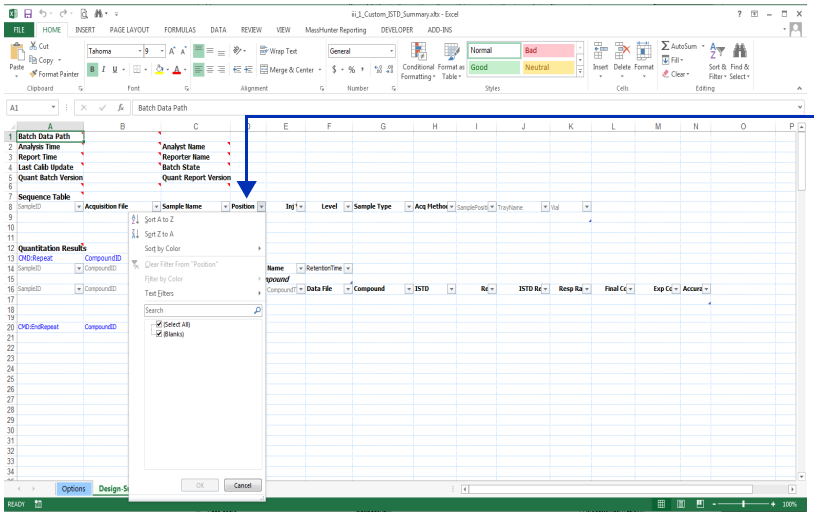


Figure 27 Selecting the **Position** cell in Excel

Task 2. Delete a column from a Quantitative Analysis table (continued)

Step	Detailed instructions	Comments
	c Right-click this cell and click **Delete > Table Columns**.	• Do not press the **Delete** key on the keyboard to delete a column in a table. If you press the **Delete** key, the column header is changed and the column is not deleted.

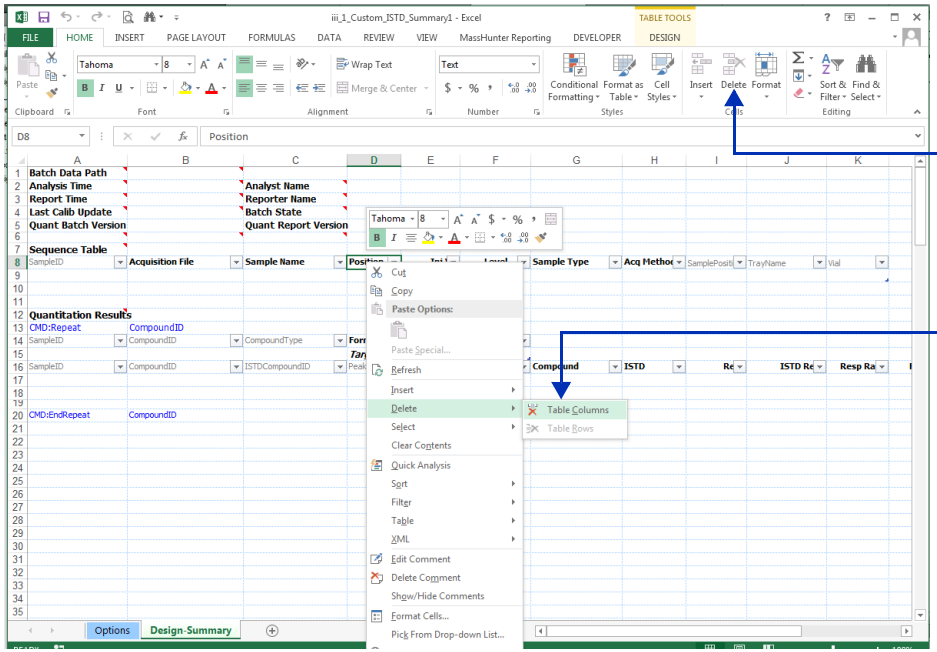
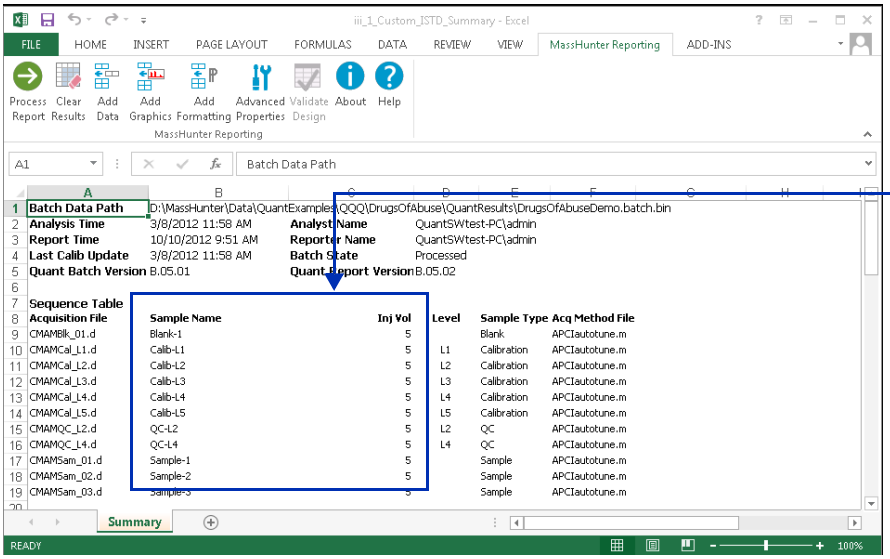


Figure 28 Deleting the **Position** column

3 Test the changes to the template.	**a** Click **Process Report**. **b** Click **Browse**. **c** Move to the **MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuseDemo** folder. **d** Select **report.results.** **e** Click **Open**. **f** Click **OK**. **g** Find the **Sequence Table**. The **Sample Name** column and the **Volume** column are adjacent.	• The Process Report command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon.

Task 2. Delete a column from a Quantitative Analysis table (continued)

Step	Detailed instructions	Comments



The Position column is no longer included in this table in the report.

Figure 29 Verifying that the **Position** column is removed

4 Save the changes to the template.

- You have to clear the results first.
- You save the template to the new name, **iii_2_Custom_ISTD_Summary.**

a Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon.

b Click **File > Save As**.

c In the **Save As** dialog box, type `iii_2_Custom_ISTD_Summary`.

d Verify the folder selected in **Save in** is correct.

e Click **Save**.

- The **Save as** type is **Excel Template**.

Task 3. Change the width of a column in a table

In this task, you change the width of a column in a table in a Quantitative Analysis template. You use the Advanced Properties dialog box to set the width of a column in a table.

Task 3. Change the width of a column in a Quantitative Analysis table

Step	Detailed instructions	Comments
1 Open the **Quantitative Analysis** template **C:\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Results_NoGraphics\iii_2_Custom_ISTD_Summary.**	• Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, **iii_2_Custom_ISTD_Summary**, where "**iii**" are your initials.	• If you did not do the previous task, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Change the width of the **Level** column to `10`.	**a** Find the table labeled **Sequence Table**. **b** Click the cell containing the word **Level**. This is the fifth column in the table.	

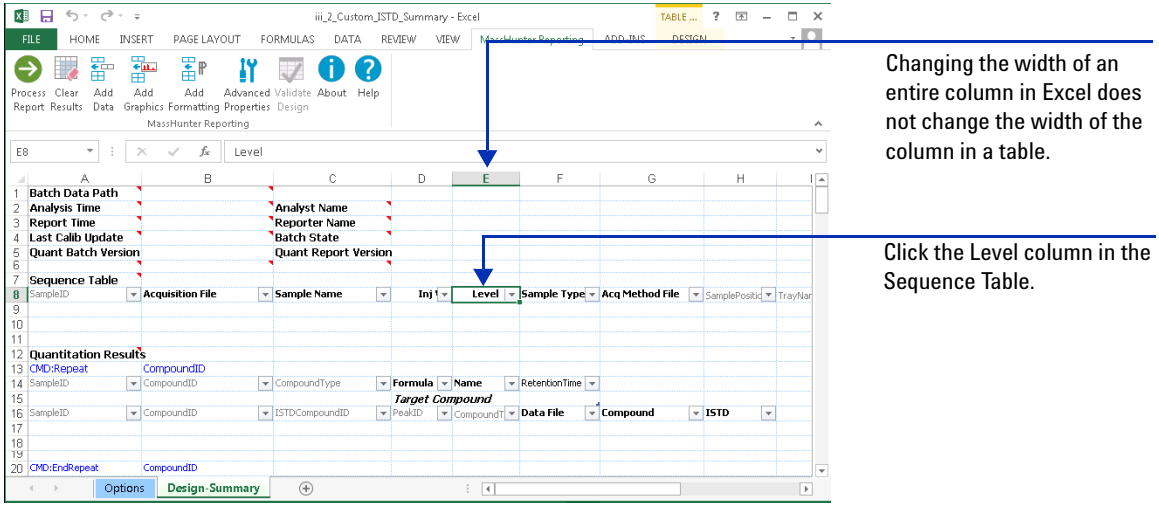
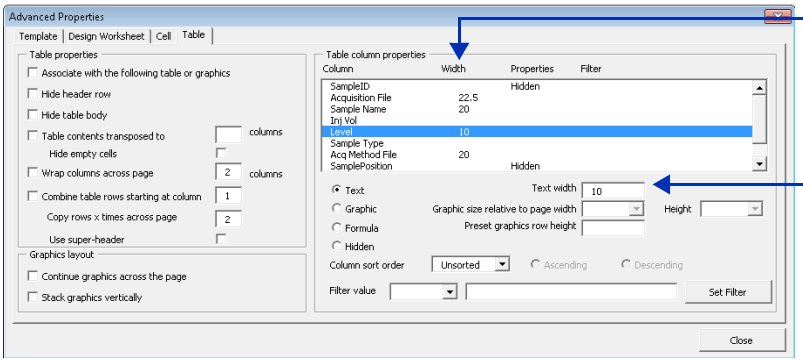


Figure 30 Selecting the **Level** column in Excel

Task 3. Change the width of a column in a Quantitative Analysis table (continued)

Step	Detailed instructions	Comments
	c Click **Advanced Properties** in the **MassHunter Reporting** tab in the **Ribbon**. **d** Type `10` in the **Text width** box. **e** Click **Close**. **f** Move the cursor over the **Level** column header to see the comment that has been added to this column.	• The **Advanced Properties** dialog box allows you to change the table in many different ways. • Any changes that you make in this dialog box take effect immediately. You can make many changes before closing this dialog box.



You can specify a column width for each column in a table. Several columns already have the width entered.

Type the new column width for the selected column here.

Figure 31 Changing the width of the Level column

Task 3. Change the width of a column in a Quantitative Analysis table (continued)

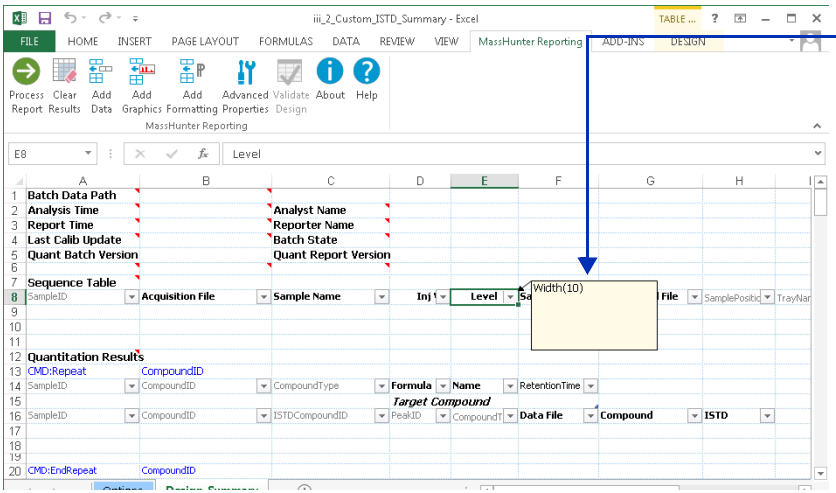
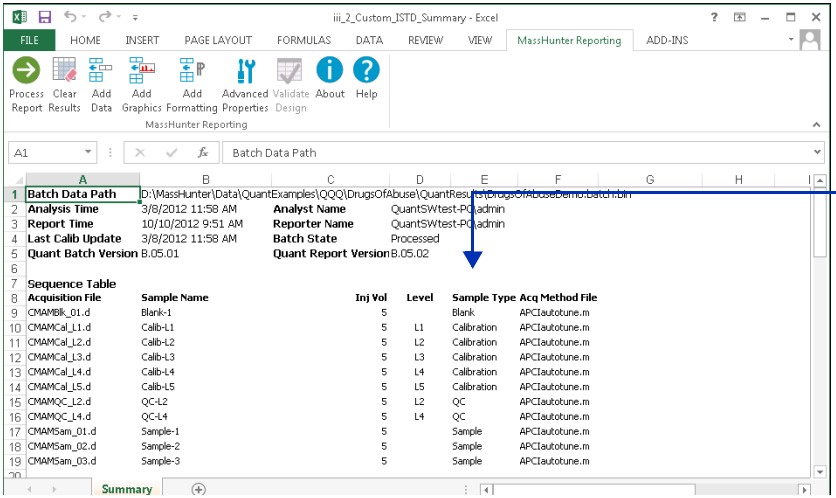
Step	Detailed instructions	Comments
		A Width comment has been added to the Level column. The Report Designer add-in reads these comments when the report is being processed and adjusts the width of the column automatically. A red triangle is added to a cell if the cell has a comment added to it. The red triangle is not visible in this cell because of the drop down box.

Figure 32 A **Width** comment has been added to the Level column

3 Test the changes to the template.	**a** Click **Process Report**. **b** Click **Browse**. **c** Move to the **\MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuseDemo** folder. **d** Select **report.results**. **e** Click **Open**. **f** Click **OK**. Find the **Sequence Table**. The **Level** column is narrower.	• The Process Report command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon.

Task 3. Change the width of a column in a Quantitative Analysis table (continued)

Step	Detailed instructions	Comments



The width of this column in the table is slightly wider.

Figure 33 Verifying changes in the width of the column after using the **Process Report** command

4 Save the changes to the template **iii_3_Custom_ISTD_Summary.**

- You have to clear the results first.

a Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon.

b Click **File > Save As**.

c In the Save As dialog box, type `iii_3_Custom_ISTD_Summary`.

d Verify the folder selected in **Save in** is correct.

e Click **Save**.

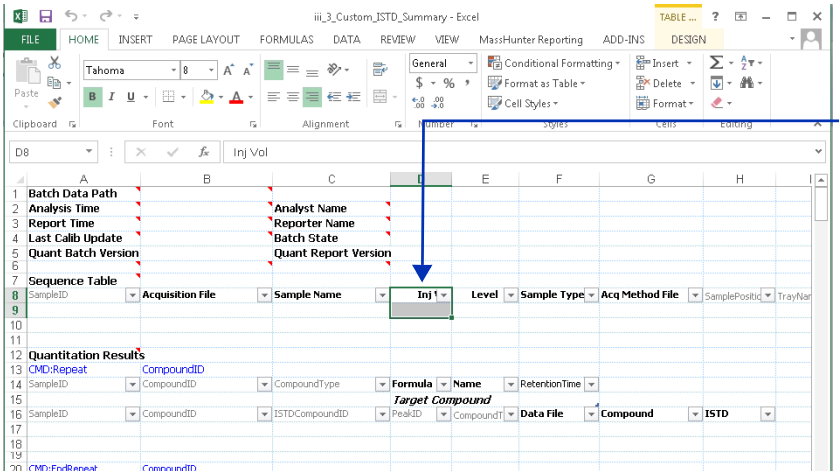
- The **Save as** type is **Excel Template**.

Task 4. Move a column in a table

In this task, you move a column in a table in a Quantitative Analysis template. If the table is filtered using the Excel filtering commands, refer to the task, Task 8. Move or delete a column in a filtered table.

Task 4. Move a column in a Quantitative Analysis table

Step	Detailed instructions	Comments
1 Open the Quantitative Analysis template **\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Results_NoGraphics\iii_3_Custom_ISTD_Summary**.	• Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, **iii_3_Custom_ISTD_Summary**, where "**iii**" are your initials.	• If you did not do the previous task, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Move the **Volume** column to the end of the table. • Move the cursor to the edge of the cell until it changes to the Move cursor.	**a** Find the table labeled **Sequence Table**. **b** Click the cell containing the word **Inj Vol**. This column is the fourth column in the table. **c** Move the cursor to the edge of the cell until the cursor changes to a four-sided arrow,  .	• The shape of the cursor changes depending upon where the cursor is pointing.



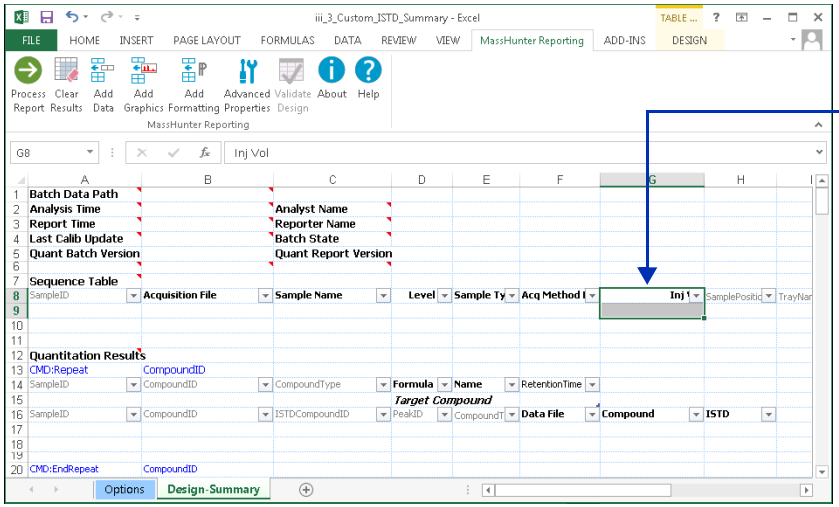
Click this cell in the **Sequence Table**.

When you move the column, the **Inj Vol** cell and the cell directly under it are moved together automatically. You do not need to manually select both cells.

Figure 34 Selecting the **Inj Vol** column in the Sequence Table

Task 4. Move a column in a Quantitative Analysis table (continued)

Step	Detailed instructions	Comments
	d Click and drag the cursor to the end of the table. You only move a column within the same table. As you drag the cursor, you can see where the column would be placed. The location between the columns changes to a hatched line. Release the mouse button when the hatched line appears between two cells. **e** Release the cursor at the end of the table.	• If you try to move the column outside of the table, the cursor changes to outline the cell where the column would be placed. If you release the mouse button when the cursor is not within the same table, two things happen. First, the label of the cell is placed in the new location. Second, the label of the column in the table is changed. You cannot undo this action. You have to rename the cell in the table and also delete the cell that was added.



The **Inj Vol column** has been moved to the end of the table.

This table has some hidden columns. You do not need to move this column after the hidden columns.

Figure 35 Moving the **Inj Vol** column to the end of the table

Task 4. Move a column in a Quantitative Analysis table (continued)

Step	Detailed instructions	Comments
3 Test the changes to the template.	**a** Click **Process Report**. **b** Click **Browse**. **c** Move to the **\MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuseDemo** folder. **d** Select **report.results.xml**. **e** Click **Open**. **f** Click **OK**. **g** Find the **Sequence Table**. The last column is now **InjVol**.	• The Process Report command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon.

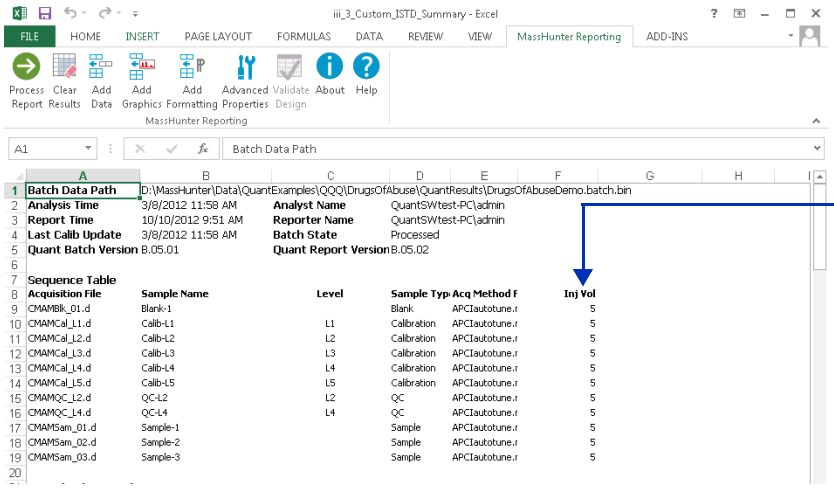


Figure 36 Verifying changes in the column header after using the **Process Report** command

4 Save the changes to the template **iii_4_Custom_ISTD_Summary**. • You have to clear the results first.	**a** Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon. **b** Click **File > Save As**. **c** In the Save As dialog box, type `iii_4_Custom_ISTD_Summary`. **d** Verify the folder selected in **Save in** is correct. **e** Click **Save**.	• The **Save as type** is **Excel Template**.

Task 5. Add a column to a table

In this task, you add a column header in a table in a Quantitative Analysis template.

Task 5. Add a column to a Quantitative Analysis table

Step	Detailed instructions	Comments
1 Open the Quantitative Analysis template **\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Results_NoGraphics\iii_4_Custom_ISTD_Summary.**	Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, **iii_4_Custom_ISTD_Summary**, where "**iii**" are your initials.	• If you did not do the previous task, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Add a column to the Sequence Table to the left of the **Acquisition File** column in the Sequence Table. • Change the name of this column to **Location**. • Change the formatting of this header to match the other headers in this table.	**a** Find the table labeled **Sequence Table**. **b** Click the cell containing the words **Acquisition File**. This column is the second column in the table.	• The **Data File** column was renamed to **Acquisition File** in "Task 1. Rename a column header in a table" on page 51.

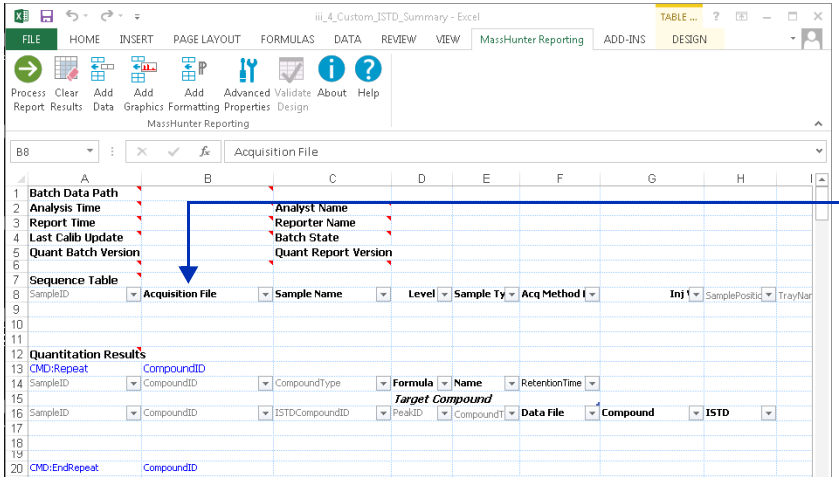
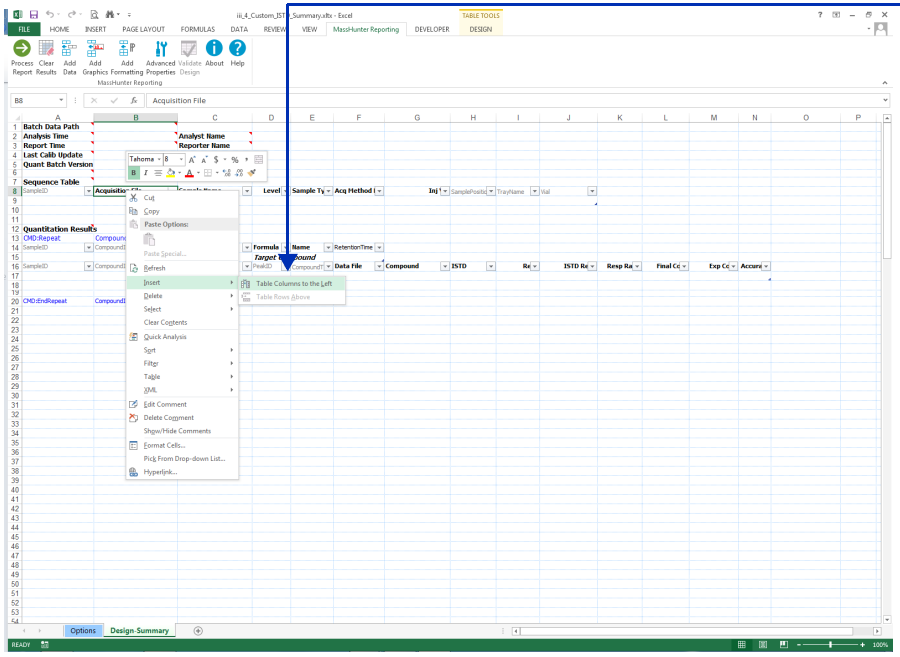


Figure 37 Selecting the Acquisition File cell in Excel

Task 5. Add a column to a Quantitative Analysis table (continued)

Step	Detailed instructions	Comments
	c Right-click this cell and click **Insert > Table columns to the left**.	• You click the column to the right of the location where you want to add a column.



Click this command. The new column is added to the left of the current column.

Figure 38 Add a column to the left of the **Acquisition File** column

d Follow the instructions in "Task 1. Rename a column header in a table" on page 51 to rename the column to **Location**.

e Type `="Laboratory 1"` in the cell directly below the cell **Location**.

f Select the cell **Location**. Right-click the cell and click the **B** icon and click the A icon in the shortcut menu.

- To add a word to a table, you first type = and then type the words inside of quotation marks. You are actually entering a simple formula.
- Headers in a table are black and bold.
- You can also change the font by using the icons in the **Font** group in the **Home** tab in the **Ribbon**.

Task 5. Add a column to a Quantitative Analysis table (continued)

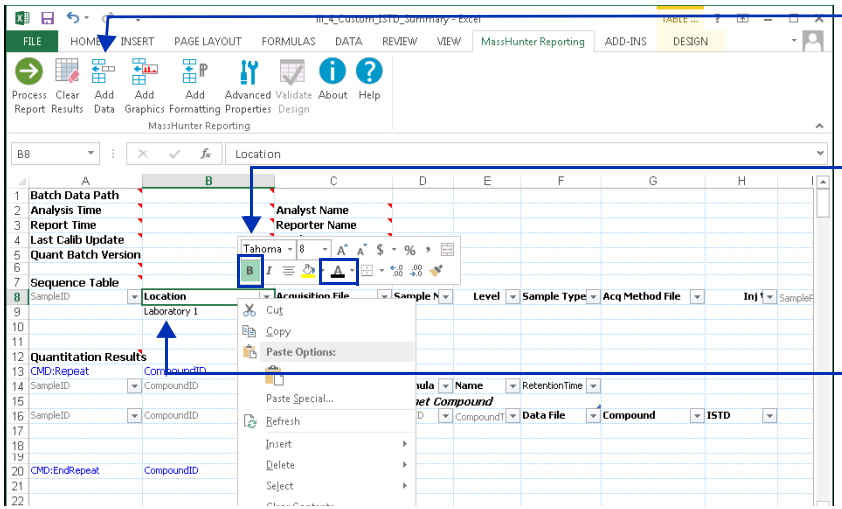
Step	Detailed instructions	Comments
		You can also use the icons in the Font group. To change the header to look like the other headers in the table, you click the Bold icon and also change the font color to black. **="Laboratory 1"** is added to this cell.

Figure 39 Change the format of the **Location** column header

3 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Move to the **\MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuseDemo** folder. **d** Select **report.results.xml**. **e** Click **Open**. **f** Click **OK**. **g** Find the Sequence Table. The first column is now **Location**.	• The Process Report command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon.

Task 5. Add a column to a Quantitative Analysis table (continued)

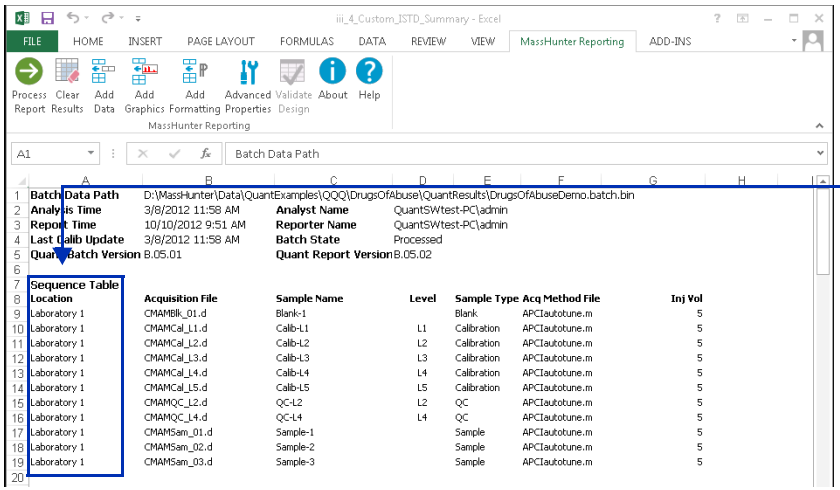
Step	Detailed instructions	Comments
		The first column is now Location. When you **Clear Results**, the formula **="Laboratory 1"** is not visible. However, it is still used whenever you process the report.

Figure 40 Verifying a new column is added to the table

4 Save the changes to the template **iii_5_Custom_ISTD_Summary.**

- You have to clear the results first.

a Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon.

b Click the **Microsoft Office button** and then click **Save As** and click **Other Formats**.

c In the Save As dialog box, type `iii_5_Custom_ISTD_Summary`.

d Verify the folder selected in **Save in** is correct.

e Click **Save**.

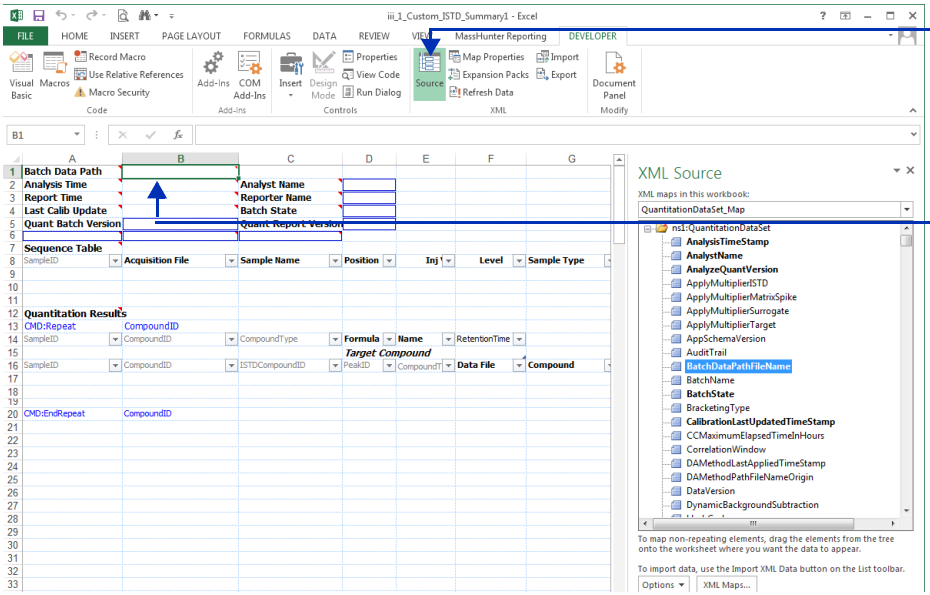
- The **Save as type** is **Excel Template**.

Task 6. Add a mapped column to a table

In this task, you add a mapped column to a table in a Quantitative Analysis template. A "mapped column" is a column that refers to information that is included in the results from the Quantitative Analysis program.

Task 6. Add a mapped column to a Quantitative Analysis table

Step	Detailed instructions	Comments
1 Open the Quantitative Analysis template **\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Results_NoGraphics\iii_5_Custom_ISTD_Summary.**	Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, **iii_5_Custom_ISTD_Summary**, where "**iii**" are your initials.	• If you did not do the previous task, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Display the XML source. • Hint: right-click a cell that is already mapped to display the shortcut menu.	**a** Find the cell containing the words **Batch Data Path**. **b** Right-click the cell next to this cell. **c** Click **XML > XML Source**.	• If the Developer tab isn't showing: **a** Click **File > Options > Customize Ribbon**. **b** Under **Main tabs**, mark **Developer**. **c** Click **OK**.



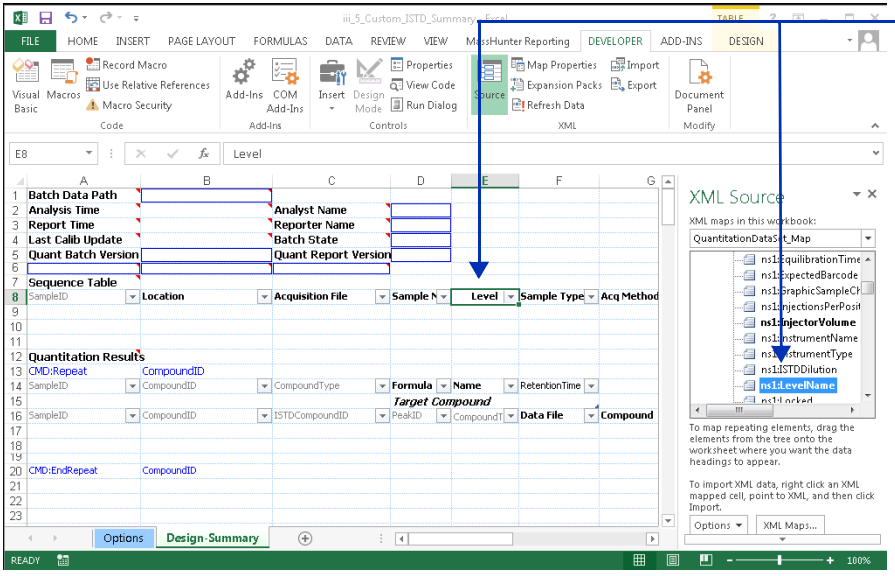
If the **Developer** tab in the Ribbon is visible, you can also click the **Source** icon in the XML

Right-click this cell and click **XML > XML Source**. You can right-click any mapped cell to select this command.

Figure 41 Displaying the XML Source task pane in Excel

Task 6. Add a mapped column to a Quantitative Analysis table (continued)

Step	Detailed instructions	Comments
3 Add the column **Barcode** to the end of the Sequence Table. • Hint: click two items in the Sequence Table to identify the correct section of the XML Source.	**a** Find the table labeled **Sequence Table.** **b** Click the **Acquisition File** column. **c** Click the **Level** column.	• As you click the mapped columns in the table, the list of elements in the XML Source window also changes. • If the element in the list is shown in Bold letters, that item is already mapped or used in the worksheet. • Elements in the same map cannot be used more than once.



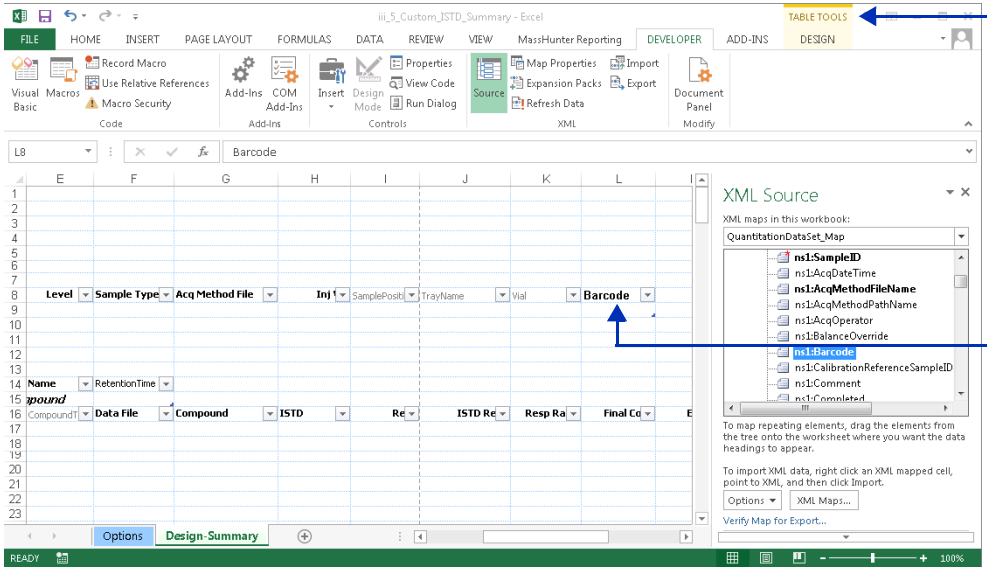
When you click the Level column, the element **ns1:LevelName** in the **XML Source** window is highlighted.

ns1: is part of the syntax of the element in the **XML Source** window. Every item in the XML Source window starts with **ns1:**.

Figure 42 Selecting the Level column in Excel

Task 6. Add a mapped column to a Quantitative Analysis table (continued)

Step	Detailed instructions	Comments
	d Scroll until the column after the end of the Sequence Table is visible. **e** In the XML Source window, scroll up to display the element **ns1:Barcode**. **f** Click and drag the element **ns1:Barcode** to the cell that is next to the **Vial** column. **g** Click the cell **Barcode**. **h** Right-click the cell and click the B icon in the shortcut menu.	• A blue triangle appears in the lower right corner of the last column in a table. After adding the column Barcode to the table, the blue triangle appears at the bottom of the Barcode column. • If you drag the element to a location that is not at the end of the table, an error is displayed. Right-click this column and click **Delete > Table Columns** to remove the column. Then, click and drag the element again to the end of the table.



In most cases, you can only add a mapped column to a table if the mapped column is from the same section in the XML source as the other columns in the table. First, you identify the section in the XML source by clicking two different columns in the table. Then, you choose one of the items that is in that same section. Items are in the same section if they are all nodes from the same element. For example, all of the elements listed between **BatchID** and **Vial** are in the same section. Finally, you drag the element to the end of the table.

Figure 43 Adding the **Barcode** column to the end of the Sequence Table

Task 6. Add a mapped column to a Quantitative Analysis table (continued)

Step	Detailed instructions	Comments
4 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Move to the **\MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuseDemo** folder. **d** Select **report.results.xml.** **e** Click **Open**. **f** Click **OK**. **g** Find the Sequence Table. **h** Scroll to the end of the Sequence Table. The **Barcode** column is now the last column in the Sequence Table.	• The Process Report command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon.

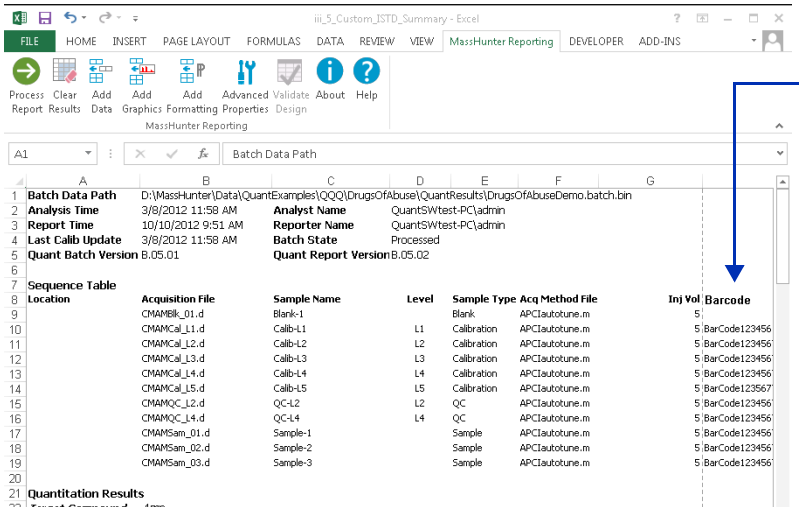


Figure 44 Verifying the Barcode column is added to the end of the Sequence Table

5 Save the changes to the template **iii_6_Custom_ISTD_Summary.** • You have to clear the results first.	**a** Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon. **b** Click **File > Save As**. **c** In the Save As dialog box, type `iii_6_Custom_ISTD_Summary`. **d** Verify the folder selected in **Save in** is correct. **e** Click **Save**.	• The **Save as type** is **Excel Template**.

You can insert a mapped column into the middle of a table. First, you add an empty column to the table. Then, you drag the mapped column to that location. Then, you have to manually change the column header.

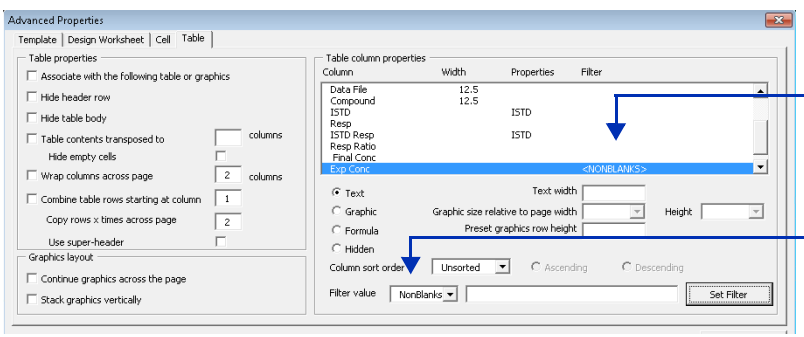
It is simpler to drag the new element to the end of the table.

Task 7. Add a filter to a table

You can add a filter to a column in a table in two different ways. If you use the Advanced Properties dialog box to add a filter, you can add a simple filter, and you can still easily move and delete a column. However, if you use Excel features to add a filter to a table, the filter can be more complex, but then you have to remove the filter before you can move or delete a column.

Task 7. Add a filter to a table in a Quantitative Analysis template

Step	Detailed instructions	Comments
1 Open the Quantitative Analysis template **\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Results_NoGraphics\iii_6_Custom_ISTD_Summary.**	• Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, **iii_6_Custom_ISTD_Summary**, where "**iii**" are your initials.	• If you did not do the previous task, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Add a filter to the Quantitation Results table using the Advanced Properties dialog box. • Only include data files that have an expected concentration.	**a** Find the second table in the section Quantitation Results. **b** Click the column labeled **Exp Conc** This column is column M in the table. **c** Click **Advanced Properties**. **d** From the **Table** tab, select **NonBlanks** in the **Filter** value box when the **Exp Conc** column is selected. **e** Click **Set Filter**. **f** Click **Close**.	• The **Advanced Properties** icon is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon.



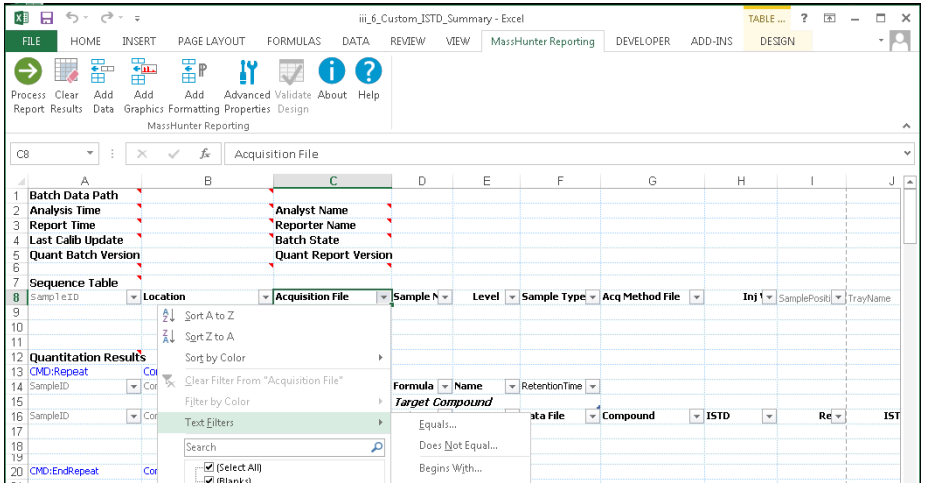
The filter is shown in the Filter column in the Table column Properties list.

Select **NonBlanks** as the **Filter Value** and then click **Set Filter.**

Figure 45 Add a filter to the Sequence Table using the Advanced Properties dialog box

Task 7. Add a filter to a table in a Quantitative Analysis template (continued)

Step	Detailed instructions	Comments
3 Add a filter to a table using Excel. • Add a text filter to the column **Acquisition File** in the Sequence Table. • Only include an Acquisition File if the file name contains **Blk** or **Cal**.	**a** Find the table labeled **Sequence Table**. **b** Click the arrow in the cell labeled **Acquisition File**. This column is column C in the table. **c** Open the list, and click **Text Filters > Contains**. The Custom AutoFilter dialog box is opened.	• A filter allows you to only include a row in the table if it passes the filter.



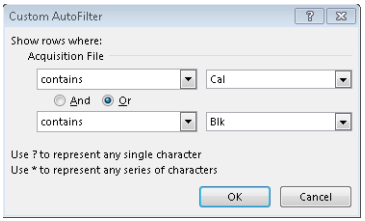
Click the arrow in the Acquisition File column and click **Text Filters > Contains.**

Figure 46 Add a filter to the Sequence Table using Excel features

d Type `Cal` in the first text field.
e Click **Or**.
f Select **contains** in the second box.
g Type `Blk` in the second text field.
h Click **OK**.

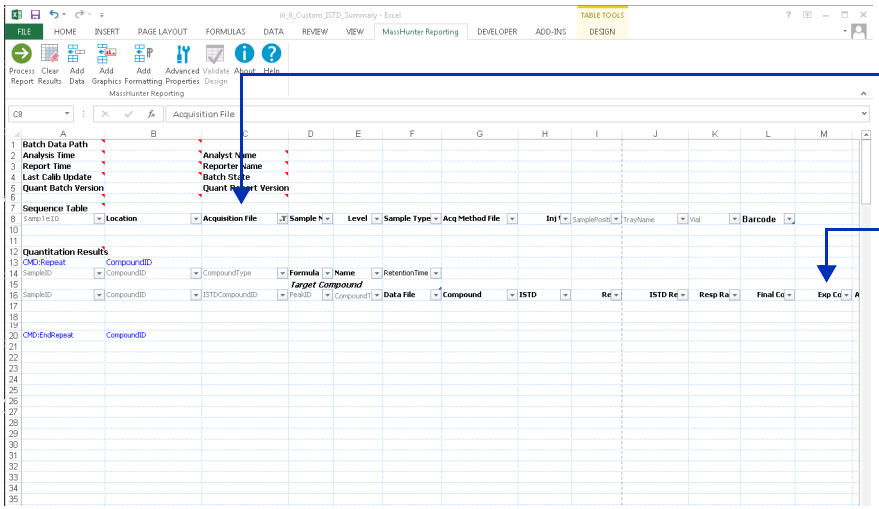
Task 7. Add a filter to a table in a Quantitative Analysis template (continued)

Step	Detailed instructions	Comments



In this example, only file names that include the letters **Cal** or **Blk** are included.

Figure 47 Setting the text filter for the **Acquisition File** column in the Sequence Table



The icon in the **Acquisition File** column is changed to show that an Excel filter is applied.

The icon in the **Exp Conc** column is not changed when a filter is added using the **Advanced Properties** dialog box.

Figure 48 A filter is added to the **Acquisition File** column

Task 7. Add a filter to a table in a Quantitative Analysis template (continued)

Step	Detailed instructions	Comments
4 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Move to the **\MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuseDemo** folder. **d** Select **report.results.xml.** **e** Click **Open**. **f** Click **OK**. **g** Find the **Sequence Table**. The only acquisition files that are included contain either **Cal** or **Blk**. **h** Find the **Quantitation Results** table. The only acquisition files that are included have an expected concentration that is not blank. All of the blanks and samples have been removed.	• The Process Report command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon.

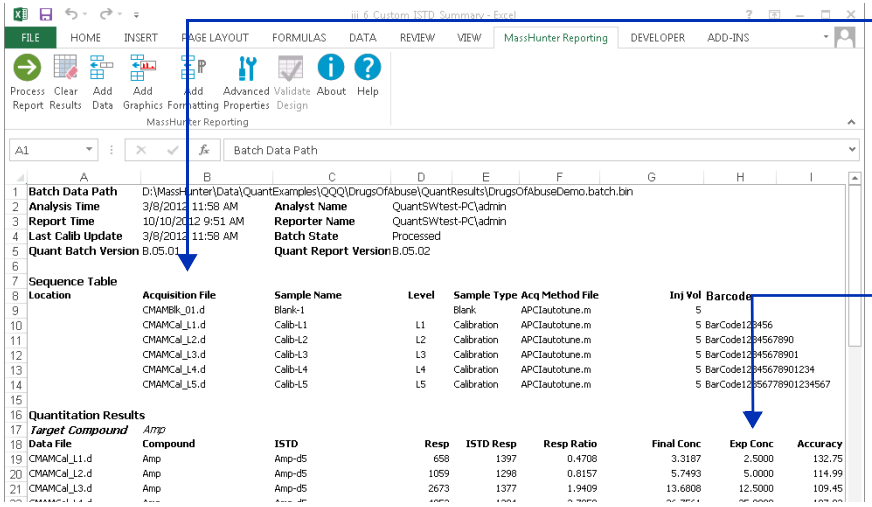


Figure 49 Verifying changes in the rows that are included in the filtered tables

Task 7. Add a filter to a table in a Quantitative Analysis template (continued)

Step	Detailed instructions	Comments
5 Save the changes to the template **iii_7_Custom_ISTD_Summary** • You have to clear the results first.	**a** Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon. **b** Click **File > Save As**. **c** In the Save As dialog box, type `iii_7_Custom_ISTD_Summary`. **d** Verify the folder selected in **Save in** is correct. **e** Click **Save**.	• The **Save as type** is **Excel Template**.

Task 8. Move or delete a column in a filtered table

You can add a filter to a column in a table in two different ways. If you use the Advanced Properties dialog box to add a filter, you can still easily move and delete a column. However, if you use Excel features to add a filter to a table, you have to remove the filter before you can move or delete a column.

Task 8. Move or delete a column in a filtered table in a Quantitative Analysis template

Step	Detailed instructions	Comments
1 Open the Quantitative Analysis template **\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Results_NoGraphics\iii_7_Custom_ISTD_Summary**.	• Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, **iii_7_Custom_ISTD_Summary**, where "**iii**" are your initials.	• If you did not do the previous task, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Delete the Inj Vol column. • Hint: you only click the column header if you want to delete the column.	**a** Find the Sequence Table. **b** Select the column labeled **Inj Vol** and the cell beneath it**.** This column is column H in the table. **c** Right-click the **Inj Vol** column and try to click **Delete > Table Columns**. You cannot because this command is grayed out. **d** Click only the cell labeled **Inj Vol**. **e** Right-click the **Inj Vol** column and click **Delete > Table Columns**. You can delete this column now.	• The Sequence Table has an Excel filter added to it.
3 Move the Barcode column. • You have to remove the filter before you can move a column.	**a** Find the **Sequence Table**. **b** Click the column labeled **Barcode** and on the cell beneath it**.** This column is column K in the table. **c** Move the cursor to the edge of the cell until the cursor changes to a four-sided arrow,  . **d** Click and drag the **Barcode** column and try to move it between two other columns. Excel displays an error message that you cannot shift cells in a filtered range or table. **e** Click **OK** in the error message.	• You cannot move a column if you have added a filter to the table using Excel. You cannot move the column between two columns. Instead, you are asked whether or not "to replace the contents of the destination cells."

Task 8. Move or delete a column in a filtered table in a Quantitative Analysis template (continued)

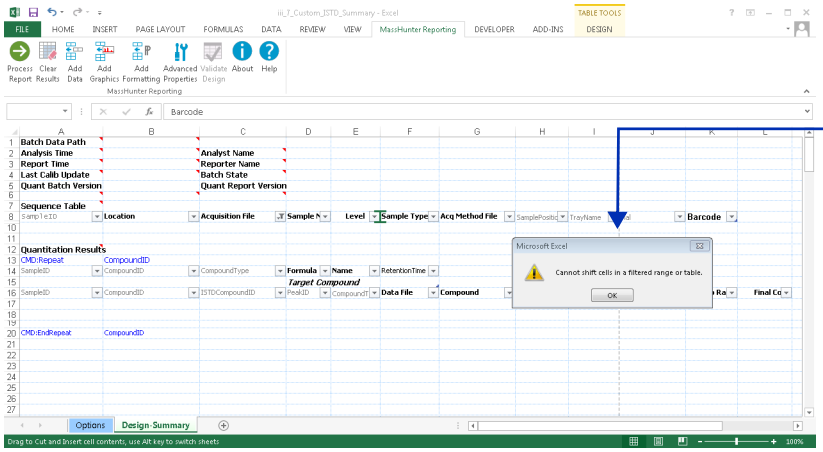
Step	Detailed instructions	Comments
		If you try to move the **Barcode** column, Excel shows you this error or a similar error.

Figure 50 A filter is added to the **Acquisition File** column

Task 8. Move or delete a column in a filtered table in a Quantitative Analysis template (continued)

Step	Detailed instructions	Comments
	f Click the column labeled **Acquisition File.** This column is column C in the table. **g** Click the **arrow** in the cell labeled **Acquisition File**. This column is the third column in the table. **h** Click **Text Filters > Custom Filter**. The Custom AutoFilter dialog box is opened. **i** Write down the filter. This filter is "contains Cal or Blk." **j** Click **Cancel**. **k** Click the **arrow** in the cell labeled **Acquisition File**. This column is the third column in the table. **l** Click **Clear Filter From "Acquisition File"**. **m** Move the **Barcode** column directly after the Acquisition File column. **n** Click the **arrow** in the cell labeled **Acquisition File**. This column is column C in the table. **o** Click **Text Filters > Contains**. The Custom AutoFilter dialog box is opened. **p** Type `Cal` in the first text field. **q** Click **Or**. **r** Select **contains** in the second box. **s** Type Blk in the second text field. **t** Click **OK**.	• Moving a column in a filtered table is a four step process: **a** Write the name of the filter. **b** Remove the filter. **c** Move the column. **d** Add the filter again.

Task 8. Move or delete a column in a filtered table in a Quantitative Analysis template (continued)

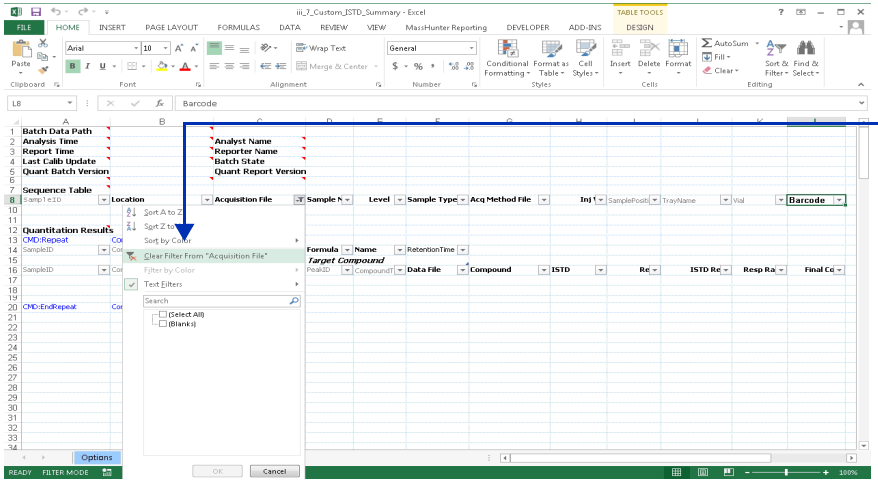
Step	Detailed instructions	Comments
		Remove the filter from the column.

Figure 51 The filter is removed from the **Acquisition File** column

- Follow the instructions in "Task 4. Move a column in a table" on page 61 to move the **Barcode** column.
- Follow the instructions in "Task 7. Add a filter to a table" on page 73 to add the filter to the Acquisition File column.

Task 8. Move or delete a column in a filtered table in a Quantitative Analysis template (continued)

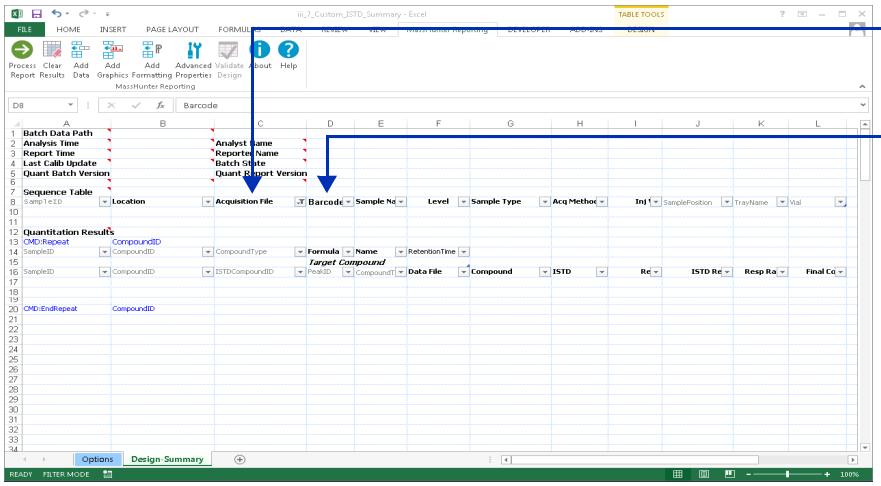
Step	Detailed instructions	Comments
		The **Acquisition File** column has the text filter again. The **Barcode** column is now after the **Acquisition File** column.
4 Delete the **Resp Ratio** column. • You can click the column header or both the column header and the cell below if you want to delete this column.	**a** Find the second table in the **Quantitation Results** section. **b** Click the column labeled **Resp Ratio** and on the cell beneath it**.** This column is column K in the table. **c** Right-click the **Resp Ratio** column and click **Delete > Table Columns**. The column is deleted.	• The second table in the Quantitation Results section has a filter added to it using the Advanced Properties dialog box.
5 Move the **Final Conc** column to directly after the **Exp Conc** column. • You do not have to remove the filter before you move this column.	**a** Find the second table in the Quantitation Results section. **b** Click the column labeled **Final Conc**. This column is column L in the table. **c** Move the cursor to the edge of the cell until the cursor changes to a four-sided arrow,  . **d** Click and drag the **Final Conc** column and move it after the **Exp Conc** column.	• Follow the instructions in "Task 4. Move a column in a table" on page 61 to move the **Final Conc** column.

Figure 52 The Barcode column is moved and the filter has been added again

Task 8. Move or delete a column in a filtered table in a Quantitative Analysis template (continued)

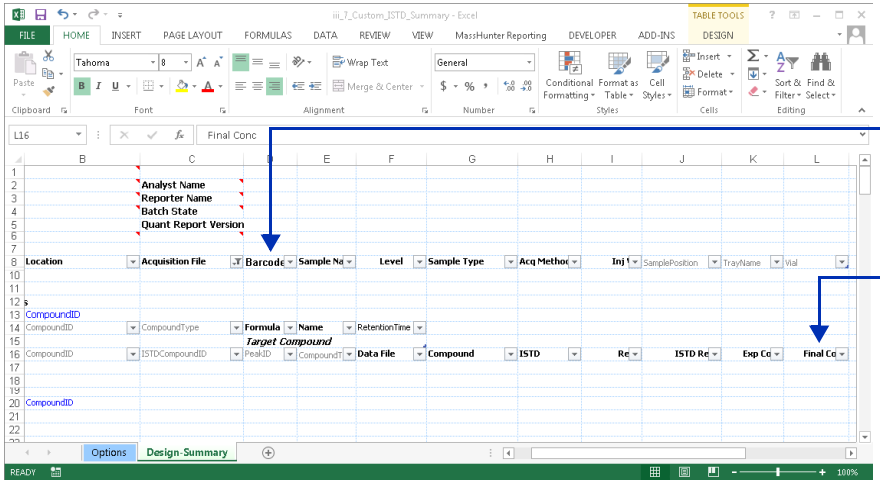
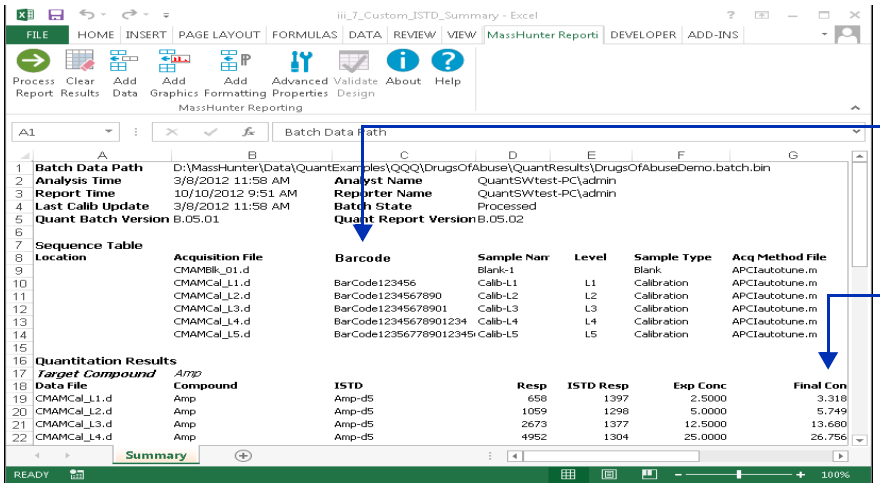
Step	Detailed instructions	Comments
		

Figure 53 The **Barcode** column and the **Final Conc** column are moved

6 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Move to the **\MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuseDemo** folder. **d** Select **report.results.xml**. **e** Click **Open**. **f** Click **OK**. **g** Find the Sequence Table. The only acquisition files that are included contain either **Cal** or **Blk**. **h** Find the Quantitation Results table. The only acquisition files that are included have an expected concentration that is not blank. All of the blanks and samples have been removed.	• The Process Report command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon.

Task 8. Move or delete a column in a filtered table in a Quantitative Analysis template (continued)

Step	Detailed instructions	Comments



The **Barcode** column is moved to after the **Acquisition File.**

The **Final Conc** column is moved to after the **Exp Conc** column.

Figure 54 Verifying that columns are moved in both filtered tables

7 Save the changes to the template **iii_8_Custom_ISTD_Summary**.

- You have to clear the results first.

a Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon.
b Click **File > Save As**.
c In the Save As dialog box, type `iii_8_Custom_ISTD_Summary`.
d Verify the folder selected in **Save in** is correct.
e Click **Save**.

- The **Save as type** is **Excel Template**.

Exercise 4
Additional ways to customize a table

In these tasks, you learn additional ways to customize a table.

Each exercise is presented in a table with three columns:

- **Steps** – Use these general instructions to proceed on your own to explore the program.
- **Detailed Instructions** – Use these if you need help or prefer to use a step-by-step learning process.
- **Comments** – Read these to learn tips and additional information about each step in the exercise.

Task 1. Add a table to a template

You can easily add a table to a template by using the commands in the **Add Data** menu in the **MassHunter Reporting** tab in the Ribbon. A different set of commands is available for Qualitative Analysis templates and Quantitative Analysis templates. Also, different types of Qualitative Analysis templates have different sets of commands.

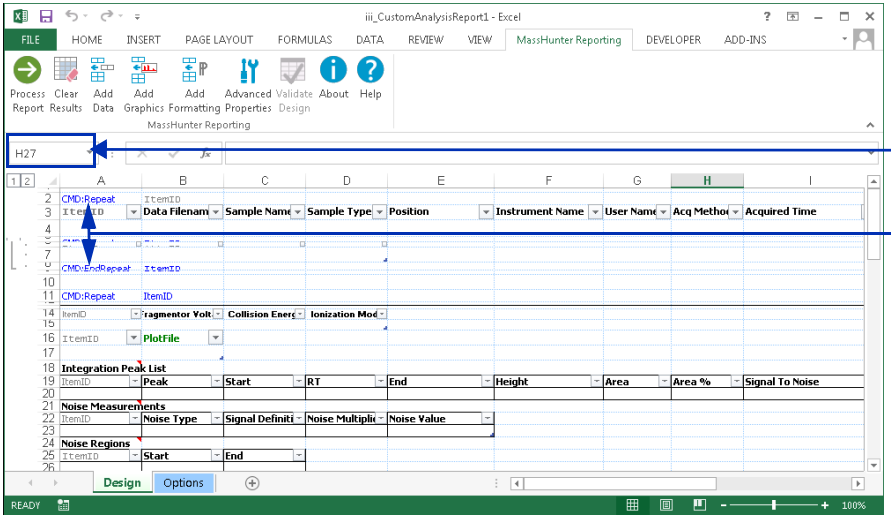
When you add a table to a template using the Add Data commands, a new XML map is added automatically. If you remove this table from the template in the future, make sure to also delete the XML map that was created. Reports print more quickly when you have fewer XML maps. You can delete unused XML maps in the using the XML maps button in the XML Maps dialog box which you get to by clicking the XML Maps button in the XML Source pane.

Task 1. Add a table to a Qualitative Analysis template

Step	Detailed instructions	Comments
1 Open the Qualitative Analysis template, **\MassHunter\Report Templates\Qual\Letter\ iii_CustomAnalysisReport**.	Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 30 to open the template, **iii_CustomAnalysisReport**, where "**iii**" are your initials.	• If you did not create this template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Add a second table to show additional Sample Information. • Add the table inside the Repeat section.	**a** Find the first table in the template. The first two items are **ItemID** and **Data Filename**. **b** Click the first cell in row 5. The rows below this row are very narrow.	• The first table is repeated for each file in the results. The Report Designer repeats all of the rows between CMD:Repeat and CMD:EndRepeat for each data file. The ItemID is different for each data file.

Task 1. Add a table to a Qualitative Analysis template (continued)

Step	Detailed instructions	Comments



The current position in the template is shown here.

All of the rows between the CMD:Repeat row and the CMD:EndRepeat row are repeated for each ItemID. ItemID identifies different data files.

Figure 55 Selecting the **first cell** in row 5

c	Click **Add Data > Sample Information** in the **MassHunter Reporting** tab in the Ribbon.	• Extra rows are automatically added to the template for the new table.

Task 1. Add a table to a Qualitative Analysis template (continued)

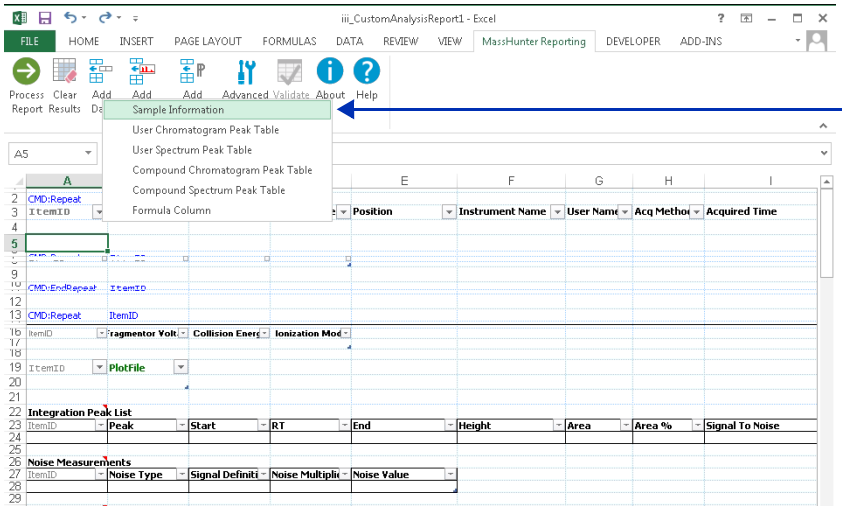
Step	Detailed instructions	Comments
		Click this command. The new table is added below row 5. The commands in the **Add Data** menu are different for the Qualitative Analysis and Quantitative Analysis Program. Different types of Qualitative Analysis templates also have different commands.

Figure 56 Add a second Sample Information table

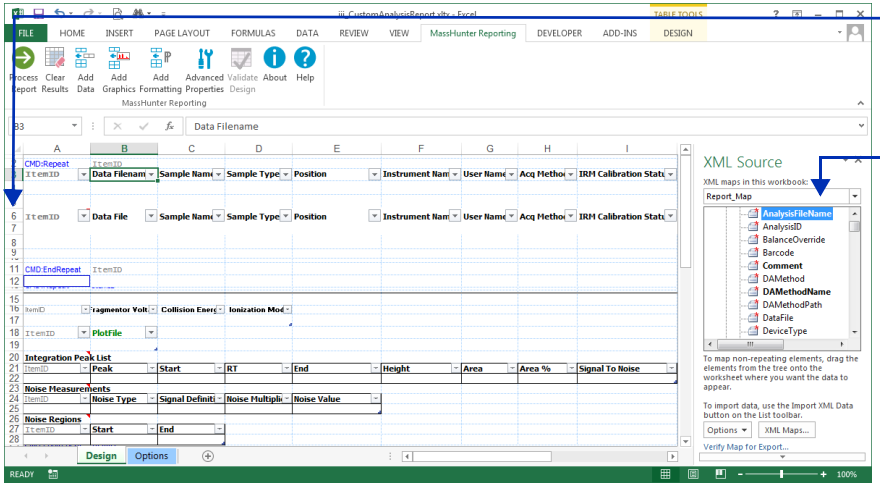
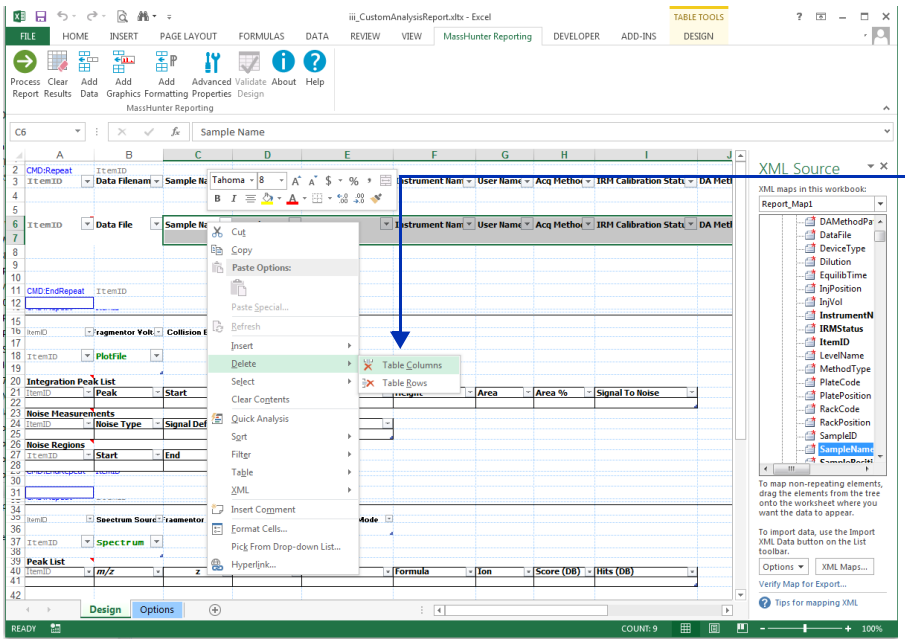
		The new table is added below row 5. The XML Source pane is opened automatically. When a table is added, a new XML map is automatically added.

Figure 57 Add a second Sample Information table

Task 1. Add a table to a Qualitative Analysis template (continued)

Step	Detailed instructions	Comments
3 Compare the columns in the two tables. • The XML Map changes depending on which table you are looking at. • The names of some of the columns are different.	**a** Click the **Data Filename** column in the first table. The XML map is Report_Map. **b** Click the **Data File** column in the second table. The XML map is Report_Map1.	• You can only map an item from an XML map one time. If you want to map an item a second time, you need to add a second map. This second map is added automatically when the new table is added.



Select the columns that you want to delete. Right-click and click **Delete** > **Table Columns**. All of the columns that are selected are removed.

Figure 58 Delete multiple columns in the second Sample Information table

Task 1. Add a table to a Qualitative Analysis template (continued)

Step	Detailed instructions	Comments
4 Change the second table to include only the following columns: • ItemID • Data File • Injector Volume • Dilution	**a** Click the **Sample Name** column in the second table. The XML map is Report_Map1. **b** Delete all of the columns in the table that are after the **Data File** column. **c** Click the **Data File** column in the second table. **d** Add the mapped columns, **Inj Vol and Dilution**. **e** Rename the **Inj Vol** column to **Injector Volume**.	• You can delete more than one table column at the same time. • Follow the instructions in "Task 2. Delete a column from a table" on page 54 to remove the columns. • You click one of the items in the table first to make sure that the correct XML map is selected. All of the columns in a table are mapped using the same XML map. The **Report_Map1** map is selected. • Follow the instructions in "Task 6. Add a mapped column to a table" on page 68 to add the columns. • Follow the instructions in "Task 1. Rename a column header in a table" on page 51 to rename the columns.

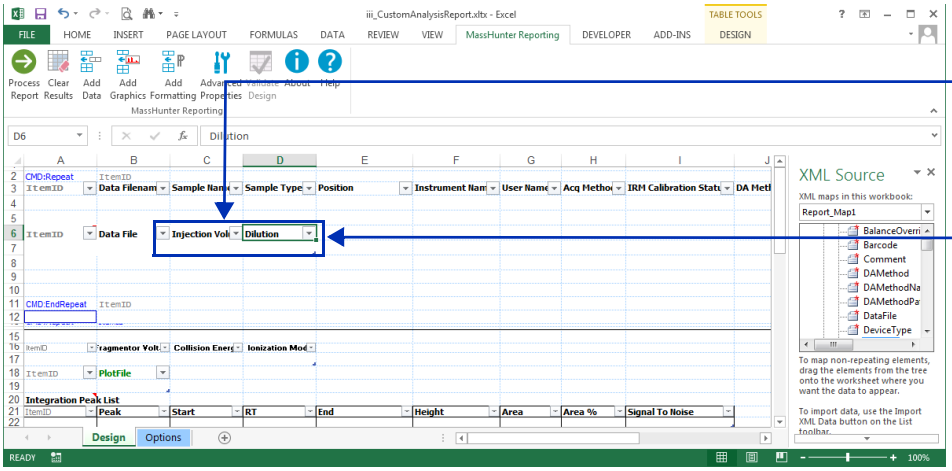
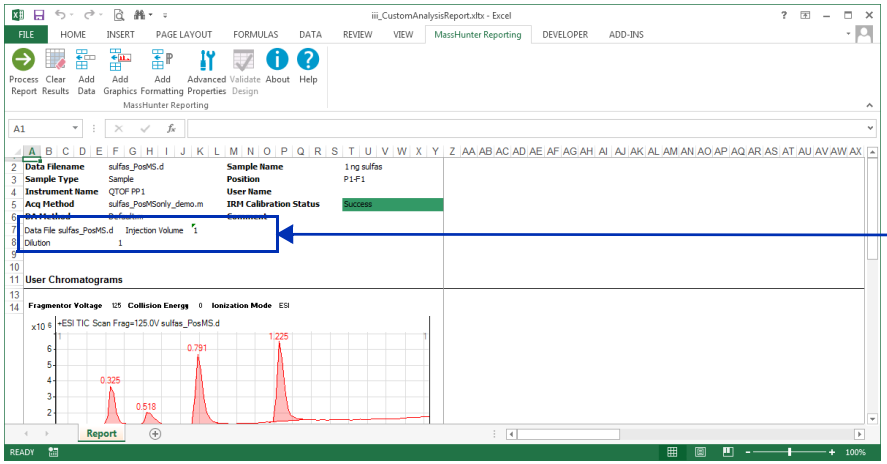


Figure 59 The **Injector Volume** and **Dilution** columns are added to the second table

Task 1. Add a table to a Qualitative Analysis template (continued)

Step	Detailed instructions	Comments
5 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Move to the **\MassHunter \Reports\Temp** folder. **d** Double-click one of the folders that contains analysis results. **e** Select **Report.xml**. **f** Click **Open**. **g** Click **OK**. **h** Find the Injector Volume and the Dilution columns.	• The **Process Report** command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon.



The first table is transposed and shows the information next to the column header.

The second Sample Information table shows the **Injector Volume** and the **Dilution**.

Figure 60 Verifying a new Sample Information table is added to the template

6 Save the changes to the template. • You have to clear the results first. • You save the template to the new name, **iii_1_Custom AnalysisReport**.	**a** Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon. **b** Click the **Microsoft Office button** and then click **Save As** and click **Other Formats**. **c** In the Save As dialog box, type `iii_1_CustomAnalysisReport`. **d** Verify the folder selected in **Save in** is correct. **e** Click **Save**.	• The **Save as type** is **Excel Template**.

4 Additional ways to customize a table

Task 1. Add a table to a template

Task 2. Format a table (Transposing and Hiding headers)

You can easily format a table using the commands in the Advanced Properties dialog box in the **MassHunter Reporting** tab in the Ribbon.

When a table is first added to a template, it is not transposed. The column headers appear in one row and the values appear directly below the column headers. If a table is transposed, then the "column headers" appear next to the values instead. Each column in the table is either printed in its own row or in a series of columns across the page. A few tables (for example, the Sample Information table in the Qualitative Analysis program) are transposed by default.

Another way to format a table is to hide the column headers. If you add a repeating section, you can turn on this feature to avoid repeating the column headers throughout the report.

Task 2. Format a table in a Qualitative Analysis template

Step	Detailed instructions	Comments
1 Open the Qualitative Analysis template, **\MassHunter\Report Templates\Qual\Letter\ iii_1_CustomAnalysisReport**.	Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 30 to open the template, ***iii*_1_CustomAnalysisReport,** where "**iii**" are your initials.	• If you did not create this template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Format the second table. • Do not transpose the second sample information table. • Set the width of each column to 15.	**a** Click a column in the second table. **b** Click **Advanced Properties** which is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon. **c** Clear the **Table contents transposed to** check box. **d** Select each Column under Table column properties. **e** Type `15` in the **Text width** field.	• By default, when you add a Sample Information table, the Table contents transposed to check box is marked. This check box is on the **Table** tab of the Advanced Properties dialog box. • Normally, a table is shown with the column headers in one row and the information in the table below each of these column headers. If a table is transposed, then the column header is printed next to the information. You can specify how many columns to use to show the information.

Task 2. Format a table in a Qualitative Analysis template (continued)

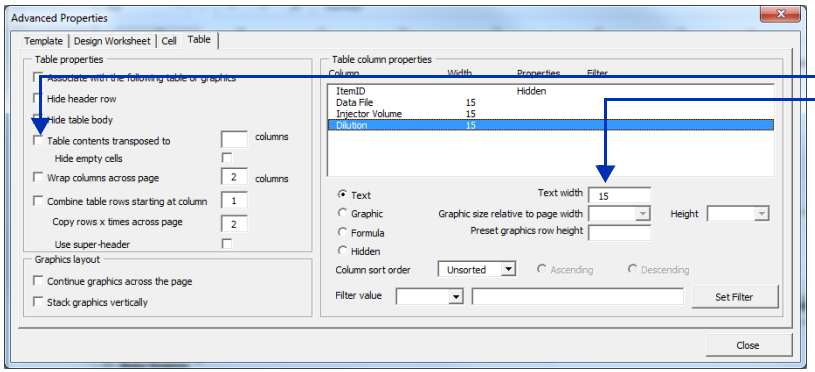
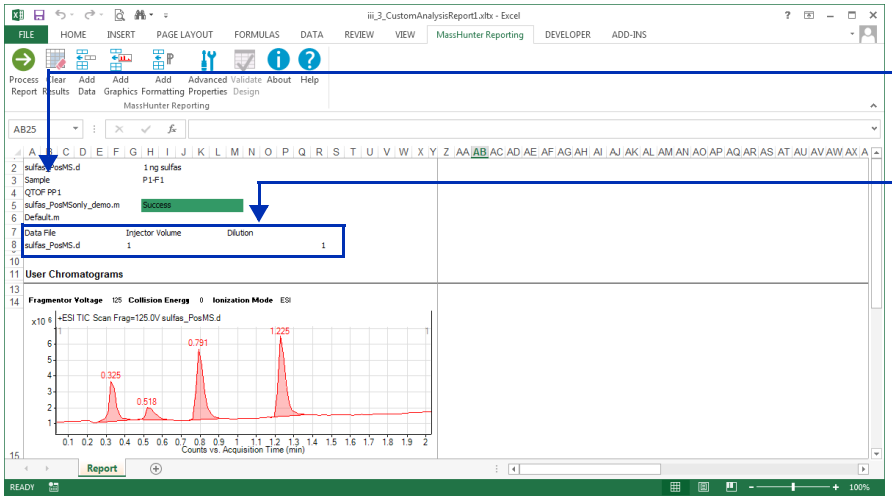
Step	Detailed instructions	Comments
		The **Table contents transposed to** check box is cleared. The width of each column in the table is set to 15 using the **Text width** field.

Figure 61 Changing table properties in the Advanced Properties dialog box

3 Format the first table. • Hide the header row.	**a** Click a column in the first table. **b** Click the Advanced Properties dialog box. **c** Mark the **Hide header row** check box under Table properties. **d** Click **Close**.	• You do not need to close the Advanced Properties dialog box to switch to a different table.
4 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Move to the **\MassHunter \Reports\Temp** folder. **d** Double-click one of the folders that contains analysis results. **e** Select **Report.xml.** **f** Click **Open**. **g** Click **OK**.	• The **Process Report** command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon.

Task 2. Format a table in a Qualitative Analysis template (continued)

Step	Detailed instructions	Comments



The first table is transposed and the header row is hidden.

The second Sample Information table is not transposed. The column header is above the information.

Figure 62 Verifying a new Sample Information table is added to the template

5 Save the changes to the template, **iii_2_CustomAnalysisReport**.

- You have to clear the results first.

a Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon.

b Click the **Microsoft Office button** and then click **Save As** and click **Other Formats**.

c In the Save As dialog box, type `iii_2_CustomAnalysisReport`, where "`iii`" are your initials.

d Verify the folder selected in **Save in** is correct.

e Click **Save**.

- The **Save as type** is **Excel Template**.

Task 3. Add a formula column to a table

In this task, you add a formula column to a table. In the Add Data menu, you click the Add Formula command to add a column to the table that contains a formula. An Excel comment is added to the cell to let the Report Designer add-in know that the column contains a formula.

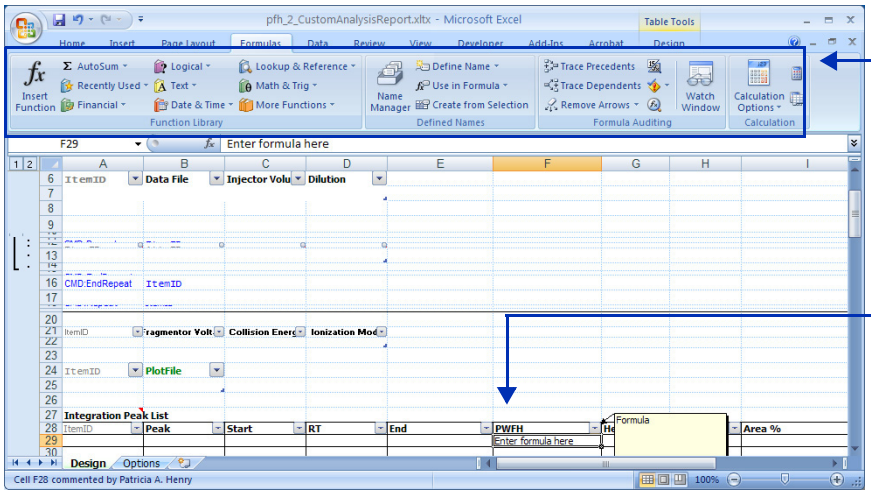
In this exercise, you will add a simple formula to a column in a table. To learn more about formulas, please refer to the online Help for Microsoft Excel. Also, many books have been written about creating formulas in Microsoft Excel.

Task 3. Add a formula column to a Qualitative Analysis table

Step	Detailed instructions	Comments
1 Open the Qualitative Analysis template **\MassHunter\Report Templates\Qual\Letter\ iii_2_CustomAnalysisReport**, where *iii* are your initials.	Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 30 to open the template, **iii_2_CustomAnalysisReport**, where "**iii**" are your initials.	• If you did not do the previous task, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Add a formula column. • Add it to the right of the column **End** in the Integration Peak List Table. • Label the column **PWFH**. • Change the formula to show the difference of the start of the peak and the end of the peak.	**a** Find the table labeled **Integration Peak List**. **b** Click the cell containing the words **End**. This column is the fifth column in the table. **c** Click **Add Data > Formula Column** in the **MassHunter Reporting** tab in the Ribbon. **d** Follow the instructions in "Task 1. Rename a column header in a table" on page 51 to rename the column to **PWFH**. **e** Click the **Formulas** tab in the Ribbon. **f** Hide the **XML Source** pane, if it is visible.	• The **Add Data > Formula Column** command adds the column to the right of the column selected. • **PWFH** is an abbreviation for Peak Width Full Height. • You can manually enter formulas if you know the syntax, without using the Excel Function Arguments dialog box.

Task 3. Add a formula column to a Qualitative Analysis table (continued)

Step	Detailed instructions	Comments



This tab in the Ribbon helps you add a formula to the table. For information about formulas and functions, see the online Help for Microsoft Excel.

The new column **PWFH** is to the right of the End column. The Excel comment, **Formula** is added to this column.

Figure 63 Add a formula column to the right of the **End** column

g Click the **Insert Function** button in the Function Library group in the **Formulas** Tab in the Ribbon

h In the **select a category** list, select **Math & Trig**.

i In the **Select a function** list, select **SUM**.

j Click **OK**.

k Click the **Number1** box in the Function Arguments dialog box.

l Click the cell in the **End** column that is next to the formula cell. This cell contains the actual results.

m Click the **Number2** box.

n Type – in this box.

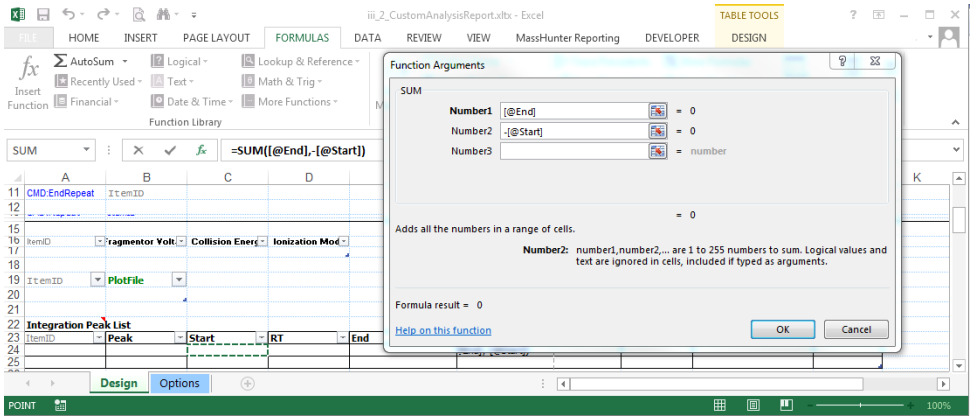
o Click the cell in the **Start** column that is in the same row as this formula. The reference to this cell is added after the "-".

p Click **OK**.

- By placing a "-" in the Number2 box, you are actually subtracting the second number.
- Excel allows you to create many different formula. This is only one simple formula that you can enter.
- To show the formulas in a template, click the **Formulas** tab. Under Formula Auditing, click the **Show Formula** button. You have to turn this feature off before trying to process the report.

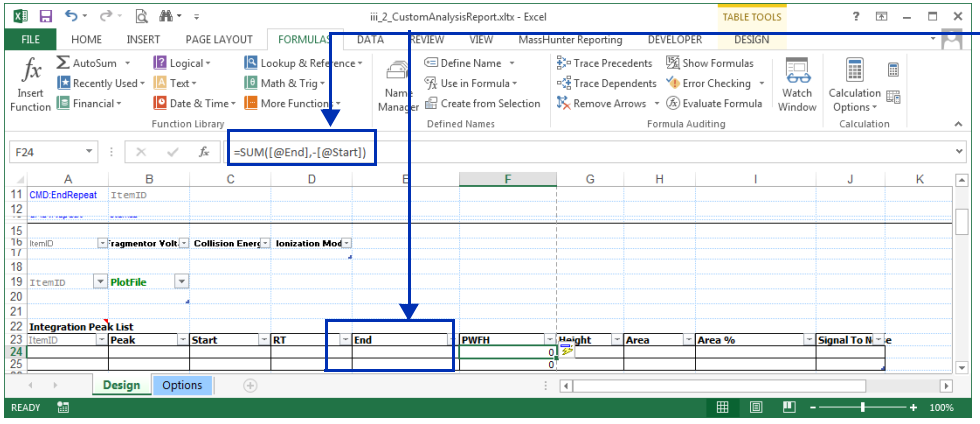
Task 3. Add a formula column to a Qualitative Analysis table (continued)

Step	Detailed instructions	Comments



By clicking in the template, you select the cells to add. Excel automatically adds the correct syntax to refer to this cell.

Figure 64 Using the Insert Function tool to add a formula to the RT Window column

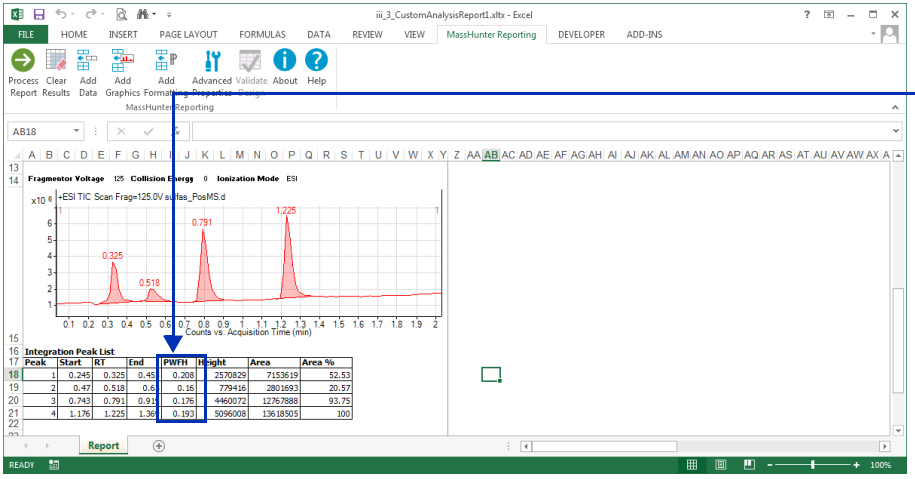


A formula starts with the equal sign. This formula is a sum of the two items listed. The blue part of the formula refers to the value in the **End** column. It is color-coded to match the outline of the cell in the **Integration Peak**

Figure 65 The formula has been added to the Integration Peak List table

Task 3. Add a formula column to a Qualitative Analysis table (continued)

Step	Detailed instructions	Comments
3 Test the changes to the template.	**a** Click the **MassHunter Reporting** tab in the Ribbon. **b** Click **Process Report**. **c** Click the **Browse** button. **d** Move to the **\MassHunter \Reports\Temp** folder. **e** Double-click one of the folders that contains analysis results. **f** Select **Report.xml**. **g** Click **Open**. **h** Click **OK**. **i** Find the Integration Peak List table. The **PWFH** column contains the difference between the **End** and the **Start** of the peak.	• The Process Report command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon.



The new column **PWFH** is included in the table after the **End** column. Each cell in this row contains the value of End - Start.

For example, in the first row, 0.453 - 0.245 = 0.208.

Figure 66 Verifying the formula column in the Integration Peak List table

Task 3. Add a formula column to a Qualitative Analysis table (continued)

Step	Detailed instructions	Comments
4 Save the changes to the template, **iii_3_CustomAnalysisReport**, where **iii** are your initials.	**a** Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon. **b** Click the **Microsoft Office button** and then click **Save As** and click **Other Formats**. **c** In the Save As dialog box, type *iii*_3_CustomAnalysisReport, where *iii* are your initials. **d** Verify the folder selected in **Save in** is correct. **e** Click **Save**.	• The **Save as type** is **Excel Template**.

Task 4. Add an ISTD column to a Quantitative Analysis template

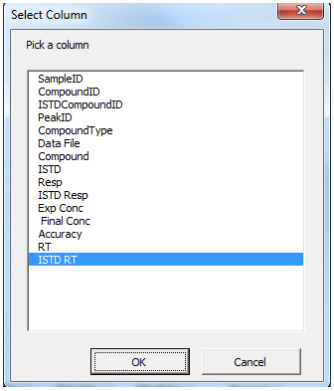
In the Quantitative Analysis program, a compound can be an internal standard (ISTD). You can include information about the internal standard in the same row in table as the related compound by adding an ISTD column.

Task 4. Add an ISTD mapped column to a Quantitative Analysis table

Step	Detailed instructions	Comments
1 Open the Quantitative Analysis template, **\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Results_NoGraphics\Parts\iii_8_Custom_ISTD_Summary** template.	Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, **iii_8_Custom_ISTD_Summary**, where "**iii**" are your initials.	• If you do not have this template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Add two columns to the Target Compound table. • Add the Retention Time column and change the name to **RT**. • Add the ISTD Retention Time column and change the name to **ISTD RT**.	**a** Follow the instructions in "Task 6. Add a mapped column to a table" on page 68 to add the Retention Time column to the end of the table. **b** Follow the instructions in "Task 1. Rename a column header in a table" on page 51 to change the name of the column to **RT**. **c** Right-click the **RT** column header and click the **B** button to make the header match the font in the other headers. **d** Right-click the **RT** column header and click the **Format Cells** command. **e** Click the **Alignment** tab. **f** Select **Right (Indent)** in the Horizontal list. Click **OK**. **g** Click the **RT** column header. **h** Click the **Add Data > ISTD Column** command. **i** Select **RT** from the Select Column dialog box. **j** Click **OK**. **k** If necessary, right-click the **ISTD RT** column header and click the **B** button to make the header match the font in the other headers.	• An ISTD column is added to the right of the selected column. • You can only add an ISTD column if the corresponding column for the compound is part of the table. That is why you added the Retention Time column first, and then you added the ISTD column. • (optional) You right-click the value for the RT and the ISTD RT and click the Format Cells command to select the number category and to select the number of decimal places. • (optional) You can set the width of the RT and ISTD RT column.

Task 4. Add an ISTD mapped column to a Quantitative Analysis table (continued)

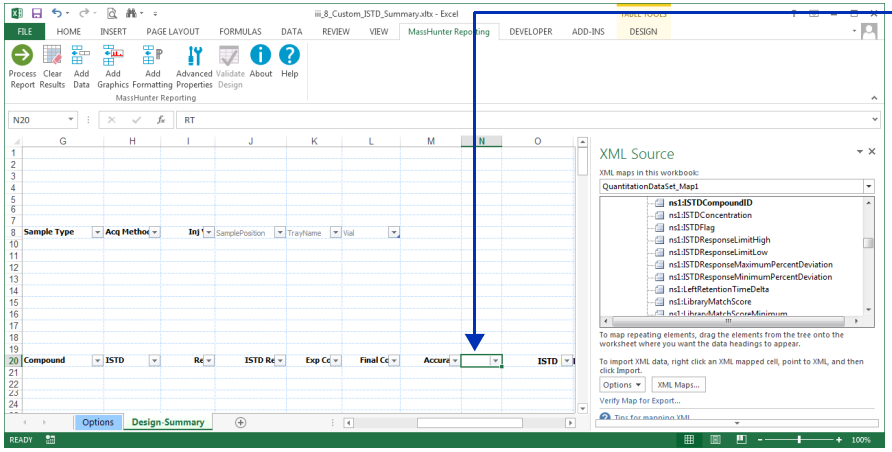
Step	Detailed instructions	Comments



Some columns in this list start with the word **ISTD**. These columns are already internal standard columns. Do not select any of these columns.

The column **ISTDCompoundID** has to be part of the table to add an ISTD column. This column is automatically added when you add an ISTD column if it is not already included. The **ISTDCompoundID** column is a hidden column.

Figure 67 Select the RT column

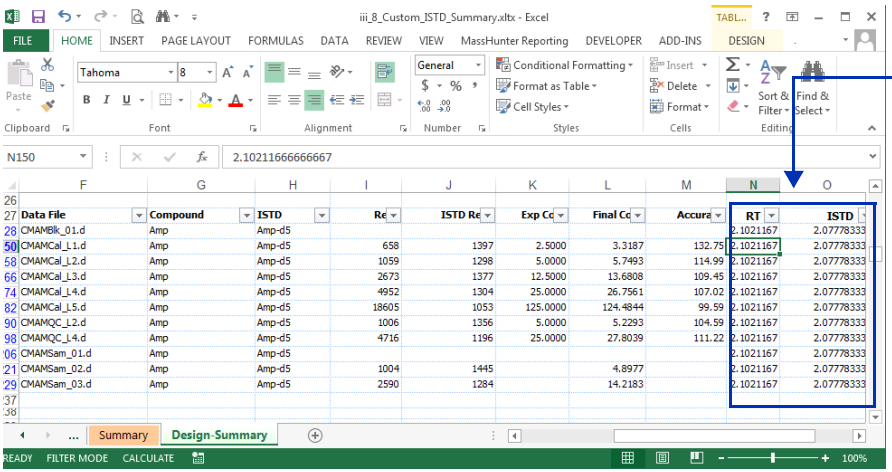


In the **Target Compound** table, you cannot see the **RT** column header because it is hidden behind the arrow. If you click this column, you can see the Column header in the Formula Bar.

Figure 68 The RT column and the ISTD RT column are part of the table

Task 4. Add an ISTD mapped column to a Quantitative Analysis table (continued)

Step	Detailed instructions	Comments
3 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Move to the **\MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuseDemo** folder. **d** Select **report.results.xml**. **e** Click **Open**. **f** Click **OK**. **g** Find the Target Compound Table. **h** Scroll to the end of the Sequence Table. The **Barcode** column is now the last column in the Sequence Table.	• The Process Report command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon.



The last two columns in the **Target Compound Table** are the **RT** and **ISTD RT** columns.

The **RT** column is the retention time of that compound. The **ISTD RT** column is the retention time for the internal standard for that compound.

Figure 69 Verifying the RT and ISTD RT columns are added to the end of the table

4 Save the changes to the template, **iii_9_Custom_ISTD_Summary**. • You have to clear the results first.	**a** Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon. **b** Click **File > Save As**. **c** In the Save As dialog box, type `iii_9_Custom_ISTD_Summary`. **d** Verify the folder selected in **Save in** is correct. **e** Click **Save**.	• The **Save as type** is **Excel Template**.

Task 5. Add a column that is already mapped

If an element in the XML Source is already being used in the template, it is shown in Bold letters in the XML Source. If you want to include the element again in a different part of the template, you need to add an additional map to the template.

When you add a table to a template using the Add Data commands, a new map is added automatically. You can add a new map file manually and then manually add the information from this map to the template. You cannot use more than one map in a table, so you cannot add items from this map to an existing table.

Usually, you will not need to do this task.

Task 5. Add a column that is already mapped to a Qualitative Analysis template

Step	Detailed instructions	Comments
1 Open the Qualitative Analysis template **\MassHunter\Report Templates\Qual\Letter\ iii_3_CustomAnalysisReport**, where **iii** are your initials.	Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 30 to open the template, **iii_3_CustomAnalysisReport**, where "**iii**" are your initials.	• If you did not create this template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Add the item **AnalysisFileName** to the first column in row 10.	**a** Find the second table in the template. The items in this table are **ItemID**, **Data File**, **Injector Volume** and **Dilution**. **b** In the table, click **Data File**. **c** Right-click and click **XML > XML Source**. **d** Click the **Dilution** column. **e** Try to add the **AnalysisFileName** item to the end of the table. An error message is displayed.	• In the XML Source window, both of these items are shown in bold which means that this item is already being used. • See "Task 6. Add a mapped column to a table" on page 68 for instructions on adding a mapped column to a table.

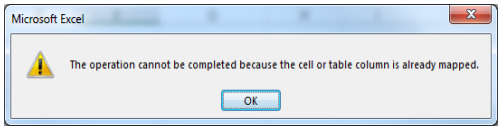
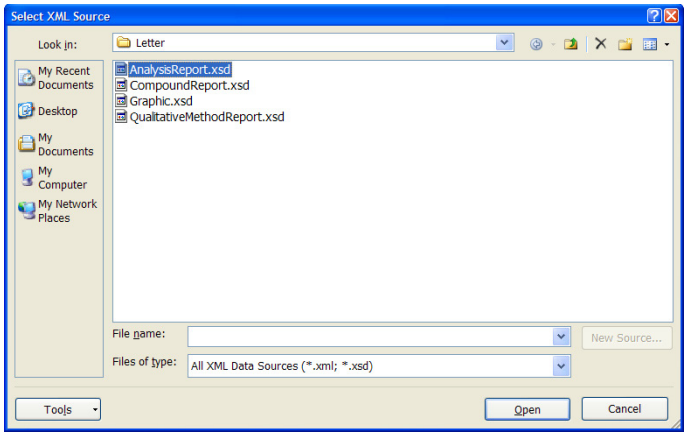


Figure 70 Error shown if you try to map a column two times

Task 5. Add a column that is already mapped to a Qualitative Analysis template (continued)

Step	Detailed instructions	Comments
	f Click **XML Maps** in the XML Source pane. The XML Maps dialog box is opened. **g** Click **Add** in the XML Maps dialog box. **h** Move to the **Report Templates/Qual/Letter** folder. **i** Select **AnalysisReport.xsd** for this template. **j** Click **Open**. **k** Click **OK**.	• Two maps are already available in the XML Maps dialog box. • The map files are in the same folder as the templates. The Qualitative Analysis program has a different map file for each type of template.



AnalysisReport.xsd - Analysis report

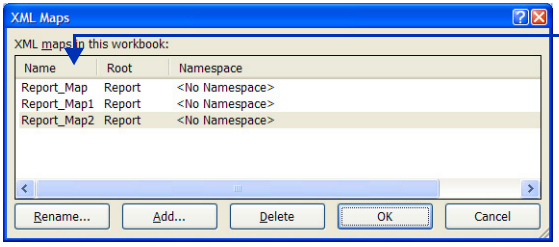
CompoundReport.xsd - Compound report

Graphic.xsd - Graphic report

QualitativeMethodReport.xsd - Qualitative Analysis Method Report

For a Quantitative Analysis template, the XML Source file is **batch.results.xsd**.

Figure 71 Add another map file



Report_Map - original map file

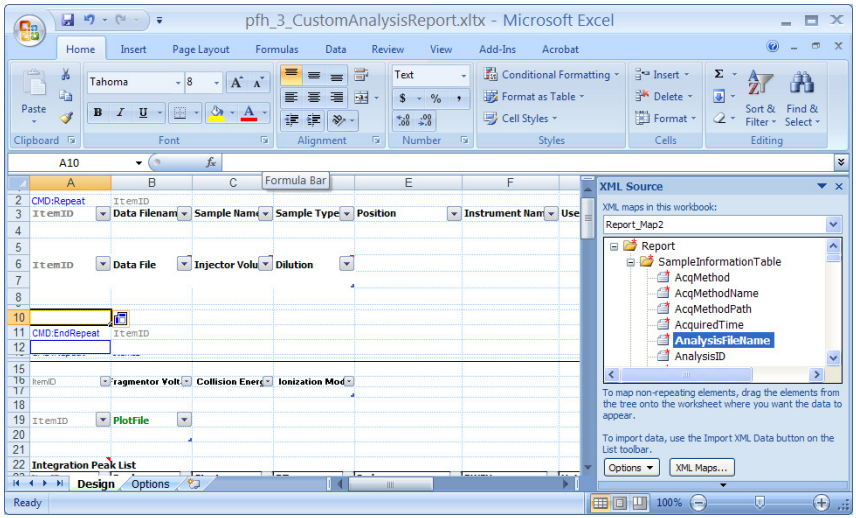
Report_Map1 - automatically added in Task 1 when the table was added

Report_Map2 - added manually in this task

Figure 72 Three XML maps are available in this template

Task 5. Add a column that is already mapped to a Qualitative Analysis template (continued)

Step	Detailed instructions	Comments
	l Select **Report_Map2** in the XML Source pane. **m** Add the mapped column, **AnalysisFileName** in the first column of row 10.	



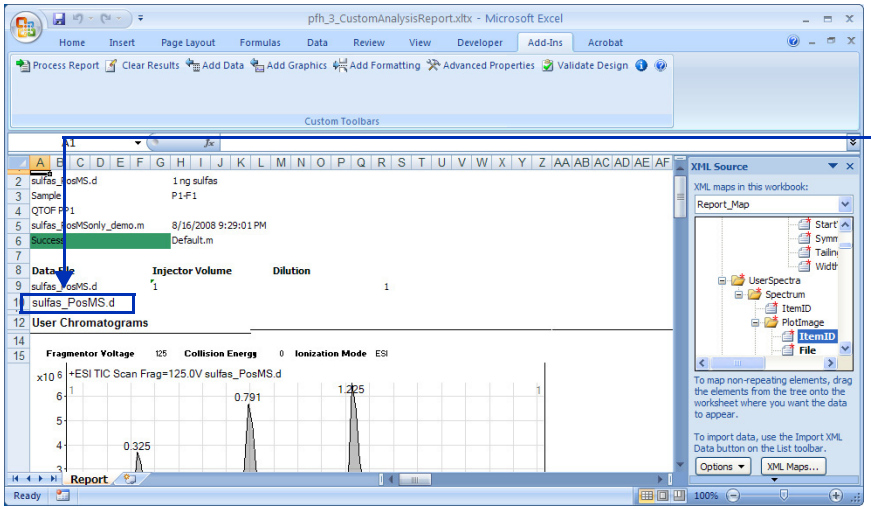
The **AnalysisFileName** is added to the first column in row 10. Because this cell is not part of a table, the column header is not automatically added above the value.

Figure 73 Add the AnalysisFileName item

3 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Move to the ***\MassHunter\Reports\Temp*** folder. **d** Double-click one of the folders that contains analysis results. **e** Select ***Report.xml***. **f** Click **Open**. **g** Click **OK**. **h** Find the first column in row 10. Verify that the **AnalysisFileName** is included	• The **Process Report** command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon.

Task 5. Add a column that is already mapped to a Qualitative Analysis template (continued)

Step	Detailed instructions	Comments



The AnalysisFileName is added after the second Sample Information table.

Figure 74 Verifying that the AnalysisFileName is repeated

4 Save the changes to the template.
- You have to clear the results first.
- You save the template to the new name, **iii_4_Custom AnalysisReport**, where **iii** are your initials.

a Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon.
b Click the **Microsoft Office button** and then click **Save As** and click **Other Formats**.
c In the Save As dialog box, type *iii*_4_CustomAnalysisReport.
d Verify the folder selected in **Save in** is correct.
e Click **Save**.
- The **Save as type** is **Excel Template**.

Exercise 5
Graphics

In this exercise, you learn how to add graphics to a Quantitative Analysis template. In Task 2, you also learn how to print those graphics more compactly.

Each exercise is presented in a table with three columns:

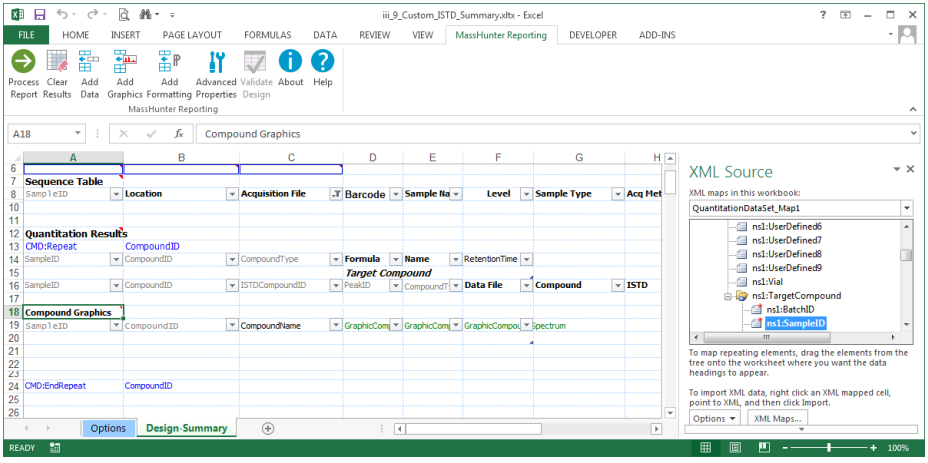
- **Steps** – Use these general instructions to proceed on your own to explore the program.
- **Detailed Instructions** – Use these if you need help or prefer to use a step-by-step learning process.
- **Comments** – Read these to learn tips and additional information about each step in the exercise.

Task 1. Adding graphics to a template

You can easily add graphics to a template using the commands in the Add Graphics menu. The Report Designer add-in has a different set of commands available in this menu for the Quantitative Analysis program and for each type of template in the Qualitative Analysis program.

Task 1. Add graphics to a Quantitative Analysis template

Step	Detailed instructions	Comments
1 Open the Quantitative Analysis template, **\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Results_NoGraphics\Parts\iii_9_Custom_ISTD_Summary template.**	Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, **iii_9_Custom_ISTD_Summary**, where "**iii**" are your initials.	• If you do not have this template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Add target compound graphics. • Add them in the Quantitation Results repeating section.	**a** Click in the first column in the last rows before the CMD:EndRepeat CompoundID row. **b** Click **Add Graphics > Compound Graphics**.	• Refer to "Task 3. Add a single repeating section" on page 125 for an explanation of repeating sections. • Three different graphics are added in the Compound Graphics table.



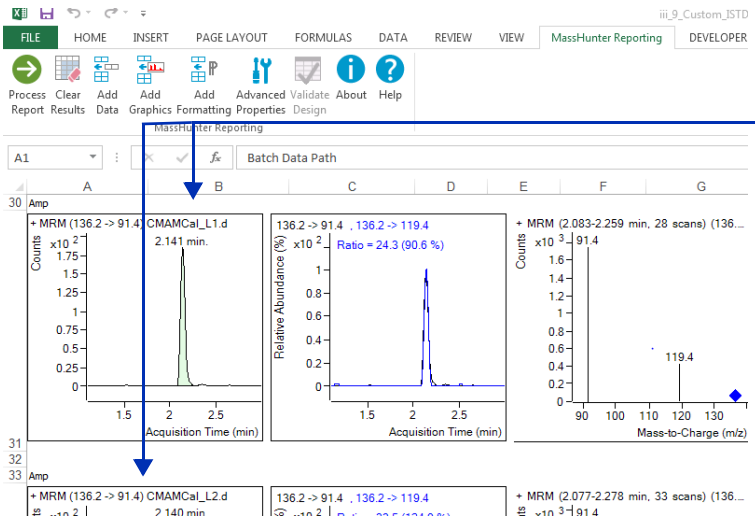
You can quickly find any graphics in the template because they are shown in green in the template.

The graphics are included in the **CompoundID** repeating

Figure 75 Select the **RT** column

Task 1. Add graphics to a Quantitative Analysis template (continued)

Step	Detailed instructions	Comments
3 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Move to the **\MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuseDemo** folder. **d** Select **report.results.xml**. **e** Click **Open**. **f** Click **OK**. **g** Close the **XML Source** pane. **h** Find the Compound Graphics section. The three compound graphics are shown in the same row.	• The Process Report command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon.



The Compound Graphics for each data file are shown in different rows.

All of the graphics for the first compound are shown together.

Figure 76 The compound graphics are added after the Target Compound table

4 Save the changes to the template, ***iii*_10_Custom_ISTD_Summary.** • You have to clear the results first.	**a** Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon. **b** Click **File > Save As**. **c** In the Save As dialog box, type *iii*_10_Custom_ISTD_Summary. **d** Verify the folder selected in **Save in** is correct. **e** Click **Save**.	• The **Save as type** is **Excel Template**.

Task 2. Display multiple graphics per row

If you have graphics in a template, you can specify the relative width and height for those graphics.

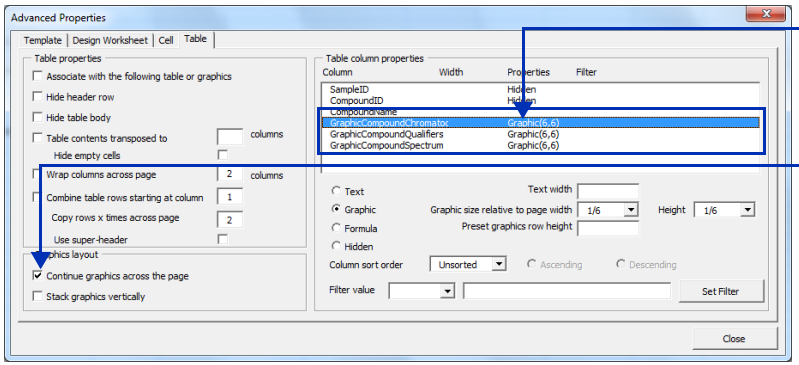
You can also mark whether or not to print graphics side-by-side. Normally, only graphics that are in the same row of the table are printed side-by-side. However, you can specify that graphics from different rows are printed side-by-side.

Task 2. Use the side-by-side graphics feature in a Quantitative Analysis template

Step	Detailed instructions	Comments
1 Open the Quantitative Analysis template, **\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Results_NoGraphics\Parts\iii_10_Custom_ISTD_Summary**.	Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, **iii_10_Custom_ISTD_Summary**, where "**iii**" are your initials.	• If you do not have the **iii_10_Custom_ISTD_Summary** template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Change the size of the graphics in the Compound Graphics table. • Make the width of each graphic 1/6th of the width of the page. • Make the height of each graphics 1/6th of the height of the page.	**a** Click one of the graphics in the Compound Graphics table. **b** Click **Advanced Properties** in the **MassHunter Reporting** tab in the Ribbon. **c** Select **1/6** for the **Graphic size relative to page width** and **Height** boxes for each graphic. **d** Mark the **Continue graphics across the page** check box. **e** Click **Close**.	• Make sure to change the width and height for each graphic.

Task 2. Use the side-by-side graphics feature in a Quantitative Analysis template (continued)

Step	Detailed instructions	Comments



Set the relative graphic width and height for each of the graphics.

Mark the Continue graphics across the page check box. This check box controls whether or not different rows of graphics can be printed on the same line.

The **Stack graphics vertically** check box changes how the graphics are organized on the page. If this check box is cleared, then the related graphics are printed side-by-side. If this check box is marked, then related graphics are printed on consecutive rows.

Figure 77 Select the RT column

3 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Move to the **\MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuseDemo** folder. **d** Select **report.results.xml**. **e** Click **Open**. **f** Click **OK**. **g** Close the **XML Source** pane. **h** Find the first Compound Graphics section. Six different graphics are printed in the same row.	• The Process Report command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon.

Task 2. Use the side-by-side graphics feature in a Quantitative Analysis template (continued)

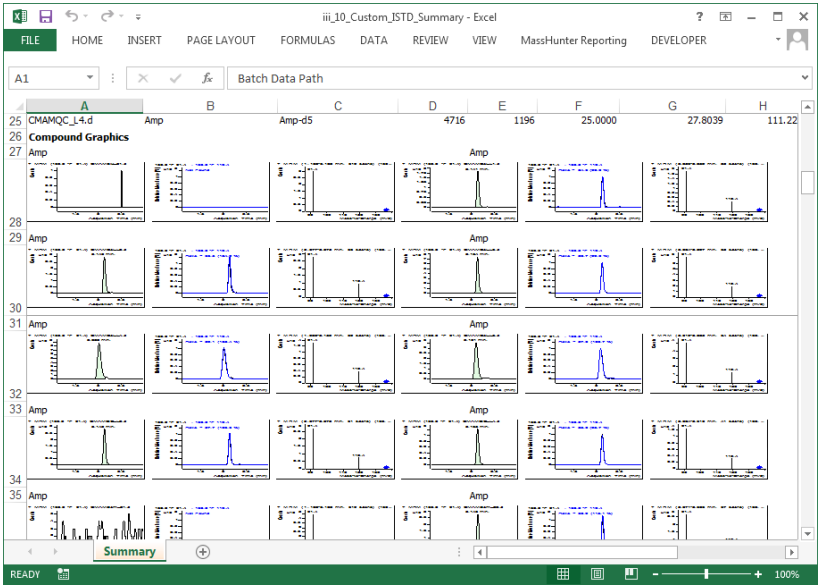
Step	Detailed instructions	Comments
		Six different graphics are printed in each row. Each is one sixth the width of the page and one sixth the height of the page. Also, the graphics from two different data files are printed on the same line. You read the graphics from left to right on the page. For example, the graphics for the second data file are printed to the right of the graphics for the first data file.
4 Save the changes to the template, **iii_11_Custom_ISTD_ Summary**. • You have to clear the results first.	**a** Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon. **b** Click **File > Save As**. **c** In the Save As dialog box, type `iii_11_Custom_ISTD_Summary`. **d** Verify the folder selected in **Save in** is correct. **e** Click **Save**.	• The **Save as type** is **Excel Template**.

Figure 78 Graphics are printed side-by-side when you mark **Continue graphics across the page**

Exercise 6
Advanced topics

In this exercise, you learn how to use some of the advanced features in the MassHunter Report Designer add-in.

Each exercise is presented in a table with three columns:

- **Steps** – Use these general instructions to proceed on your own to explore the program.
- **Detailed Instructions** – Use these if you need help or prefer to use a step-by-step learning process.
- **Comments** – Read these to learn tips and additional information about each step in the exercise.

Task 1. Add a page break and a sheet break

You can add a page break or a sheet break anywhere in a template.

If you add a page break, the report automatically puts the next information in the report at the beginning of a new page.

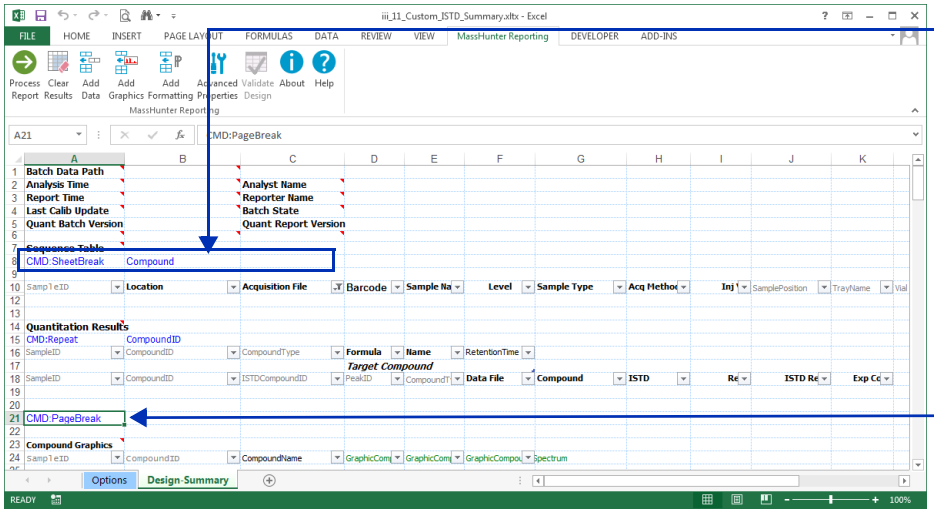
A sheet break is similar to a page break; the report automatically puts the next information in the report at the beginning of a new page. It also places the information on a new worksheet. When you add a sheet break, you can select an item that is already part of the template to label the new worksheet. This is important because you can include the name of the worksheet in the header or footer of the report. See "Task 2. Customize the footer of the Qualitative Analysis template" on page 32 or "Task 5. Customize the footer of the Quantitative Analysis Excel template" on page 42 for more information.

Task 1. Add a page break and a sheet break

Step	Detailed instructions	Comments
1 Open the Quantitative Analysis template, **\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Results_NoGraphics\Parts\iii_11_Custom_ISTD_Summary**.	Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, ***/ii*_11_Custom_ISTD_Summary**, where "**iii**" are your initials.	• If you do not have this template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Add a sheet break to the Quantitation Results section. • Select Compound to label the worksheet.	**a** Select the row containing the **SampleID** column in the Quantitation Results section. **b** Right-click the row and click **Insert**. A row is added above the table. **c** Click the first column in this new row. **d** Click **Add Formatting > Sheet Break** in the **MassHunter Reporting** tab in the Ribbon. **e** Select **Compound**. **f** Click **OK**.	• You can only select an item that is included between that row and the end of the template to use as the label for the worksheet. • If the item is not part of the template, you can add it to the template and hide that column or cell. • If you do not want to specify an item to use to label the new worksheet, click **Cancel**. The CMD:Sheet Break command is still added to the template.

Task 1. Add a page break and a sheet break (continued)

Step	Detailed instructions	Comments
3 Add a page break before the graphics in the Quantitation Results section.	**a** Click the first column in the row that is above the Compound Graphics label. **b** Click **Add Formatting > Page Break** in the **MassHunter Reporting** tab in the Ribbon.	• A page break only starts a new page. It does not change the worksheet label.



When you add a Sheet Break, you select an item to use to label the new worksheet. If you do not select an item, then the name of the design worksheet is used to label each of the new worksheets.

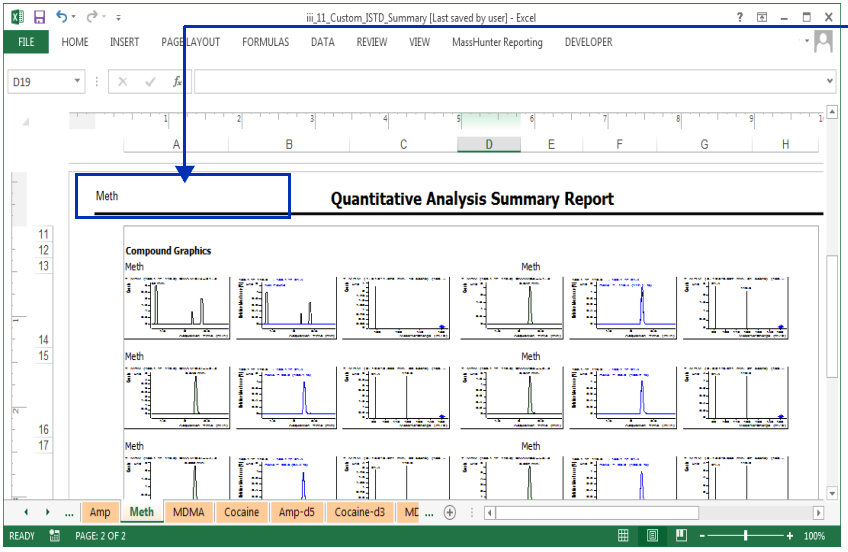
You do not select a column when you add a Page Break.

Figure 79 Adding a Sheet Break and a Page Break

4 Add the sheet name to the header of the worksheet.	**a** Click the **View** tab. **b** Click the **Page Layout** button. **c** Click the left portion of the header. **d** Click the **Header & Footer Tools** tab. **e** Click the **Sheet Name** button under **Header & Footer Elements** in the **Header & Footer Tools** tab. **f** Click outside of the header area. **g** Click **Normal** in the Workbook Views group in the **View** tab in the Ribbon.	• The footer also contains the Sheet Name in the left hand section.

Task 1. Add a page break and a sheet break (continued)

Step	Detailed instructions	Comments
5 Test the changes to the template.	**a** Click the **MassHunter Reporting** tab. **b** Click **Process Report**. **c** Click the **Browse** button. **d** Move to the **\MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuseDemo** folder. **e** Select **report.results.xml**. **f** Click **Open**. **g** Click **OK**. **h** Click the **Meth** worksheet. Each worksheet is labeled with the name of a different compound. **i** Click the **View** tab in the Ribbon. **j** Click the **Page Layout** button or the **Page Break Preview** button. **k** The compound graphics are printed starting at the top of the next page.	• The Process Report command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon.



The header contains the name of the WorkSheet. The name of the worksheet is set when using the **CMD:SheetBreak** command.

The graphics are printed at the top of a new page because of the CMD:PageBreak command that is added.

Figure 80 The Compound Graphics are printed at the start of the page. The worksheets are labeled with the compound name

Task 1. Add a page break and a sheet break (continued)

Step	Detailed instructions	Comments
6 Save the changes to the template, **iii_12_Custom_ISTD_ Summary.** • You have to clear the results first.	**a** Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon. **b** Click **File > Save As**. **c** In the Save As dialog box, type *iii*_12_Custom_ISTD_Summary. **d** Verify the folder selected in **Save in** is correct. **e** Click **Save**.	• The **Save as type** is **Excel Template**.

Task 2. Use Test Mode

Once Test Mode is enabled, you can process the report, one step at a time. When you click Process Report, three steps are performed. Using the Test Mode commands, you can pause after any of the steps:

1. Click **Import XML Data** to see the data that is imported into the Design worksheets. At this point, you can see the raw imported data, before any filtering. For MassHunter Quantitative Analysis, you see the data from the entire batch.
2. Click **Copy Data to Report** to see the data after it is filtered and copied to the report worksheets.
3. Click **Format Report** to see the data after it is formatted, and the graphics are imported.

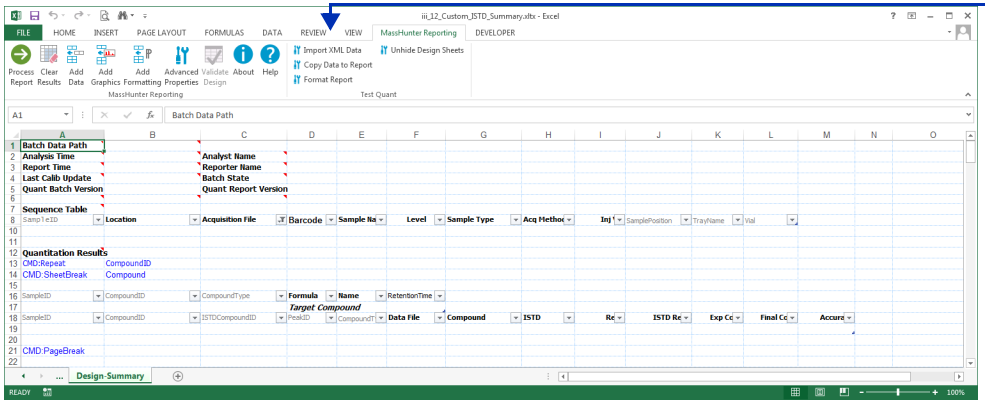
If you click **Unhide Design Sheets**, you can view the Design worksheets at the same time as the final report. The Design worksheets are hidden after the Format Report step.

Task 2. Use Test mode

Step	Detailed instructions	Comments
1 Make a backup copy of the file **MassHunter Reporting Quant.config**.	**a** Open the Windows Explorer program. **b** Move to the **C:\Program Files\Microsoft Office\Office12\Library** folder. **c** Right-click the **MassHunter Reporting Quant.config** file and click **Copy**. **d** Click **Edit > Paste** to add a copy of the config file to the current folder. **e** Right-click the new file, **Copy of MassHunter Reporting Quant.config** and click **Rename**. **f** Type *backup_MassHunter Reporting Quant.config*.	• If you want to enable Test Mode in the Report Designer for Qualitative Analysis add-in, you change the **MassHunter Reporting Qual.config** file.
2 Remove the **Read-only** attribute from the original config file.	**a** Right-click the **MassHunter Reporting Quant.config** file and click **Properties**. **b** Clear the **Read-only** check box in the Attributes section, if necessary. **c** Click **OK**.	

Task 2. Use Test mode (continued)

Step	Detailed instructions	Comments
3 Change the TestMode enabled line from **False** to **True**.	**a** Right-click the **MassHunter Reporting Quant.config** file and click **Open**. You can open this file with Notepad. **b** Find the line **"<TestMode enabled="False"/>"**. **c** Change the word **False** to **True**. **d** Save the change. If you are using Notepad, click **File > Save**. **e** Close the program.	
4 Open the Quantitative Analysis template, **\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Results_NoGraphics\Parts\iii_12_Custom_ISTD_Summary**.	Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, **iii_12_Custom_ISTD_Summary**, where "**iii**" are your initials.	• If you do not have the **iii_12_Custom_ISTD_Summary** template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.

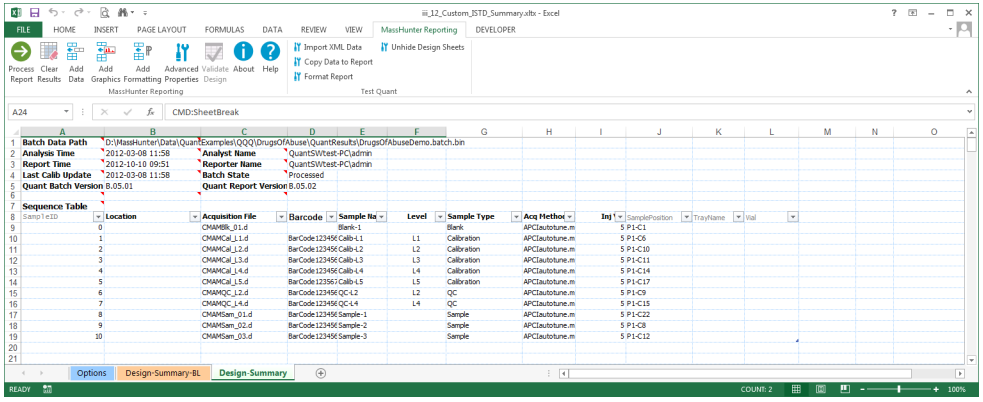


When you enable **Test Mode**, a new menu is added to the MassHunter Reporting toolbar. These commands allow you to step through processing the report which can help you determine the cause of a problem in the template.

Figure 81 The Test Mode menu

Task 2. Use Test mode (continued)

Step	Detailed instructions	Comments
5 Test the steps in the Test Quant menu.	**a** Click **Test Quant > Import XML Data.** **b** Click the **Browse** button. **c** Move to the **\MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuseDemo** folder. **d** Select **report.results.xml.** **e** Click **Open**. **f** Click **OK**.	• The Test Quant command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon. • You cannot skip a step. You must do each step in order. • Do not repeat any of the steps. You must clear the results before trying to import a different XML Data file.

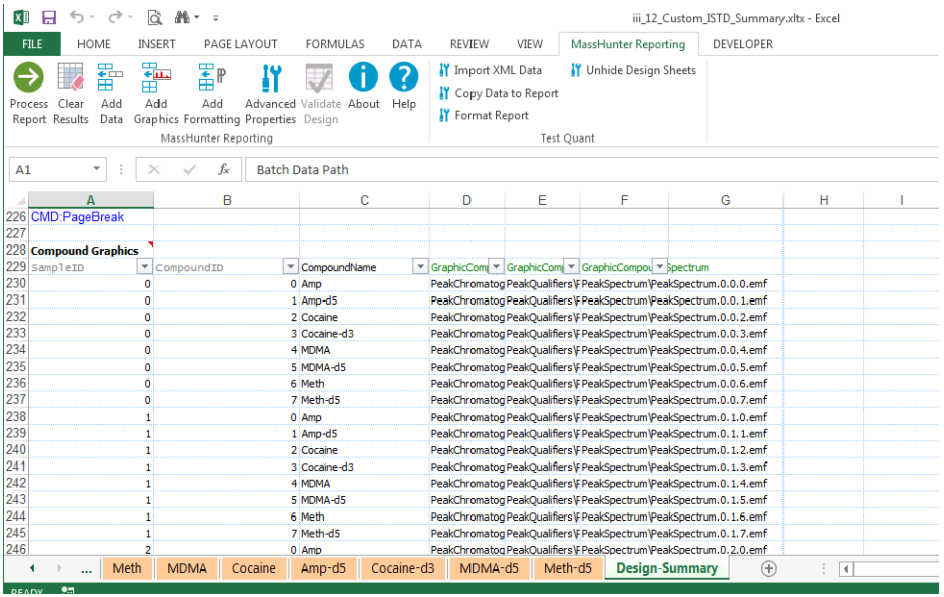


After the first step, the data is added to the template, but it is not filtered or copied to the report worksheets or formatted.

Figure 82 After the **Test Quant > Import XML Data** step

Task 2. Use Test mode (continued)

Step	Detailed instructions	Comments
	g Click **Test Quant > Copy Data to Report.**	

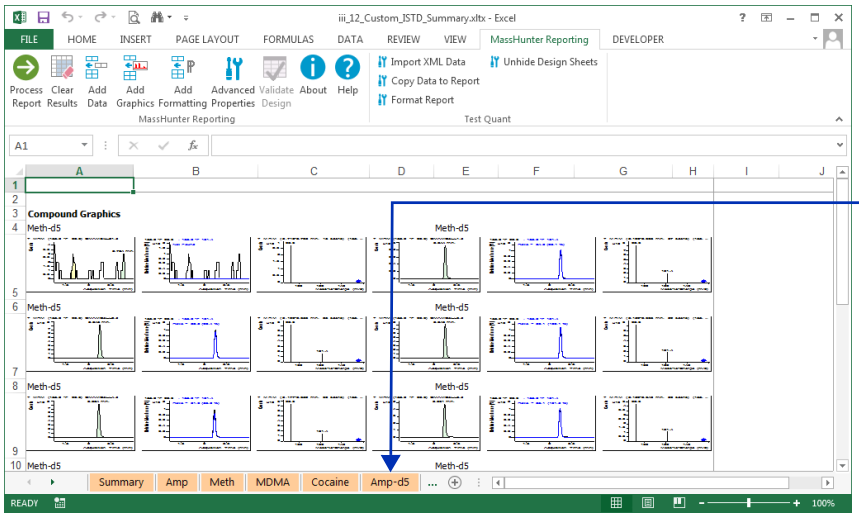


After the second step, the data is placed onto the appropriate worksheet and it is filtered, but it is not formatted. Also, the graphics are not included in the report yet.

Figure 83 After the **Test Quant > Copy Data to Report** step

Task 2. Use Test mode (continued)

Step	Detailed instructions	Comments
	h Click **Test Quant > Format Report.**	



After the third step, the graphics are included in the report and the data is formatted.

The **Unhide Design Sheets** command allows you to see the Design-Summary worksheet while you are looking at the results. After the Format Quant step, the Design worksheets are hidden.

Figure 84 After the **Test Quant > Format Quant** step

6 Clear the results and close Excel.	**a** Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon. **b** Click the **Microsoft Office button** and click **Close**.	• You can use the **Clear Results** command after any of the steps.

Task 3. Add a single repeating section

A repeating section allows you to organize the rows in a table differently. It also allows you to group different tables together. In "Task 4. Add a nested repeating section" on page 129, you group different tables together using a nested repeating section.

In this task, you add a single repeating section which lets you change how the data in a table is included. When you add a table to a template, the add-in automatically creates the template using the first ID in the table and then the second ID. For example, when you add a Target Compound table to the template, the SampleID is the first ID, so the table has all of the information for each sample grouped together. By adding a repeating section, you can group all of the information about each compound together.

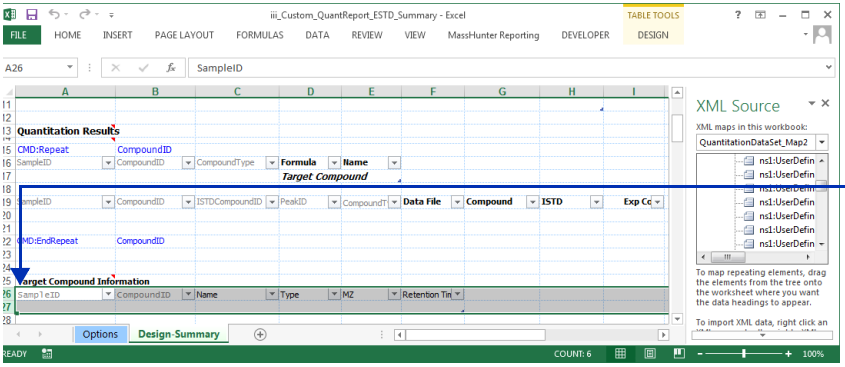
A repeating section is similar to the programming concept of a For/Next loop. **CMD:Repeat** is equivalent to "For each item in the Column Selected repeat the following lines". **CMD:EndRepeat** is equivalent to "Next" or the end of the lines to repeat.

Task 3. Add a single repeating section

Step	Detailed instructions	Comments
1 Open the Quantitative Analysis template, *\MassHunter\Report Templates\Quant\Letter\ESTD\Parts\iii_Custom_QuantReport_ESTD_Summary*.	Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, **iii_Custom_QuantReport_ESTD_Summary**, where "**iii**" are your initials.	• Make a copy of the **QuantReport_ESTD_Summary_B_04_00** template and rename it to `iii_Custom_QuantReport_ESTD_Summary`, where "`iii`" are your initials.
2 Add a repeating section at the end of the template. • Add the Target Compound table. • Repeat this table using the CompoundID.	**a** Select the first column in row 25. **b** Click **Add Data > Target Compound Table** in the **MassHunter Reporting** tab in the Ribbon. The Target Compound Information table is added at the end of the report. **c** Select rows 26 to 27. Click row 26 and drag to include row 27.	• You can also fix the headers of this table to match the headers of the other tables in this template. Right-click the headers, and click the **B** in the shortcut menu to change the font.

Task 3. Add a single repeating section (continued)

Step	Detailed instructions	Comments



Rows 26 and 27 are selected. Row 25 is not selected because that row is not being repeated.

Figure 85 Adding a single repeating section

d Click **Add Formatting > Repeating Section** in the **MassHunter Reporting** tab in the Ribbon.

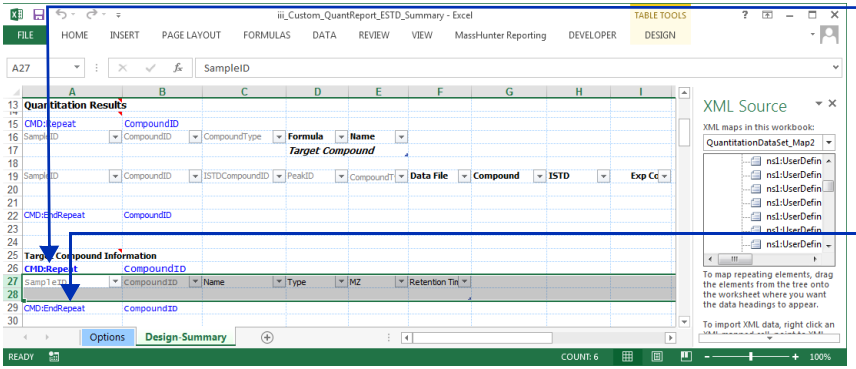
e In the Select Column dialog box, select **CompoundID**.

f Click **OK**.

- Usually, you repeat using one of the ID columns.
- To have the compound information printed together, select the CompoundID.
- Two commands are added to the template. **CMD:Repeat** is added before row 26 and **CMD:EndRepeat** is added after row 27.

Task 3. Add a single repeating section (continued)

Step	Detailed instructions	Comments



The command **CMD:Repeat** is added before the selected rows. The column that is selected is printed in the second column. This is the start of the repeating section.

The command **CMD:EndRepeat** is added after the selected rows. The column that is selected is also printed in this row. This is the end of the repeating section.

Figure 86 The repeating section is added around the Target Compound Information table

3 Test the changes to the template.

a Click **Process Report**.
b Click the **Browse** button.
c Move to the **\MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuseDemo** folder.
d Select **report.results.xml**.
e Click **Open**.
f Click **OK**.
g Scroll the report until you find the Target Compound Information table. All of the information for each compound is grouped together. The column headers are repeated between each compound because that row is part of the repeating section.

- In the Advanced Properties dialog box, you can click **Hide Header Row** if you don't want to repeat the header row for each compound.

Task 3. Add a single repeating section (continued)

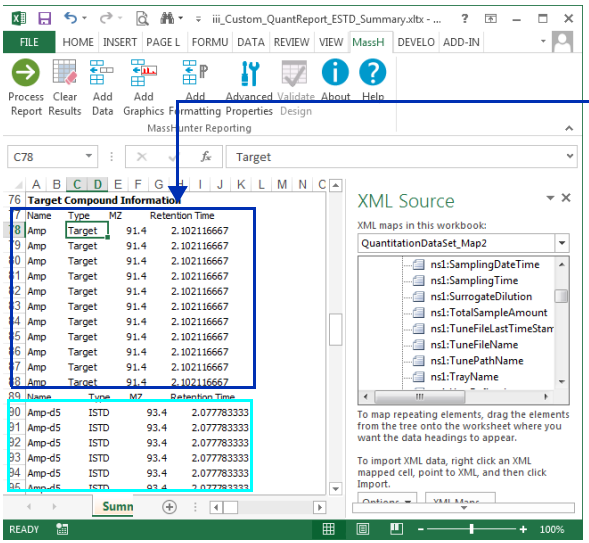
Step	Detailed instructions	Comments
		The rows about each compound are grouped together.

Figure 87 The results after adding a repeating section using the CompoundID

4 Save the changes to the template, **iii_1_Custom_QuantReport_ESTD_Summary.xlt**.

- You have to clear the results first.

a Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon.

b Click **File > Save As**.

c In the Save As dialog box, type *iii*_1_Custom_QuantReport_ESTD_Summary.

d Verify the folder selected in **Save in** is correct.

e Click **Save**.

- The **Save as type** is **Excel Template**.

Task 4. Add a nested repeating section

A repeating section allows you to organize the rows in a table differently. It also allows you to group different tables together. In "Task 3. Add a single repeating section" on page 125, you add a single repeating section which lets you change how the data in a table is organized.

In this task, you group different tables together using a nested repeating section. A nested repeating section is simply a repeating section that is within another repeating section. When repeating sections are nested, the inner repeating section needs to end before the outer repeating section ends.

- CMD:Repeat Item1
  - CMD:Repeat Item2

    Rows in the template
  - CMD:EndRepeat Item2
- CMD:EndRepeat Item1

Task 4. Add a nested repeating section

Step	Detailed instructions	Comments
1 Open the Quantitative Analysis template, **\MassHunter\Report Templates\Quant\Letter\ESTD\Parts iii_1_Custom_QuantReport_ESTD_Summary.**	Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, **iii_1_Custom_QuantReport_ESTD_Summary**, where "**iii**" are your initials.	• If you do not have the **iii_1_Custom_QuantReport_ESTD_Summary** template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Add a nested repeating section at the end of the template. • Add the Compound Graphics inside of the repeating section at the end of the report. • Add an inner repeating section repeating on the SampleID.	**a** Select row 29. **b** Right-click and click **Insert** to add a new row to the template. **c** Click the first column in row 30. **d** Click **Add Graphics > Compound Graphics** in the **MassHunter Reporting** tab in the Ribbon. **e** Select rows 27 to 32. Click row 27 and drag to include row 32.	• Do not include the rows containing the commands **CMD:Repeat** nor **CMD:EndRepeat**.

Task 4. Add a nested repeating section (continued)

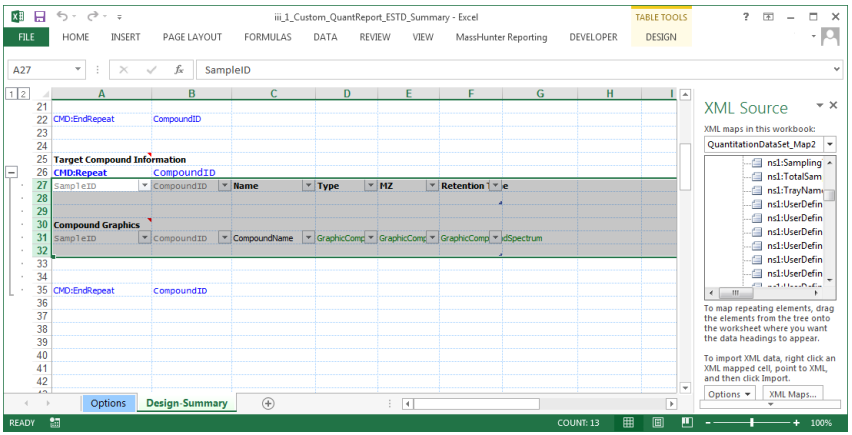
Step	Detailed instructions	Comments
		Rows 27 through 32 are selected. The **CMD:Repeat** row and the **CMD:EndRepeat** rows are not selected.

Figure 88 Selecting both tables inside of the Repeating Section

f Click **Add Formatting > Repeating Section** in the **MassHunter Reporting** tab in the Ribbon.

g In the Select Column dialog box, select **SampleID**.

h Click **OK**.

- Do not select the **CompoundID** item. The **CompoundID** has already been used in the outer repeating section.
- If we did not add an inner repeating section, then the report would be organized differently. For each compound, all of the samples in the Target Compound Information table would be included, and then all of the samples in the Compound Graphics would be included.

Task 4. Add a nested repeating section (continued)

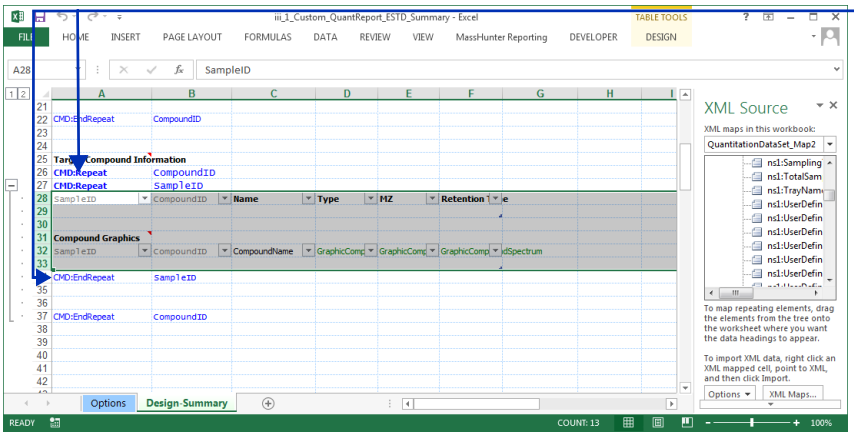
Step	Detailed instructions	Comments
		The command **CMD:Repeat** is added before the selected rows, and the command **CMD:EndRepeat** is added after the selected rows. Both of these commands are between the original **CMD:Repeat CompoundID** and **CMD:EndRepeat CompoundID** rows.

Figure 89 An inner repeating section is added which includes both tables

3 Test the changes to the template.

a Click **Process Report**.
b Click the **Browse** button.
c Move to the **\MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuseDemo** folder.
d Select **report.results.xml**.
e Click **Open**.
f Click **OK**.
g Scroll the report until you find the Target Compound Information table. All of the information for each compound is grouped together. Within each compound, the Sample Information and the Compound Graphics from each sample are grouped together.

Task 4. Add a nested repeating section (continued)

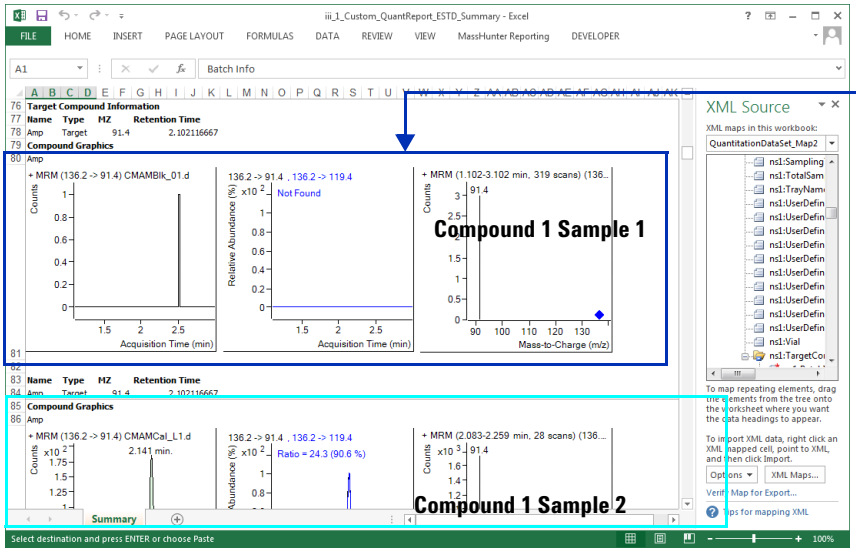
Step	Detailed instructions	Comments
		The report is organized so that all of the information for each compound is grouped together (the outer repeating section). Within each compound section, the information for each sample is grouped together.

Figure 90 The results of a repeating section using the CompoundID

4 Save the changes to the template, **iii_2_Custom_QuantReport_ESTD_Summary.xlt**.

- You have to clear the results first.

a Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon.
b Click **File > Save As**.
c In the Save As dialog box, type *iii*_2_Custom_QuantReport_ESTD_Summary.
d Verify the folder selected in **Save in** is correct.
e Click **Save**.

- The **Save as type** is **Excel Template**.

Task 5. Change values on the Options worksheet

The Options worksheet is part of every template that is shipped with the software. The values on this worksheet are used to set some of the formatting options. The values in the first table are only used if the **Use Options** value is set to True. Many of the Quantitative Analysis templates set this value to False, by default. Many of the Qualitative Analysis templates set this value to True by default.

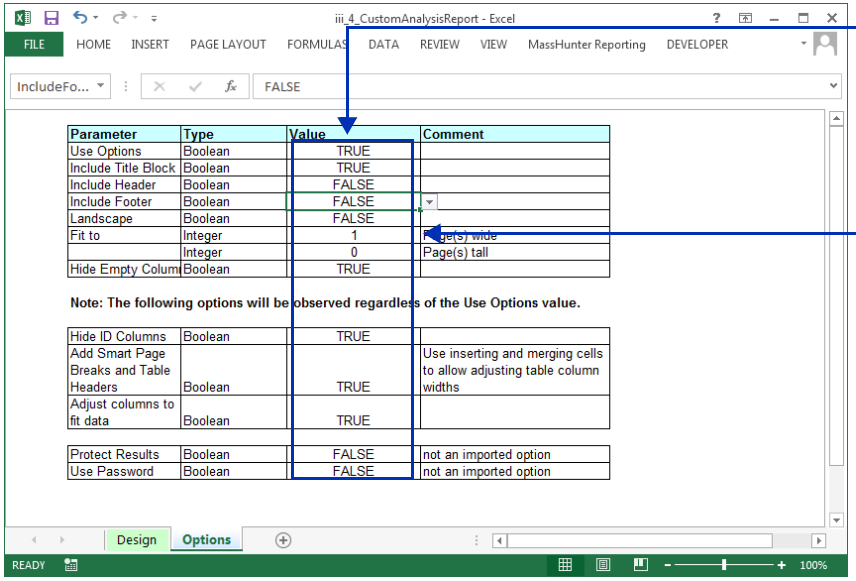
Two options that affect the speed of report generation are **Add Smart Page Breaks** and **Adjust Columns to Fit Data**. These options are needed for proper formatting of a report. However, if you are only interested in creating output for a LIMS system, you may choose to set both off these options to **FALSE**.

Task 5. Change values on the Options worksheet

Step	Detailed instructions	Comments
1 Open the Qualitative Analysis template **\MassHunter\Report Templates\Qual\Letter\ iii_4_CustomAnalysisReport**, where **iii** are your initials.	Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 30 to open the template, **iii_4_CustomAnalysisReport**, where "**iii**" are your initials.	• If you did not create this template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Switch to the Options worksheet. • Set **Use Options** to True • Set **Include Header** to False • Set **Include Footer** to False	**a** Click the **Options** worksheet at the bottom of the program. **b** Find the **Use Options** row. **c** Select **True** in the Value column. **d** Find the **Include Header** row. **e** Select **False** in the Value column. **f** Find the **Include Footer** row. **g** Select **False** in the Value column.	• Only change the values in the Value column. • The Options in the first section only change the report if the Use Options value is True. • The Options in the second section are not affected by the Use Options value. • If you have a template that is missing an option, you can add that option to the options template by copying the option line from a template that does have that line. You have to remember to explicitly name the Value cell of that row to the value that was shown in the old template.

Task 5. Change values on the Options worksheet (continued)

Step	Detailed instructions	Comments



Each cell in the Value column is explicitly named. You can see the name of the cell here.

Only change the Value column. In this example, the Include Header and Include Footer values are set to False. The header and footer will not be printed in the report.

Figure 91 Change the values in the Options worksheet

3 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Move to the **\MassHunter \Reports\Temp** folder. **d** Double-click one of the folders that contains analysis results. **e** Select **Report.xml**. **f** Click **Open**. **g** Click **OK**. **h** Click the **Microsoft Office button** and click **Print > Print Preview**.	• The **Process Report** command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon.

Task 5. Change values on the Options worksheet (continued)

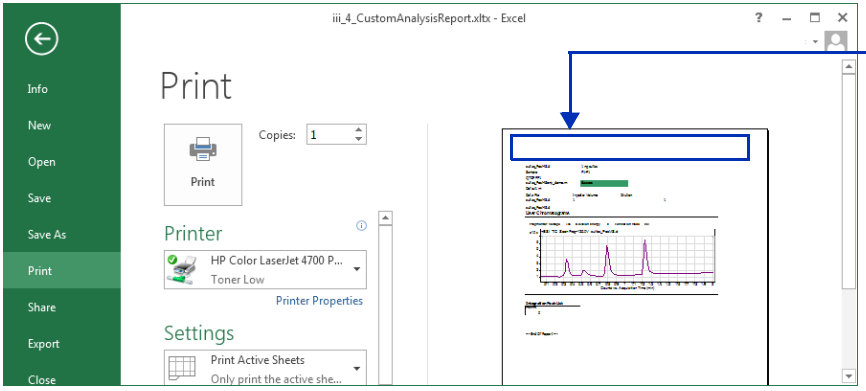
Step	Detailed instructions	Comments
		The header and the footer are not included in the report. The Qualitative Analysis program lets you set several of these options in the user interface. The values you set here are overridden by the values in the Qualitative Analysis user interface when you print from the Qualitative Analysis programs.

Figure 92 Verifying that the header and footer are not shown

4 Save the template to **iii_5_CustomAnalysisReport**, where **iii** are your initials.
- You have to clear the results first.

a Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon.
b Click **File > Save As**.
c In the Save As dialog box, type `iii_5_CustomAnalysisReport`.
d Verify the folder selected in **Save in** is correct.
e Click **Save**.

- The **Save as type** is **Excel Template**.
- See the MassHunter Report Designer Training for more information on the different options.

Task 6. Add a formula using the IF function

One of the Excel functions that you can use in a formula is the IF function. The **IF** function has the following format:

=IF(LogicalTest,Value If True, Value If False)

This formula allows you to do one of two actions, depending on whether the logical test is true or not.

In this example, you check whether or not a formula is found for a peak. If the formula is not found, then the text "Not Found" is printed. If the formula is found, then the formula is printed.

The **IF** function is very powerful. See the Excel online Help for more information on this feature.

Task 6. Add a formula using the IF function

Step	Detailed instructions	Comments
1 Open the Qualitative Analysis template **\MassHunter\Report Templates\Qual\Letter\ iii_5_CustomAnalysisReport**, where **iii** are your initials.	Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 30 to open the template, **iii_5_CustomAnalysisReport,** where "**iii**" are your initials.	• If you did not create this template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Add a formula column to the second Peak List table. • If the formula is not defined, print "Not Found." • If the formula is defined, print the formula.	**a** Find the **Formula** column in the Peak List table that is at the end of the report. **b** Click the **Formula** column. **c** Click **Add Data > Formula Column** in the **MassHunter Reporting** tab in the Ribbon. **d** Click the **Formulas** tab.	• See the online Help for Excel for a complete description of the IF formula and other possible formulas.

Task 6. Add a formula using the IF function (continued)

Step	Detailed instructions	Comments

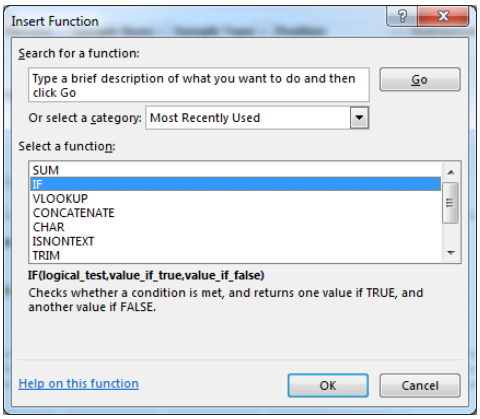


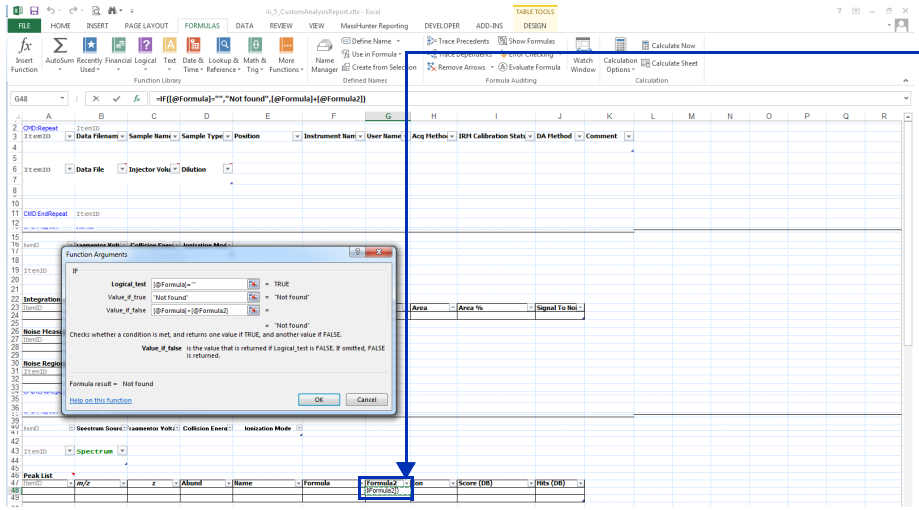
Figure 93 Select the IF Function

e Click **Insert Function**.

f In the **Select a function** dialog box, select **IF**.

g Click **OK.**

- See the online Help for Excel for a complete description of the IF formula and other possible formulas.



You click the cell in the Formula column in the table to get [Formula] added to the Logical_test and the Value_if_false boxes.

Figure 94 Enter the formula using the Function Arguments dialog box

Task 6. Add a formula using the IF function (continued)

Step	Detailed instructions	Comments
	h Click the **Logical_test** box. **i** Click the cell in the Formula column. **j** Type =" " in the Logical_test box. **k** Type `Not Found` in the **Value_if_true** box. **l** Click the **Value_if_false** box. **m** Click the cell in the Formula column. **n** Click **OK**.	
3 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Move to the **\MassHunter \Reports\Temp** folder. **d** Double-click one of the folders that contains analysis results. **e** Select **Report.xml.** **f** Click **Open**. **g** Click **OK**. **h** Find the Peak Table at the end of the report. **i** Compare the Formula column and the Formula2 column.	• The **Process Report** command is part of the MassHunter toolbar in the **MassHunter Reporting** tab in the Ribbon. • This template has more than one Peak Table. Make sure that you find the Peak Table at the end of the template. • Make sure that the results contain compounds that have the formula defined.

Task 6. Add a formula using the IF function (continued)

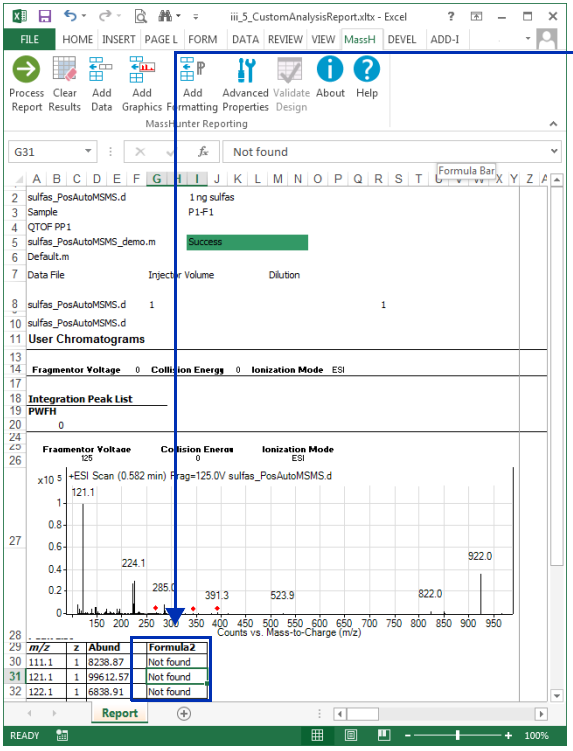
Step	Detailed instructions	Comments
		When the cell in the Formula column is empty, the Formula2 column contains Not Found. You can hide the original column using the Advanced Properties dialog box. You select the **Formula** column and click the **Hidden** button. The formula is visible in the **Formula2** column.

Figure 95 The empty cells in the Formula column are replaced with **Not Found** in the Formula2 column

4 Save the template to **iii_6_CustomAnalysisReport**, where **iii** are your initials.

- You have to clear the results first.

a Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon.

b Click **File > Save As**.

c In the Save As dialog box, type `iii_6_CustomAnalysisReport`.

d Verify the folder selected in **Save in** is correct.

e Click **Save**.

- The **Save as type** is **Excel Template**.

Task 7. Use the VLOOKUP function

In this task, you use the function VLOOKUP in a template to look up limits for different compounds. The VLOOKUP function allows you to look in a table to find a specific value, and then it returns another value in that row. The main steps that you need to do are:

1. Add a tab that contains the lookup table.
2. Add the formula column to the table that uses the VLOOKUP function.
3. Add a second formula column that uses the value returned by the VLOOKUP function.

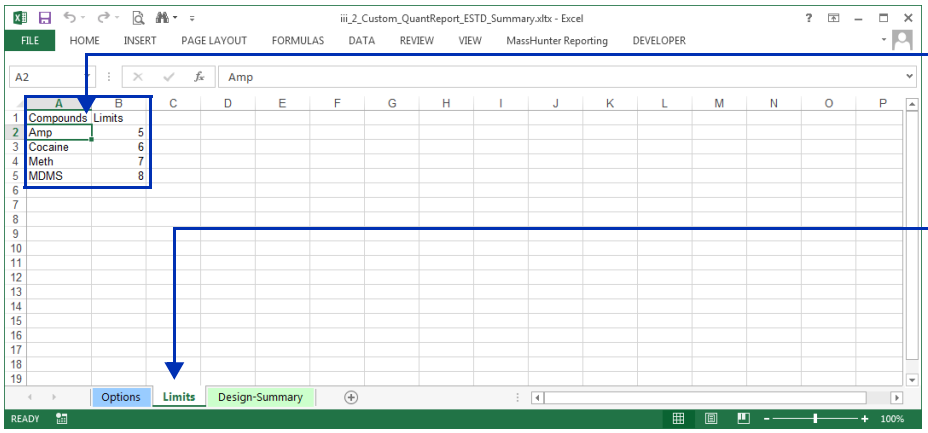
The VLOOKUP function does slow down processing of the report, so you want to make the VLOOKUP range as small as possible.

Task 7. Use the VLOOKUP function to add a Limits column

Step	Detailed instructions	Comments
1 Open the Quantitative Analysis template, **\MassHunter\Report Templates\Quant\Letter\ESTD\Parts\iii_2_Custom_QuantReport_ESTD_Summary**.	Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, **iii_2_Custom_QuantReport_ESTD_Summary**, where "**iii**" are your initials.	• If you do not have the **iii_2_Custom_QuantReport_ESTD_Summary** template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.
2 Add a new worksheet to the template that contains the VLOOKUP range. For this example, we will use the following arbitrary values • Amp 5 • Cocaine 6 • Meth 7 • MDMA 8	**a** Press **Shift** and **F11**. A new worksheet is added. **b** Click the first column in row 1. **c** Type `Compounds`. **d** Click the second column in row 1. **e** Type `Limits`. **f** Enter the four compound names in the Compounds column. **g** Enter the four limits in the Limits column. **h** Right-click the tab at the bottom of the worksheet. **i** Click **Rename**. **j** Type `Limits` and press **Enter**.	• You can also click the **Insert Worksheet** tab that is next to the other tabs at the bottom of the program. • Instead, you can add the lookup table to the **Options** tab. The **Options** tab is not printed when the report is printed.

Task 7. Use the VLOOKUP function to add a Limits column (continued)

Step	Detailed instructions	Comments



The **Compounds** and **Limits** columns are added to the worksheet.

The name of the worksheet is changed to **Limits**.

Figure 96 Adding the new worksheet and renaming it Limits

k Click **Advanced Properties** in the **MassHunter Reporting** tab in the Ribbon.

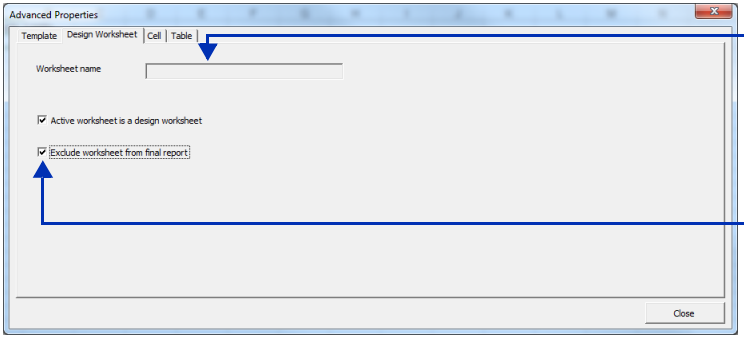
l Click the **Design Worksheet** tab.

m Mark the **Active worksheet is a design worksheet** check box.

n Mark the **Exclude worksheet from final report** check box.

o Click **Close**.

- If the **Exclude worksheet from final report** check box is marked, this worksheet is not printed when the report is printed.



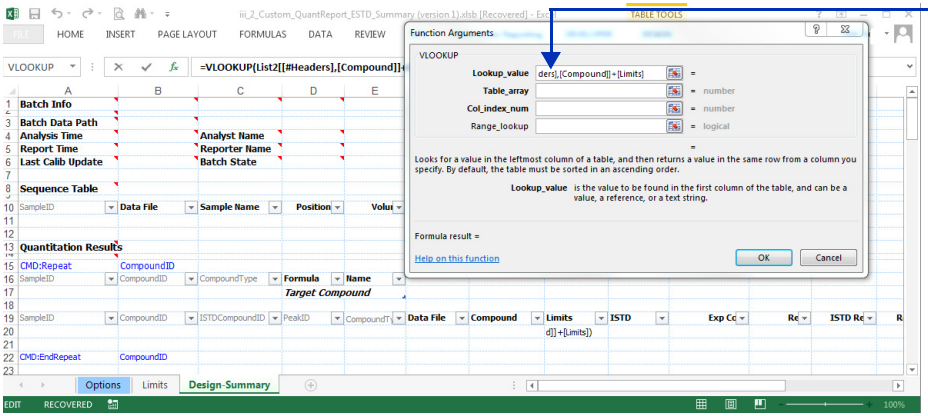
The name of the worksheet is shown in this dialog box, but you cannot edit it in this tab.

Mark both check boxes in this dialog box.

Figure 97 Advanced Properties dialog box

Task 7. Use the VLOOKUP function to add a Limits column (continued)

Step	Detailed instructions	Comments
3 Add the VLOOKUP formula column.	**a** Click the **Design-Summary** worksheet tab. **b** Find the **Compound** column in the second Quantitation Results table. **c** Click **Add Data > Formula Column**. **d** Rename the new column `Limits`. **e** Click the cell containing the words **Enter formula here**. **f** Click the **Formulas** tab in the Ribbon. **g** Click **Insert Function**. **h** In the select a category box, select **Lookup & Reference**. **i** Select **VLOOKUP** in the **Select a function** list. **j** Click **OK**. **k** Click the cell containing the value in the **Compound** column.	• See Task 3. Add a formula column to a table for more information on adding a formula column.



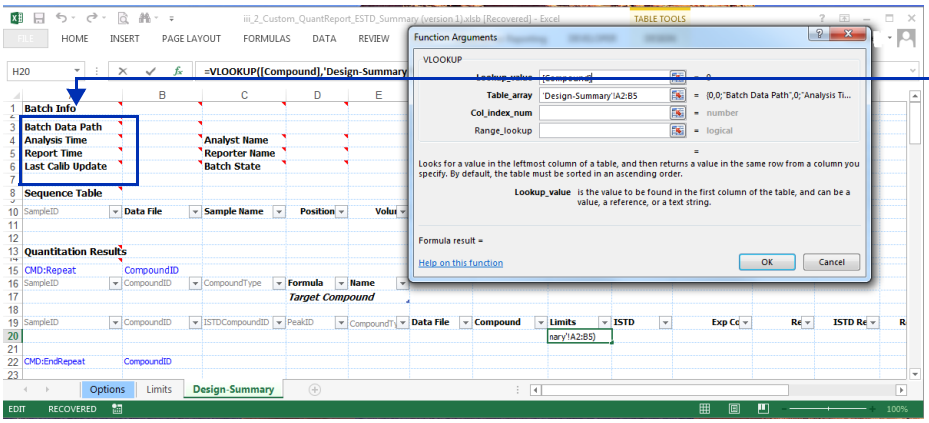
The Lookup_value is the value that you want to look up in the Limits worksheet. So, you click the cell in the Compound column that contains the results. Do not click the column header.

Figure 98 Add the Lookup_value to the Function Arguments dialog box

	l Click the **Table_array** box in the Function Arguments dialog box. **m** Click the **Limits** worksheet tab. **n** Click and drag to select the area containing the compound names and the limits.	• When you click the Limits worksheet tab, "Limits!" is added to the Table_array box.

Task 7. Use the VLOOKUP function to add a Limits column (continued)

Step	Detailed instructions	Comments



Select the area containing the compound names and limits. You do not include the column headers.

Figure 99 Add the Table_array value to the Function Arguments dialog box

o In the Table_array box, select the entire string.

p Press **F4**.

q Type `2` in the **Col_index_num** box in the Function Arguments dialog box.

r Type `False` in the **Range_lookup** box.

s Click **OK**.

- When you press **F4**, a "$" is added before each column or row reference. This makes the cell reference absolute.
- The values are in the second column in the worksheet, so you type `2` in the Col_index_num box. If the values were in the third column, you would type `3`.

Task 7. Use the VLOOKUP function to add a Limits column (continued)

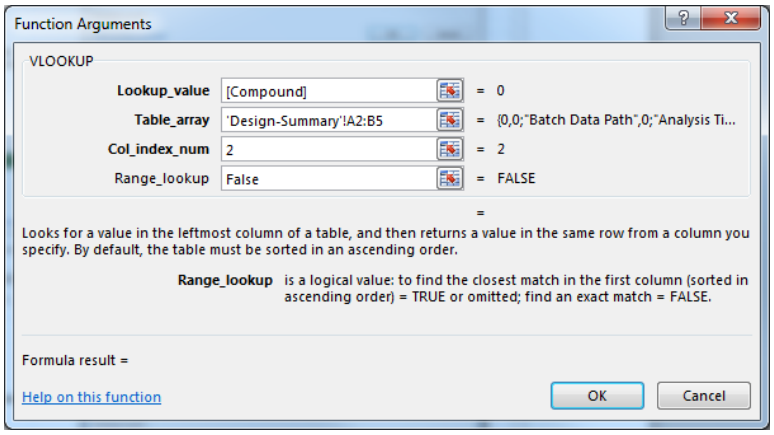
Step	Detailed instructions	Comments
		Select the area containing the compound names and limits. You do not include the column headers.

Figure 100 The Function Arguments dialog box for the VLOOKUP function

4 Add the second formula column to check if the Final Concentration is below the value in the Limits column. • If the value is below the limit, print the message **Below limit.** • Otherwise, print **Pass**.	**a** Click the **Final Conc** column in the same table. **b** Click **Add Data > Formula Column**. **c** Rename the column `Limit Check`. **d** Click the cell containing the words **Enter formula here**. **e** Click the **Formulas** tab in the Ribbon. **f** Click **Insert Function**. **g** In the select a category box, select **Logical**. **h** Select **IF** in the **Select a function** list. **i** Click **OK**. **j** Click the cell containing the value in the **Final Conc** column. **k** Type < **l** Click the cell containing the value in the **Limits** column. **m** Type `Below limit` in the **Value_if_true** box. **n** Type `Pass` in the **Value_if_false** box. **o** Click **OK**.	• See Task 6. Add a formula using the IF function for more information on adding a formula column using the IF function.

Task 7. Use the VLOOKUP function to add a Limits column (continued)

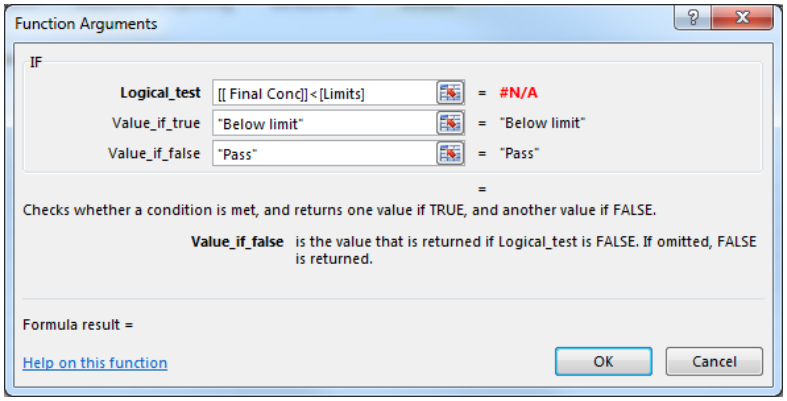
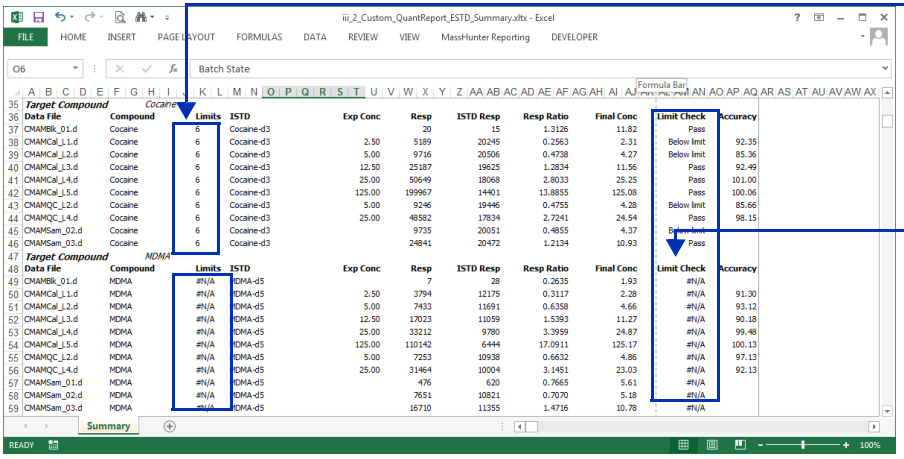
Step	Detailed instructions	Comments
		The quotation marks are automatically added when you leave the field.

Figure 101 Adding the formula to see if the Final Concentration is above the limits from the VLOOKUP function

5	Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Move to the **\MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuseDemo** folder. **d** Select **report.results.xml**. **e** Click **Open**. **f** Click **OK**. **g** Scroll to the **Quantitation Results** table. **h** Compare the results in the **Limits** column to the results in the **Final Conc** column and then check the **Limit Check** column.

Task 7. Use the VLOOKUP function to add a Limits column (continued)

Step	Detailed instructions	Comments



The **Limits** column contains the value from the Limits tab that was next to this Compound name.

The **Limit Check** column contains the word **Below Limit** if the Final Concentration is below the Limit. It contains the word **Pass** if the Final Concentration is not less than the Limit.

Figure 102 Two different formula columns were added to the Target Compound table

6 Save the changes to the template, **iii_3_Custom_QuantReport_ESTD_Summary.xlt.**

- You have to clear the results first.

a Click **Clear Results** in the **MassHunter Reporting** tab in the Ribbon.

b Click **File > Save As**.

c In the Save As dialog box, type iii_3_Custom_QuantReport_ESTD_Summary.

d Verify the folder selected in **Save in** is correct.

e Click **Save**.

- The **Save as type** is **Excel Template**.

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In This Book

This guide contains information on how to create reports using the Agilent MassHunter Workstation Qualitative Analysis program, the Agilent MassHunter Workstation Quantitative Analysis program, and how to modify templates using the Agilent MassHunter Workstation Software Report Designer add-in and Microsoft Excel.

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