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 Add-in.

Exercise 1 Creating Reports

In this exercise, you produce reports using the Qualitative Analysis program and the Quantitative Analysis program. In the Qualitative Analysis program, you select what sections to include in the reports. In the Quantitative Analysis program, you learn about the many different templates that are available.

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 and Task 7, you generate Quantitative Analysis reports.

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 74.
- Turn off any unneeded formatting options. See "Task 5. Change values on the Options worksheet" on page 135.
- 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 142.
- Print on a standalone system, if possible.
- If you are printing to a networked printer, set the Microsoft Image Writer as the default 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

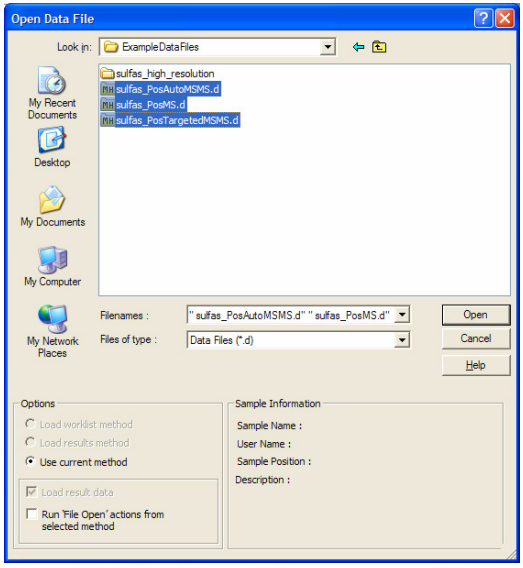
Steps	Detailed Instructions	Comments
1 Open the Qualitative Analysis program and open the data files, **sulfas-PosAutoMSMS**, **sulfas-PosMS.d** and **sulfas-PosTargetedMSMS.d** in the folder **\MassHunter\Data**, or in the folder where you copied them.	**a** Double-click the **Agilent MassHunter Qualitative 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, and 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.
• Make sure that **Use current method** is clicked. • Make sure that the check box for **Run 'File Open' actions from selected method** is clear.		

Figure 1 The Open Data File dialog box is automatically opened.

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

Steps	Detailed Instructions	Comments
	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 3 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.

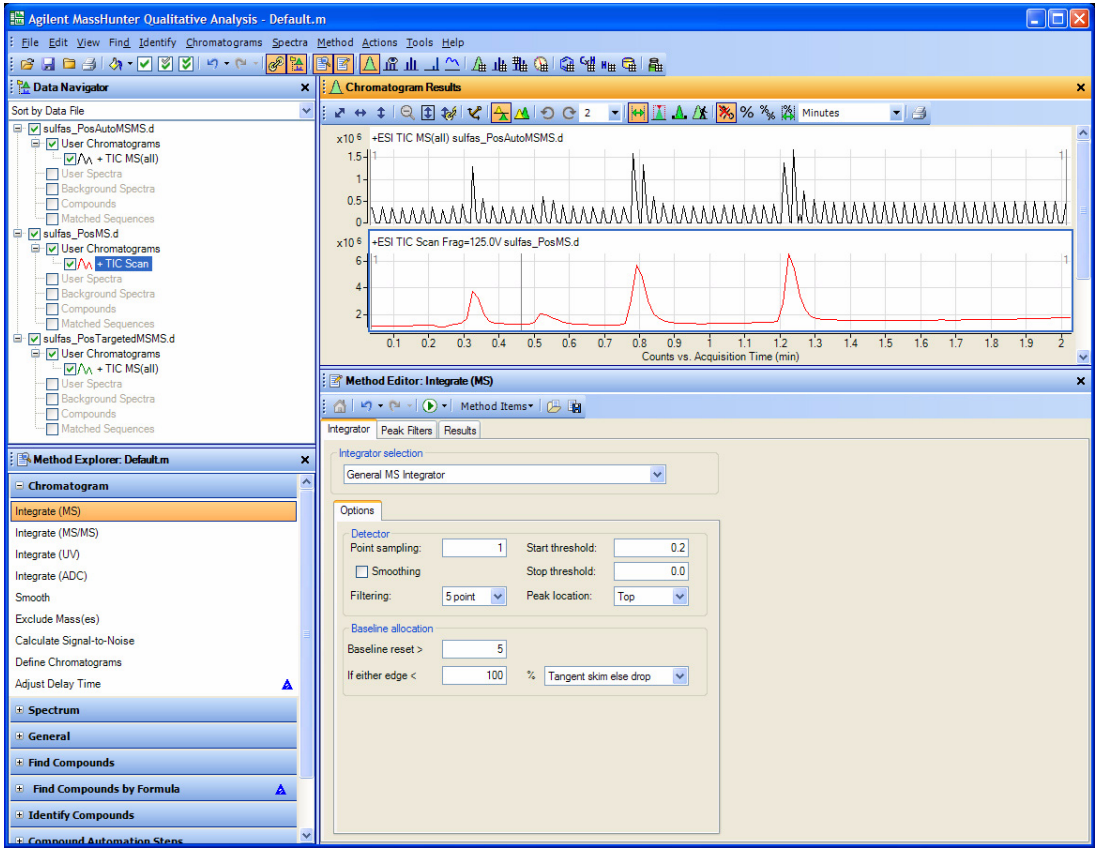
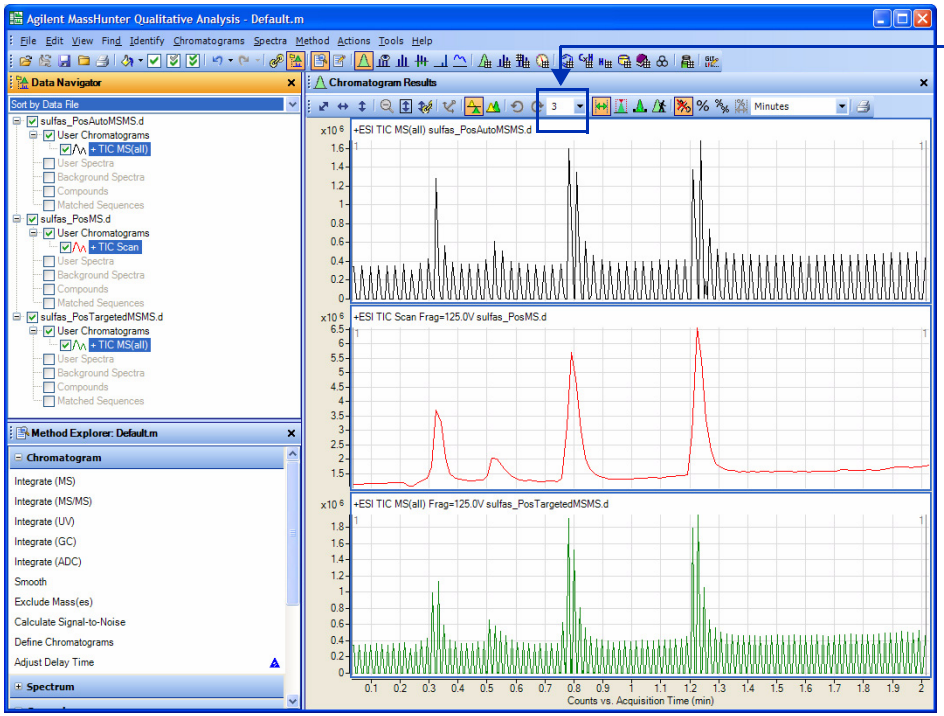


Figure 2 Qualitative Analysis main window

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

Steps	Detailed Instructions	Comments
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 **Tools > Configure for Workflow > General**. **b** Click the down arrow next to the **Maximum Number of List Panes** icon 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 the **View > Window Layouts > Load Layout** command.



Maximum Number of List Panes icon

The default method and layout are loaded.

To load the default display and plot settings, click Tools > Plot Display Options.

Figure 3 Qualitative Analysis main window with the General Workflow selected

Task 2. Print an analysis report

Whenever 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 **Tools > 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 **General > 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, then the peak 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 2. Print an analysis report (continued)

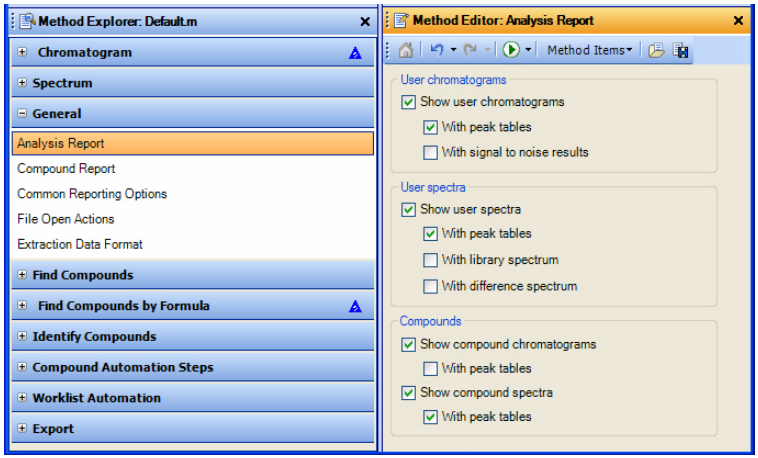
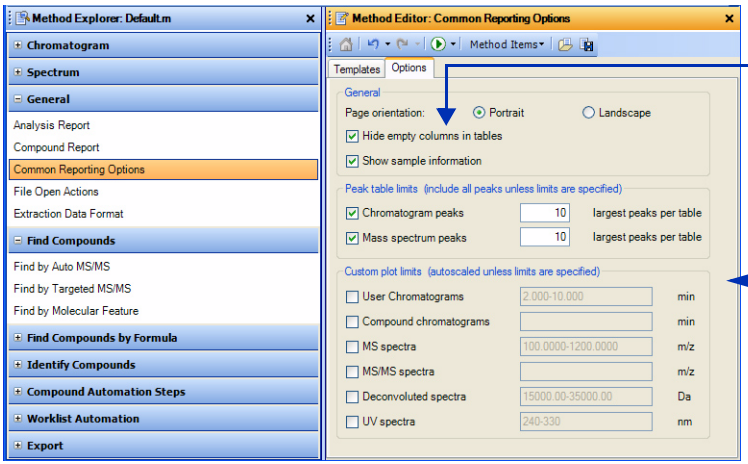
Steps	Detailed Instructions	Comments
		**Before printing the analysis report, you generate the results that you want to include. For example, if you want to include compound chromatograms, you need to run one of the Find Compounds algorithms.** **If you want to increase the speed of printing a report, remove any unnecessary graphics. Including graphics in a report slows down report generation.**
3 Select the template to use when printing this report.	**a** In Method Explorer, click **General > 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 that are 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 will print on A4 size paper. • Three different analysis report templates are available in each folder.

Figure 4 Analysis Report section in the Method Editor

Task 2. Print an analysis report (continued)

Steps	Detailed Instructions	Comments



Mark this check box if you do not want to include empty columns in any table in the report.

You can specify the plot limits to use in the report for each type of graphic.

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**.
  - From the data file shortcut menu in the Data Navigator, 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 General > 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. Please 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 **Tools > 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 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. **a** Click one of the commands in the **Find** menu to find compounds. **b** In Method Explorer, click **General > Compound Report**. **c** Mark the check boxes for any additional sections you want to print. **d** 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

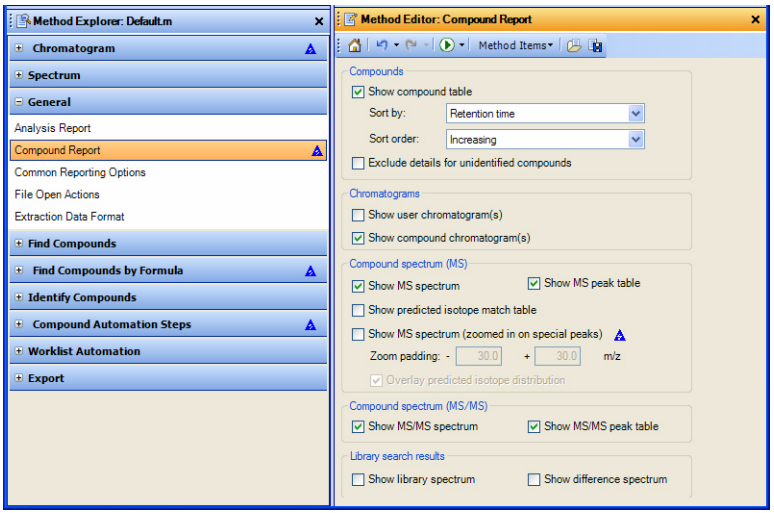
Step	Detailed Instructions	Comments
		**To increase the speed of creating a report, remove any unnecessary graphics. Including graphics in a report slows down the creation of reports.**

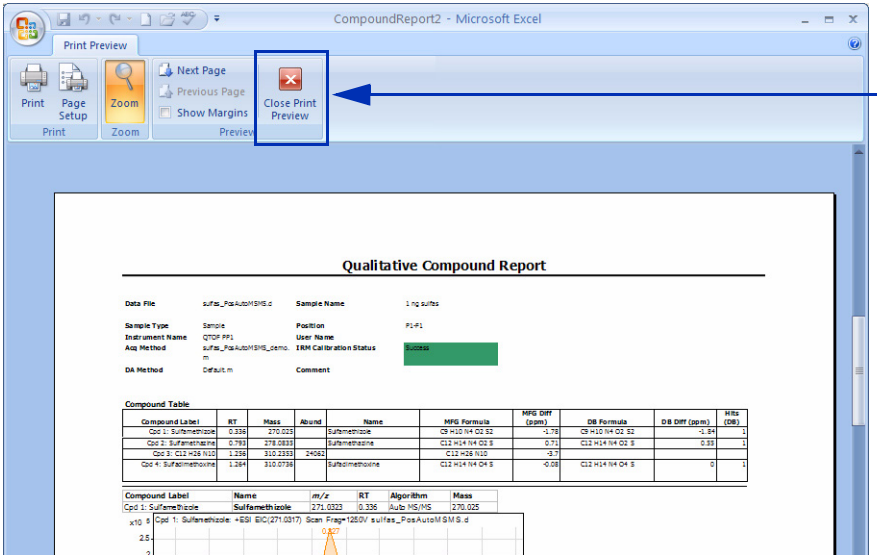
Figure 6 Compound Report tab in the Method Editor

3 Select the template to use when printing this report.	**a** In Method Explorer, click **General > Common Reporting Options**. **b** Verify that the correct **Report template folder** is selected. **c** Verify that the correct **Compound report template** is being used. **d** Click the **Options** tab. **e** Verify the settings on this tab.	• The report templates that are 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 will print on A4 size paper. • Several different compound report templates are available in each folder.

Task 3. Print a compound report

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, you select the printer to use 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 Analysis Report** in the **Actions** menu.
		• You can also 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.	**a** 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 **Tools > 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 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.xltx or graphicfullpage.xltx.	**a** In Method Explorer, click **General > Common Reporting Options**. **b** Verify that the correct **Report template folder** is selected.	• The report templates that are 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 will 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.xltx template is used.

Task 3. Print a graphics report

Step	Detailed Instructions	Comments

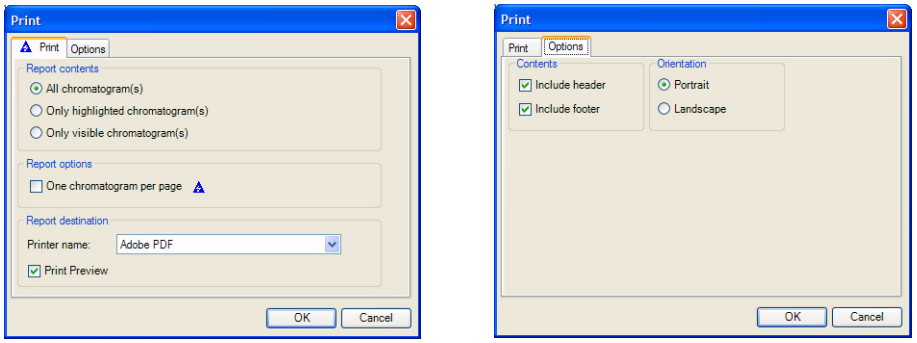
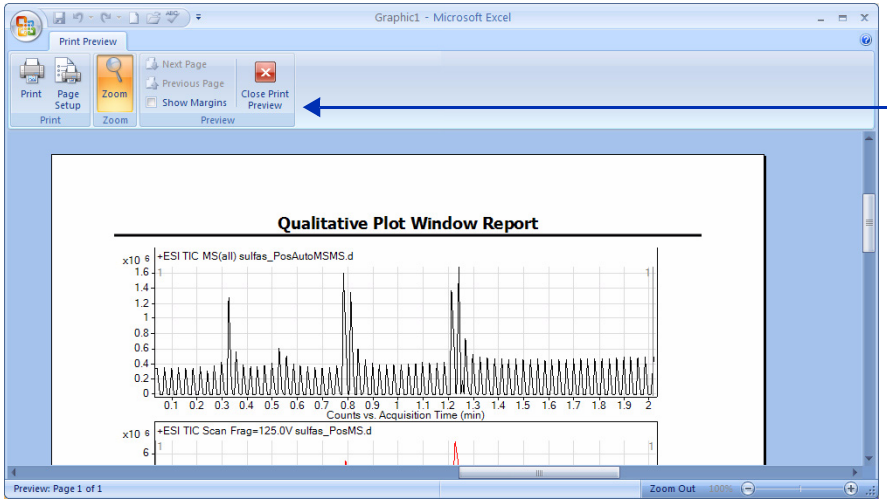


Figure 8 The Print and Options tab in the Print dialog box



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

Figure 9 The Print Preview window showing the Plot Window Report

4 Close the Print Preview window.

a 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 template that does not include a lot of graphics. Many templates are included with the Quantitative Analysis program. Some of these templates include graphics, and some do not. Reports that do not include graphics print more quickly. If possible, select a template that does not include graphics. 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 74.
- Turn off any unneeded formatting options. See "Task 5. Change values on the Options worksheet" on page 135.
- 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 142.
- Print on a standalone system, if possible.
- If you are printing to a networked printer, set the Microsoft Image Writer as the default 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** Navigate to the folder ***Your Directory*\DrugsOfAbuse\.** **d** Select a batch. You can select either DrugsOfAbuseDemo.batch.xml of ***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.

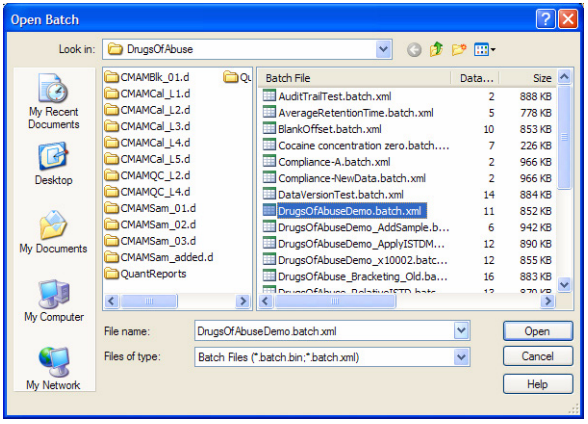


Figure 10 Open a batch file

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 2 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.

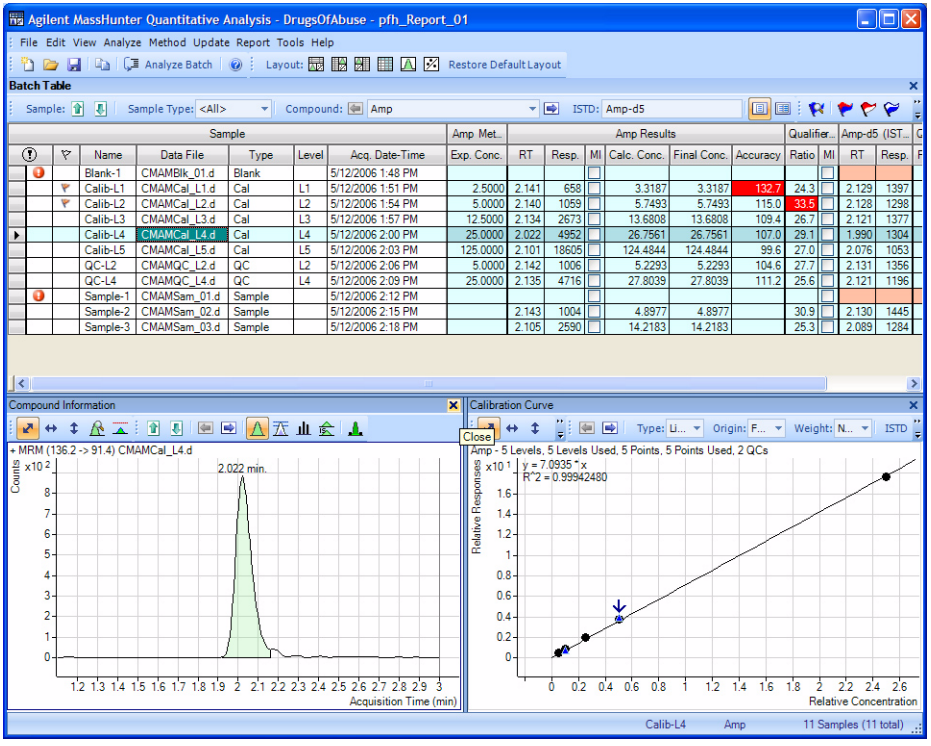


Figure 11 Quantitative Analysis program after analyzing batch

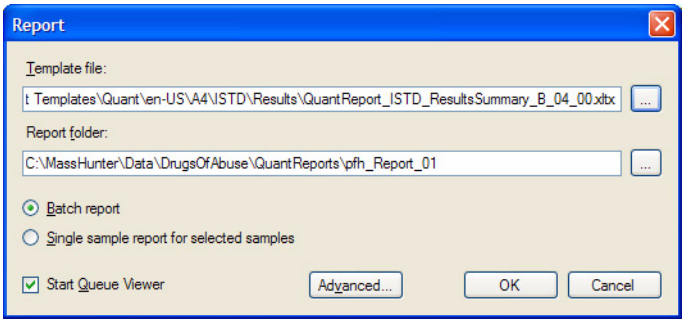
Task 6. Generate quantitation reports using the standard dialog box

In this task, you generate ISTD report using the one of the provided ISTD templates. You use the standard Report dialog box.

Task 6. Generate quantitation reports using the standard dialog box

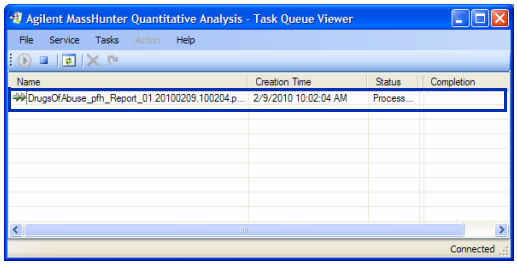
Steps	Detailed Instructions	Comments
1 If necessary, open the batch file ***iii*_Report_01.batch.xml**. • If the batch is already open, skip to step 2.	**a** To start the Quantitative Analysis program, click the **Quantitative Analysis (QQQ)** icon on your Desktop. **b** Click **Open Batch** on the toolbar to display the Open Batch dialog box. **c** Navigate to ***Your Directory*****DrugsOfAbuse** and select ***iii*_Test_01.batch.xml.** **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 options. • The first template is **Quantreport_ISTD_ResultsSummary_B_04_00.xltx** • The Reports folder should be ***Your Directory****DrugsofAbuse****QuantReports**. • The default filename is ***iii*_Test_01**, where "*iii*" are your initials.	**a** Click **Report > Generate**. The system displays the standard Report dialog box. **b** Click ... . **c** Navigate to the **Letter****ISTD****Results** folder. **d** Select **Quantreport_ISTD_ResultsSummary_B_04_00.xltx** and click **Open**. The program adds the template to the **Template file** field in the Reports pane. **e** Specify the default destination directory for saving Excel reports in the **Report folder** text box; for example, ***Your Directory*****DrugsOfAbuse****QuantReports*****iii*_Test_01**. **f** Mark the **Start Queue Viewer** check box. **g** Click the **Batch report** button.	• You can only add one report at a time using the standard Report dialog box. • The report is automatically printed to the default printer.

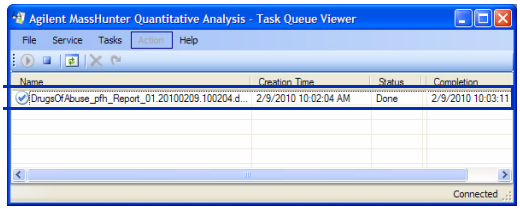
Task 6. Generate quantitation reports using the standard dialog box

Steps	Detailed Instructions	Comments
		
3 Generate the report. • View the status of the report generation in the Task Queue Viewer.	**a** Click **OK** in the Report dialog box to generate the report. **b** Click **Report > Queue Viewer** to monitor the report generation process. The system displays the Task Queue Viewer program. **c** Watch the progress of the report in the Status column.	• One job is added to the queue. The reports are printed in the order requested. You can see the status of the reports in the Queue Viewer program.

Task 6. Generate quantitation reports using the standard dialog box

Steps	Detailed Instructions	Comments





When the Status column changes to "Done", the report is finished.

d Close the **Task Queue Viewer** program.

Task 7. Generate quantitation reports using the advanced Report dialog boxes

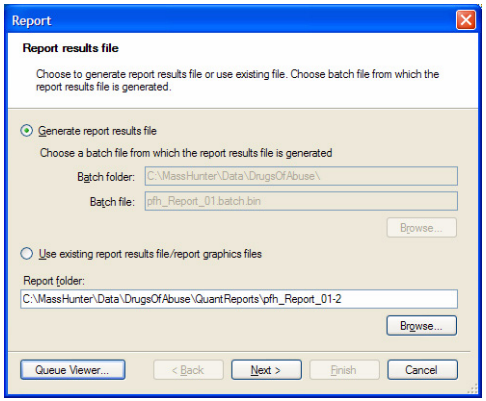
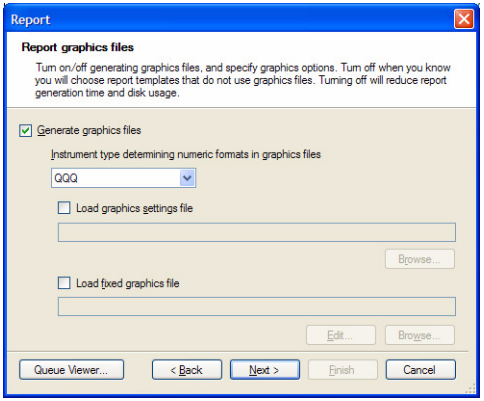
In this task, you generate ISTD and compound reports using the corresponding templates. You use the advanced Report dialog boxes. You use the advanced Report dialog boxes if you want to do any of the following:

- Specify a different printer than the default printer.
- Re-use existing graphics files.
- Specify a different numeric format for graphics than the default format.
- Create a separate report for each sample.
- Include only some of the samples in the report.
- Include only some of the compounds in the report.

Task 7. Generate quantitation reports using the advanced Report dialog boxes

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** Navigate to ***Your Directory*****DrugsOfAbuse** and select ***iii*_Test_01.batch.xml.** **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 Start to generate a report using the advanced Report dialog boxes. • The destination directory should be ***Your Directory*****DrugsofAbuse****QuantReports**. • The default filename is ***iii*_Test_01**, where "*iii*" are your initials.	**a** Click **Report > Generate**. The system displays the standard Report dialog box. **b** Click **Advanced**. **c** Click **Generate report results file**.	• If you want to generate a new report using existing report results and graphics files, you click **Use existing report results file/report graphics file**. • You can also specify the **Instrument Type determining numeric formats in graphics files**. This value is used to determine how many decimal places to show in the graphics.

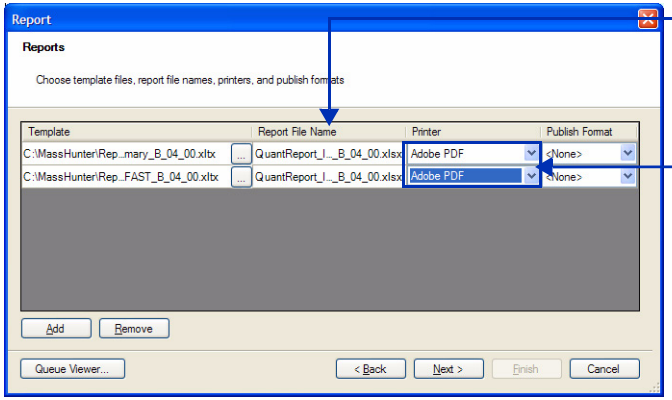
Task 7. Generate quantitation reports using the advanced Report dialog boxes

Steps	Detailed Instructions	Comments
		
3 Select the instrument type to use when generating the report. • The DrugsOfAbuse batch was generated on a Triple Quadrupole instrument. You select QQQ for this batch.	**a** Mark Generate graphics files. **b** Select **QQQ** for the Instrument type determining numeric formats in graphics files. **c** Click **Next**.	• If you mark the **Load graphics settings file** check box, you can load the graphics settings file that you saved in the Quantitative Analysis program. • You can also load a Fixed Graphics File. This file includes limits to use for the X and Y axis for the report. You can set different limits for different compounds.
		

Task 7. Generate quantitation reports using the advanced Report dialog boxes

Steps	Detailed Instructions	Comments

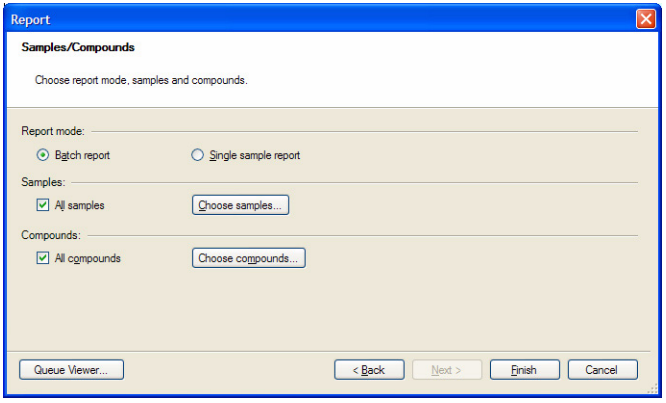
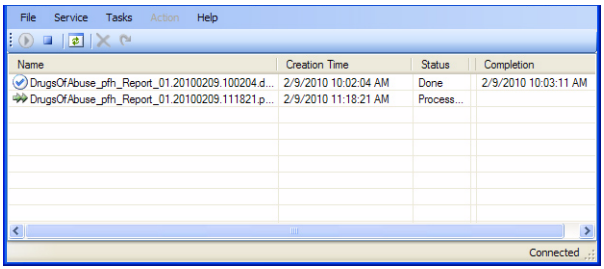
4 Add two templates.
• The first template is **Quantreport_ISTD_ResultsSummary_B_04_00.xltx**
• The second template is **QuantReport_ISTD_ResultsByCompound_FAST_B_04_00.xltx.**
• Make sure the report name is *TemplateName*.xlsx, where *TemplateName* is the exact name of the template.
	a Click **Add** under Reports. The system displays the Open dialog box.
	b Navigate to the **Letter\ISTD\Results** folder.
	c Select **Quantreport_ISTD_ResultsSummary_B_03_01.xltx** and click **Open**. The program adds the template to the Template field in the Reports pane.
	d In the Report File Name column in the Reports table, verify that the template is **QuantReport_ISTD_Results_B_03_01.xlsx**.
	e Select a printer for this report.
	f Click **Add** under Reports. The system displays the Open dialog box.
	g Select **Quantreport_ISTD_ResultsByCompound_FAST_B_04_00.xltx.** Click **Open**.
	h Verify that the template is **QuantReport_ISTD_Results_B_03_01.xlsx**.
	i Select a printer for this report.
	j Click **Next**.
		• Note that the **B_03_01** designation corresponds to the Quantitative Analysis software release, which will change over time. Therefore, the report file names may change correspondingly.
		• If you want to print to A4 paper, navigate to the A4 folder.
		• Templates are separated into the following folders:
		  • ESTD
		  • ISTD
		  • LIMs
		  • Method
		  • misc
		  • Outliers - this folder contains several folders for the different types of outliers.
		  • UnknownsAnalysis



The Report File Name is filled in automatically.

You select a printer for each template.

Task 7. Generate quantitation reports using the advanced Report dialog boxes

Steps	Detailed Instructions	Comments
5 Specify which samples and compounds to include in the report. • Select the **Batch report** option. • Select All samples. • Select All compounds.	**a** Click **Batch report**. **b** Mark **All samples**. **c** Mark **All compounds**.	• You can create a separate report for each sample by clicking **Single sample report**.
		**You can choose to print only some of the samples or some of the compounds. If you mark either of the check boxes, the appropriate dialog box is displayed to let you choose the samples or compounds to include.**
6 Generate the reports. • View the status of the report generation in the Task Queue Viewer.	**a** Click **Finish** in the Report dialog box to generate the report. **b** Click **Report > Queue Viewer** to monitor the report generation process. The system displays the Task Queue Viewer program. **c** Watch the progress of the report in the **Status** column.	• Only one job is added to the queue which will print both reports. The reports are printed in the order requested. You can see the status of the reports in the Queue Viewer program.
	 **d** Close the **Task Queue Viewer** program.	

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.xltx file and rename the file **iii_CustomAnalysisReport.xltx**	**a** Open the Windows Explorer program. **b** Navigate to the *Report Templates*\ *Qual* folder in the folder where you installed the data. **c** Navigate to the *Letter* or *A4* folder **d** Right-click the *AnalysisReport.xltx* 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, **Copy of AnalysisReport.xltx** and click **Rename**. **g** Type *iii_CustomAnalysisReport.xltx*.	• You do the same steps to open a Quantitative Analysis template. • You can (and should) change the name of the template that you modify. However, you cannot change the name of the graphics templates in the Qualitative Analysis program. Instead, you need to make a backup of the template and open the original template. When you have finished editing the template, you also save a copy of the changed template.
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.

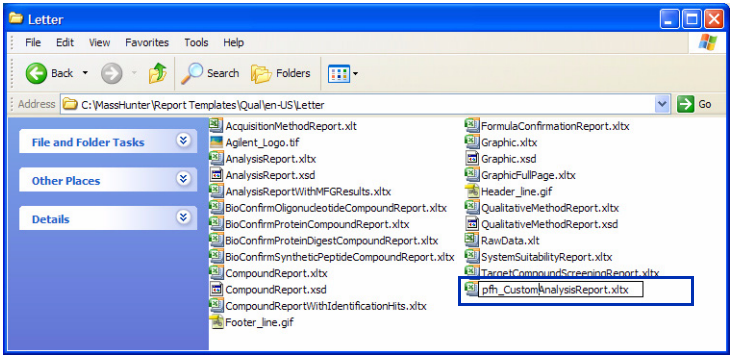


Figure 12 Report Templates\Qual\Letter folder

Task 1. Open a Qualitative Analysis template

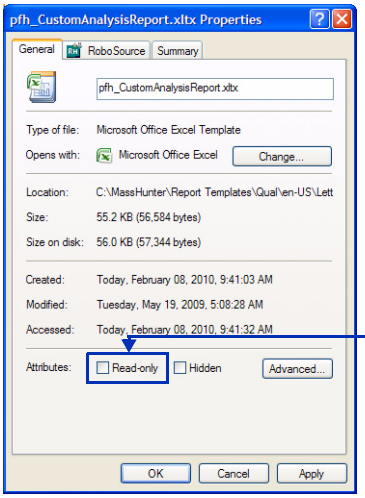
Step	Detailed Instructions	Comments
		**Clear the Read-only check box.**
3 Open the template.	• Right-click the new file and click **Open**.	

Figure 13 Properties dialog box

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 the task, "Task 1. Open a Qualitative Analysis template" on page 32.

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.	**a** 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 on any of these sections to edit that part.

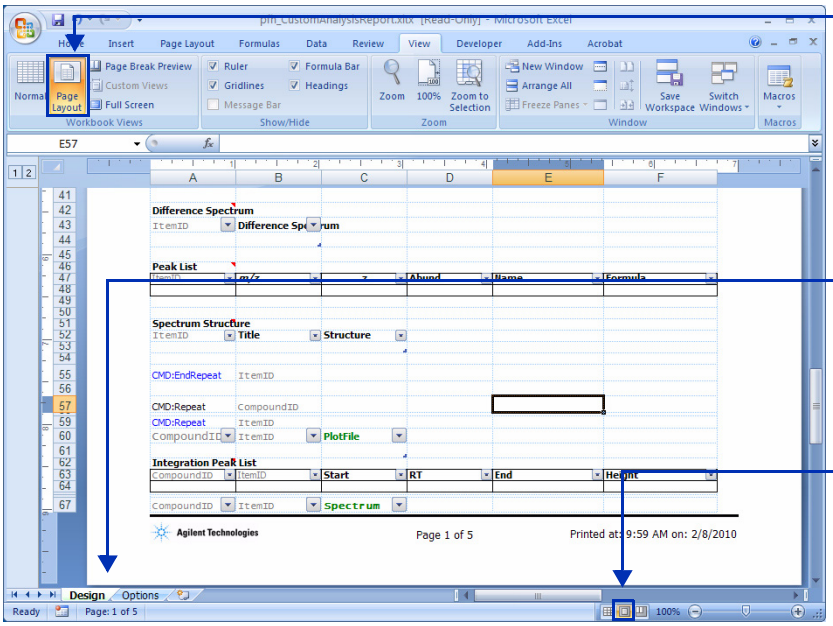
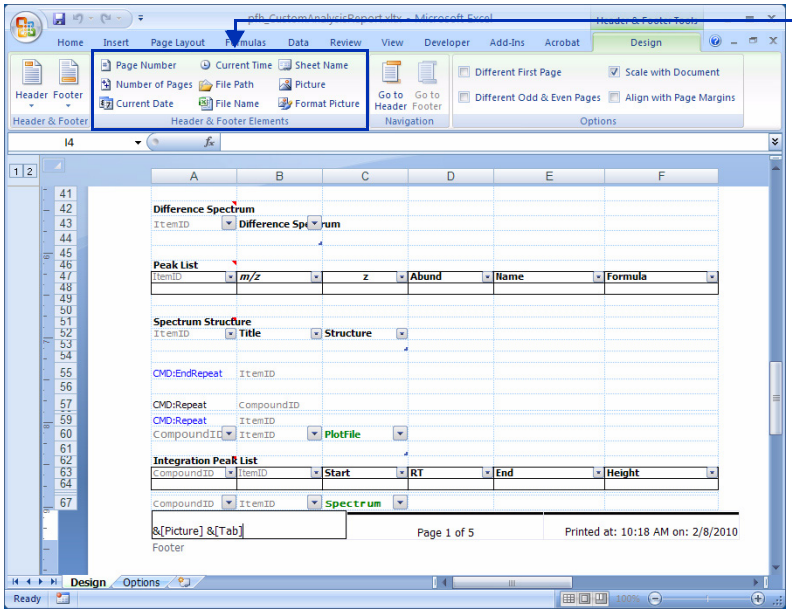


Figure 14 Switching to the Page Layout view in Excel

Task 2. Customize the footer of the Qualitative Analysis template

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** Click at the end of this text to add something to this section. **d** Type a space. **e** 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 on 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. In the task "Task 1. Add a page break and a sheet break" on page 118, you will learn how to change the sheet name.

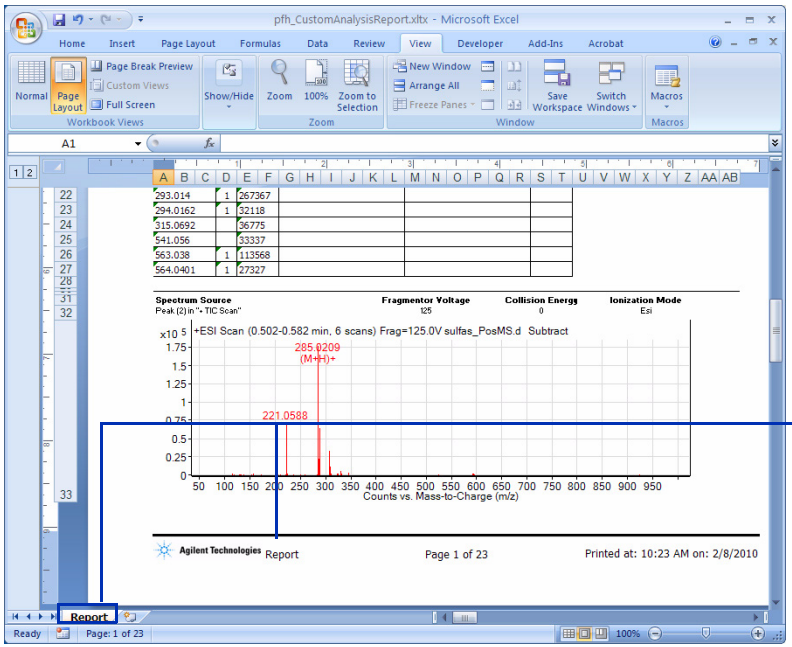
Figure 15 The Header and Footer Design Tab in Excel

Task 2. Customize the footer of the Qualitative Analysis template

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 **Add-Ins** tab. **b** Click **Process Report**. **c** Click the **Browse** button. **d** Navigate 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** 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 Add-Ins 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

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 Add-Ins tab in the Ribbon.

b Click the **Microsoft Office Button** and then click **Save**.

c (optional) To save to a different template name, click **Save As** and click **Other Formats**.

d In the Save As dialog box, type a new **File name**,

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

f Click **Save**.

- You can click **Save As > Other Formats** if you want to change the name of the template.
- The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**.
- If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *\MassHunter\Report Templates\Qual\en-US\Letter* folder.

Task 2. Customize the footer of the Qualitative Analysis template

Step	Detailed Instructions	Comments

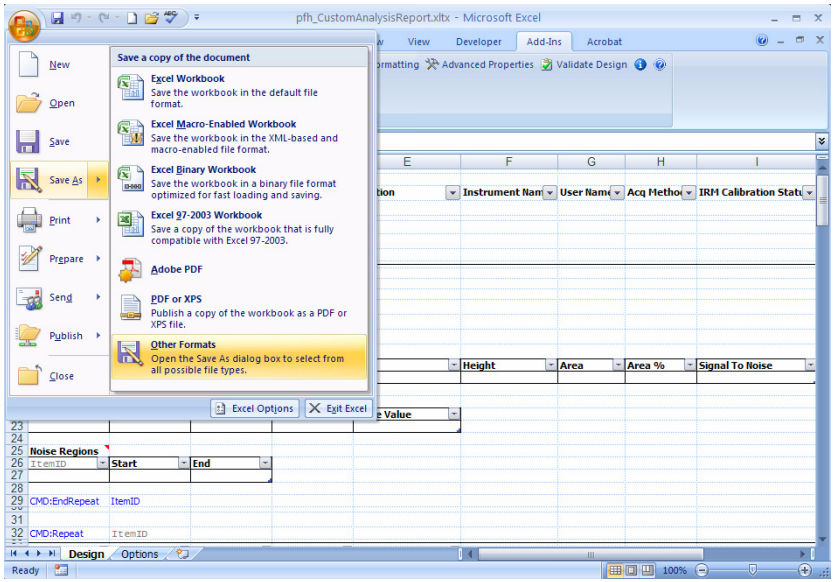


Figure 17 The Save As menu in the Microsoft Office button menu

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 **General > Common Reporting Options**. **b** Select the template ***iii*_CustomAnalysisReport.xltx** 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

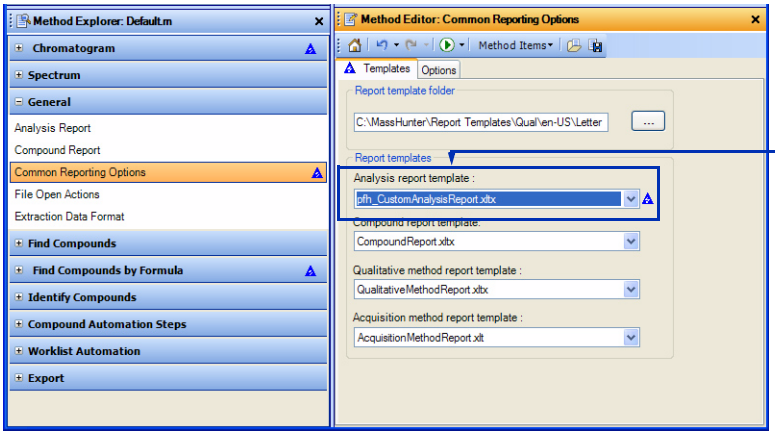
Steps	Detailed Instructions	Comments
		**You select the new report template for the Analysis report here.**

Figure 18 Analysis Report section in the Method Editor

3 Select the template to use when printing this report.	**a** In Method Explorer, click **General > 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 that are 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 will 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

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. ◦ 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**. ◦ From the data file shortcut menu in the Data Navigator, 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 General > 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 4. Open a Quantitative Analysis template

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

Task 4. Open a Quantitative Analysis template

Step	Detailed Instructions	Comments
1 Make a copy of the QuantReport_ISTD_Summary_*B_04_00*.xltx file and rename the file **iii_Custom_ISTD_Summary.xltx**	**a** Open the Windows Explorer program **b** Open the *Report Templates\Quant\en-US* folder in the folder where you installed the data. **c** Navigate to the *Letter* or *A4* folder. **d** Navigate to the *ISTD/Parts* folder. **e** Right-click the *QuantReport_ISTD_Summary_B_04_00.xltx* 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, *Copy of QuantReport_ISTD_Summary_B_04_00.xltx*, and click **Rename**. **h** Type *iii_Custom_ISTD_Summary.xltx*.	• 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*.
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.

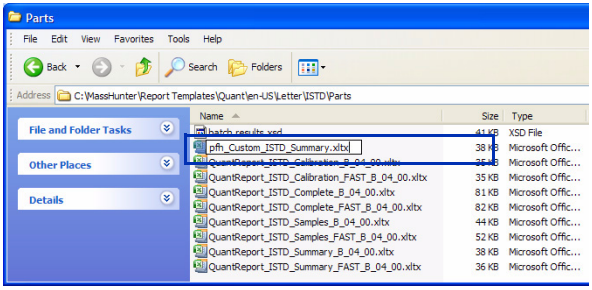


Figure 19 MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Parts folder

Task 4. Open a Quantitative Analysis template

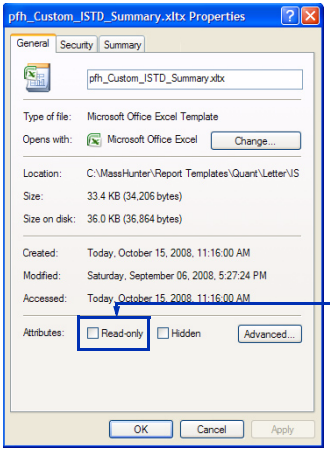
Step	Detailed Instructions	Comments
		Clear the **Read-only** check box. This check box may already be clear.
3 Open the template.	• Right-click the new file and click **Open**.	

Figure 20 Properties dialog box

Task 5. Customize the footer of the Quantitative Analysis template

In this task, you change the footer of the Quantitative Analysis template that you opened in the task, "Task 4. Open a Quantitative Analysis template" on page 42.

Task 5. Change the footer of the Quantitative Analysis template

Step	Detailed Instructions	Comments
1 Switch to the Page Layout view.	**a** 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 on any of these sections to edit that part.

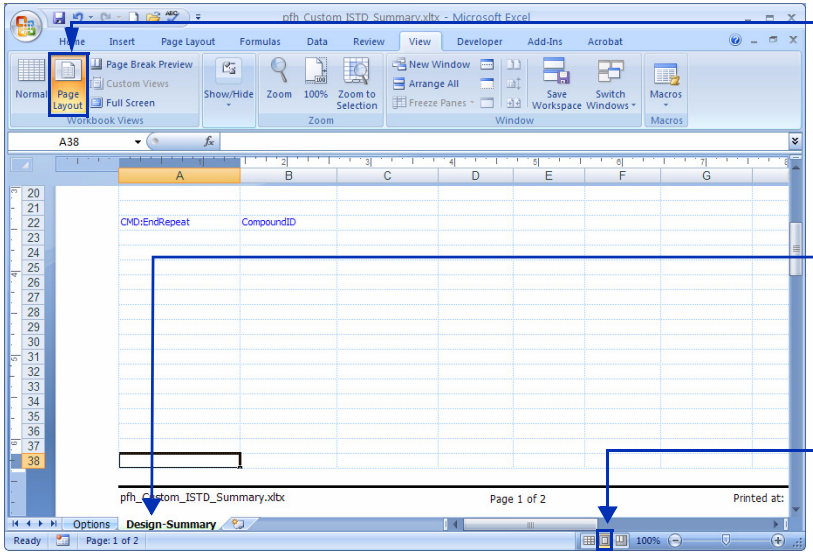
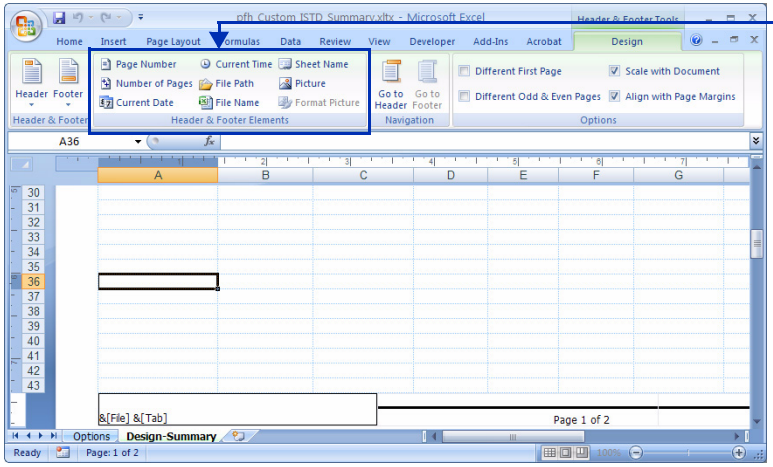


Figure 21 Switching to the Page Layout view in Excel

Task 5. Change the footer of the Quantitative Analysis template

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 **&[File]**. **c** Click at the end of this text to add something to this section. **d** Type a space. **e** 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 on one of the sections in the header or footer. You can click these buttons to quickly add these items to the header or footer.

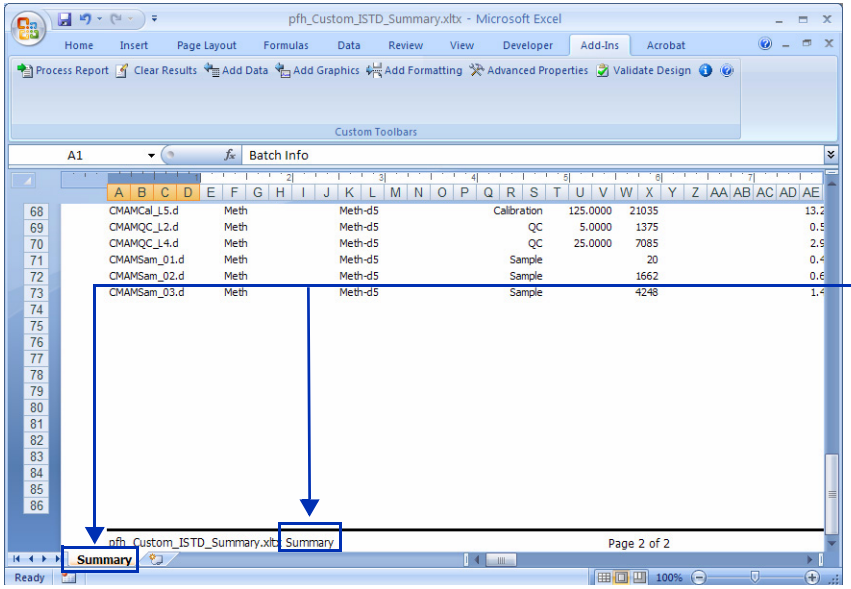
By default, the worksheet name in the template is Design-Summary. The worksheet name in the report is Summary. In a different exercise, you will learn how to change the worksheet name.

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 template

Step	Detailed Instructions	Comments
4 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Navigate to the *DrugsOfAbuse**QuantReports**DrugsOfAbuseDemo* folder. **d** Select *report.results.xml*. **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 Add-Ins 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 template

Step	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 Add-Ins tab in the Ribbon. **b** Click the **Microsoft Office Button** and then click **Save**. **c** (optional) To save to a different template name, click **Save As** and click **Other Formats**. **d** In the Save As dialog box, type a new **File name**, **e** Verify the folder selected in **Save in** is correct. **f** Click **Save**.	• You can click **Save As > Other Formats** if you want to change the name of the template. • The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**. • If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Parts* folder.

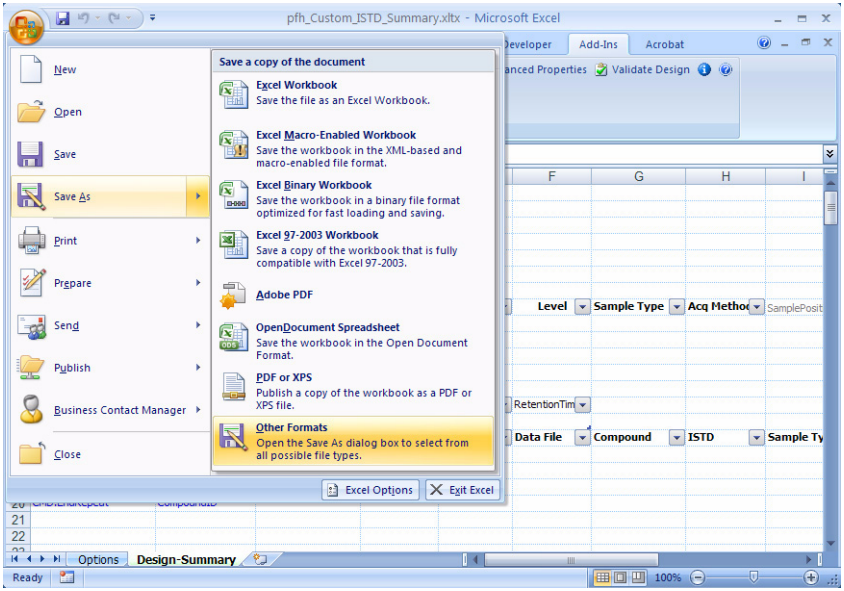


Figure 24 The Save As menu in the Microsoft Office button menu

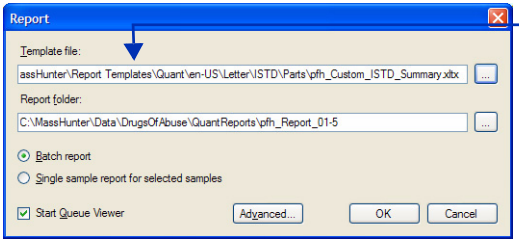
Task 6. Use the new template in the Quantitative Analysis program

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

Task 6. Use the new 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 22.	• If the Quantitative Analysis program is already running, you do not need to restart the program.
2 Open the Report dialog box. • Verify the default destination directory for reports is \ ***Your Directory*** \ **DrugsofAbuse** \ **QuantReports**. • The default filename is ***iii*_Test_01**, where "*iii*" are your initials.	**a** Click **Report > Generate**. The system displays the standard Report dialog box. **b** Click ... . **c** Specify the default destination directory for saving Excel reports in the **Report folder** text box; for example, \ ***Your Directory*** \ **DrugsOfAbuse** \ **QuantReports** \ ***iii*_Test_01**. **d** Mark the **Start Queue Viewer** check box. **e** Click the **Batch report** button. **f** Specify the default destination directory for saving Excel reports in the **Report Folder** text box; for example, \ ***Your Directory*** \ **DrugsOfAbuse** \ **QuantReports** \ ***iii*_Test_01**.	• You can also specify the **Instrument Type determining numeric formats in graphics files**. This value is used to determine how many decimal places to show in the graphics.

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

Steps	Detailed Instructions	Comments
3 Select the report template to use. • Add the template, iii_Custom_ISTD_Summary.xltx. • Make sure the report name is *iii_Custom_ISTD_Summary*.xls. By default, it is set to the name of the template.	**a** Click **Add** under Reports. The system displays the Open dialog box. **b** Navigate to the **Letter\ISTD** folder. **c** Select **iii_Custom_ISTD_Summary.xltx** and click **Open**. The program adds the template to the Template field in the Reports pane. **d** In the Report File Name column in the Reports table, verify that the template is **iii_Custom_ISTD_Summary.xltx**. **e** Mark the **Start Queue Viewer** check box.	• Click the **Advanced** button if you want to use the advanced Report dialog boxes. You use the Advanced Report dialog boxes if you want to do any of the following: • Specify a different printer than the default printer • Re-use existing graphics files • Specify a different numeric format for graphics than the default format. • Create a separate report for each sample. • Include only some of the samples in the report. • Include only some of the compounds in the report.
	**The new template is shown here.** **The default printer is used when you use the standard Report dialog boxes.**	
4 Generate the report. • View the status of the report generation in the Task Queue Viewer.	**a** Click **OK** in the Report dialog box to generate the report. **b** Click **Report > Queue Viewer** to monitor the report generation process. The system displays the Task Queue Viewer program. **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:

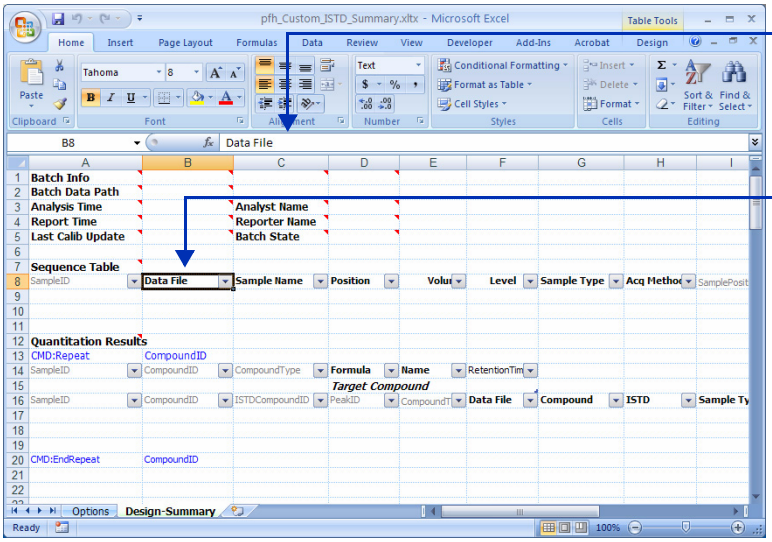
- Steps – Use these general instructions to proceed on your own to explore the program.
- Detailed Instructions – Use these if you need help or prefer to use a step-by-step learning process.
- Comments – Read these to learn tips and additional information about each step in the exercise.

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\ *iii*_Custom_ISTD_Summary.xltx template, where "*iii*" are your initials.	• Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, iii_Custom_ISTD_Summary.xltx, 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 on 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 on 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 25 Selecting the **Data File** cell in Excel

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

Step	Detailed Instructions	Comments
	c Type `Acquisition File`. You can also click in the Formula Bar to only overwrite 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.

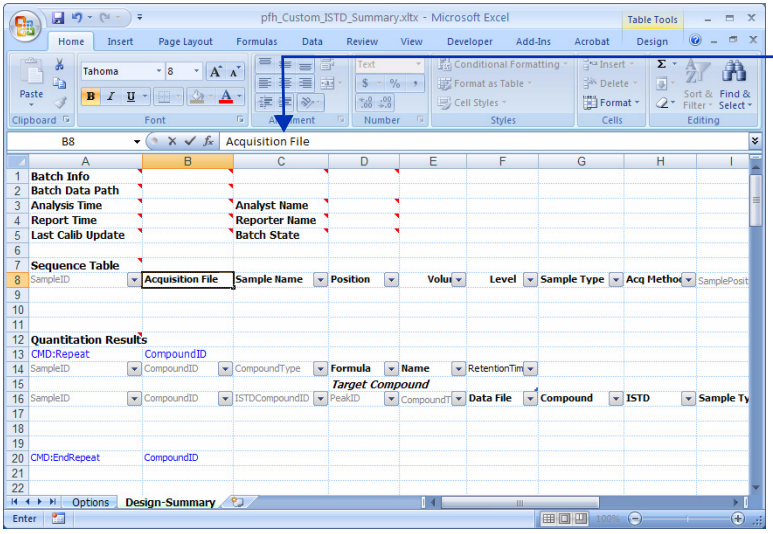
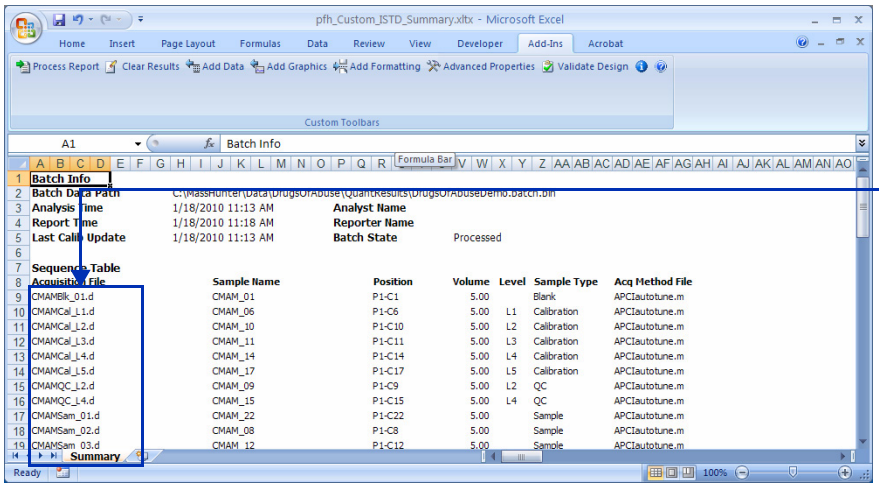


Figure 26 Changing the header of the column to **Acquisition File**

3 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Navigate to the *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 called **Acquisition File**.	• The Process Report command is part of the MassHunter toolbar in the Add-Ins 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

Step	Detailed Instructions	Comments



The column header is now Acquisition File.

Figure 27 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.xltx.

a Click **Clear Results** in the Add-Ins 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_Custom_ISTD_Summary.xltx`.

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

e Click **Save**.

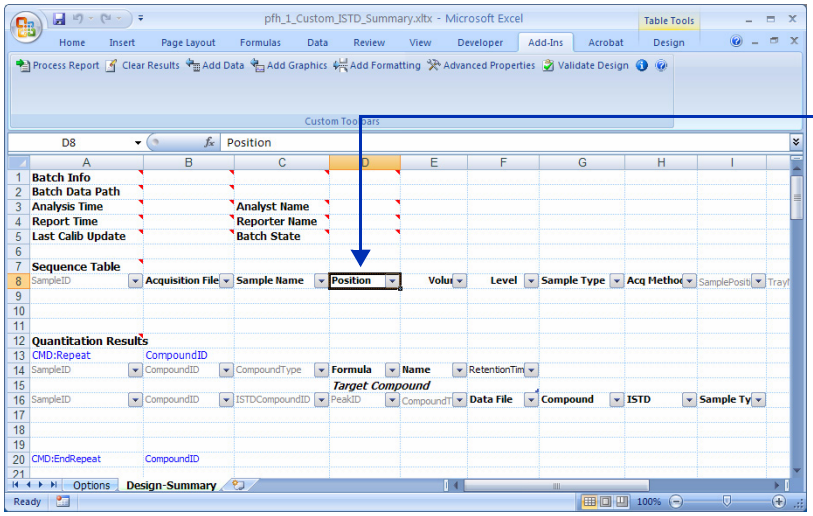
- The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**.
- If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Parts* folder.

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\Letter\ISTD\ *iii*_1_Custom_ISTD_Summary.xltx.	• Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, iii_1_Custom_ISTD_Summary.xltx, 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 on the cell containing the words **Position**. This column is the fourth column in the table.	

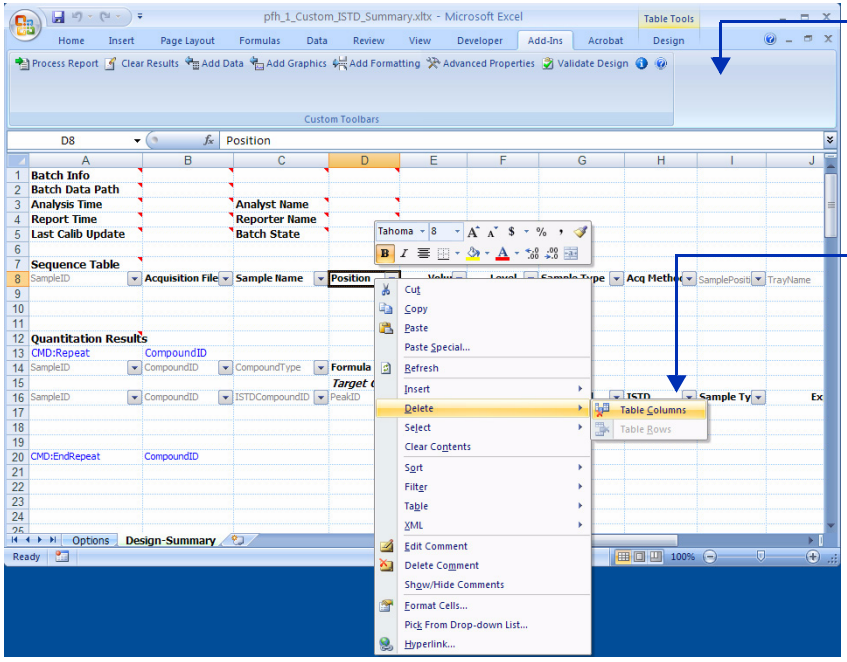


Click on this cell in the Sequence Table.

Figure 28 Selecting the **Position** cell in Excel

Task 2. Delete a column from a Quantitative Analysis table

Step	Detailed Instructions	Comments
	c Right-click this cell and click **Delete > Table Columns**.	• You cannot 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.



You can also click Delete > Table Columns in the Cells group in the Home tab in the Ribbon.

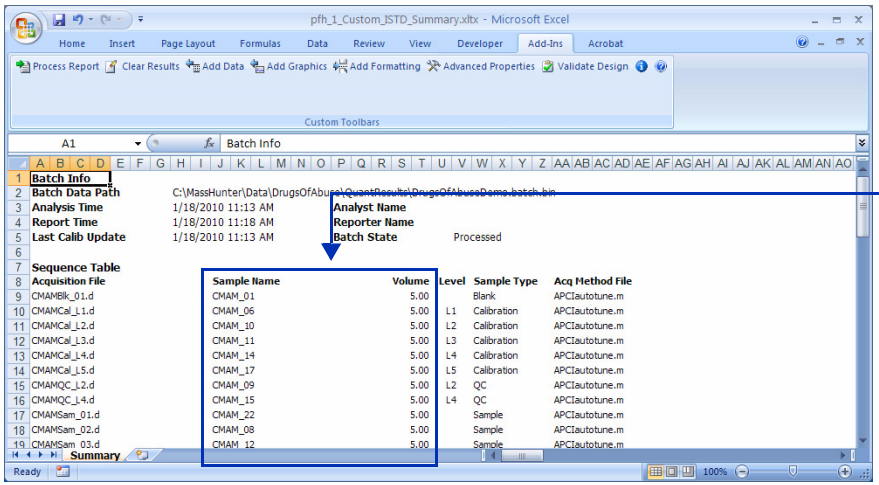
In the shortcut menu, click the command Delete > Table Columns.

Figure 29 Deleting the **Position** column

3 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Navigate to the *DrugsOfAbuse**QuantReports**DrugsOfAbuse* folder. **d** Select *report.results.xml*. **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 Add-Ins tab in the Ribbon.

Task 2. Delete a column from a Quantitative Analysis table

Step	Detailed Instructions	Comments



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

Figure 30 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.xltx.

a Click **Clear Results** in the Add-Ins 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_Custom_ISTD_Summary.xltx.

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

e Click **Save**.

- The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**.
- If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Parts* folder.

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 \MassHunter\Report Templates\Quant\Letter\ISTD\ *iii*_2_Custom_ISTD_Summary.xltx.	• Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, iii_2_Custom_ISTD_Summary.xltx, 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 on the cell containing the word **Level**. This column is the fifth column in the table.	

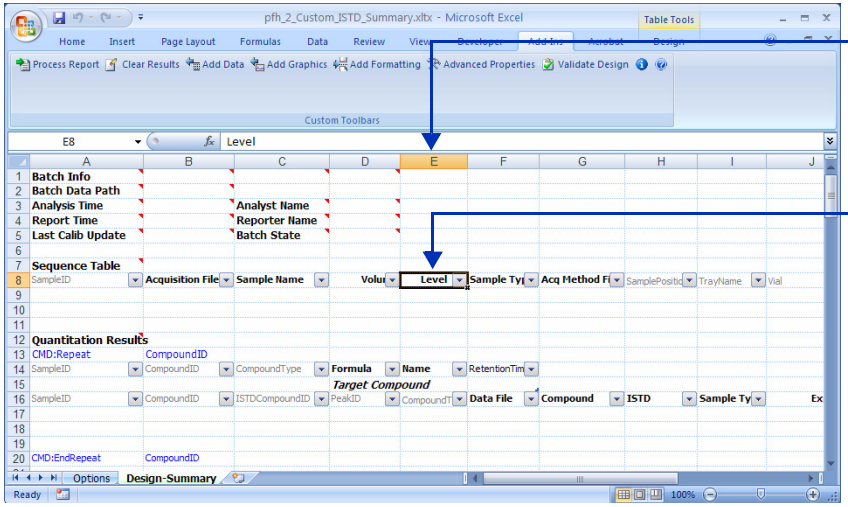
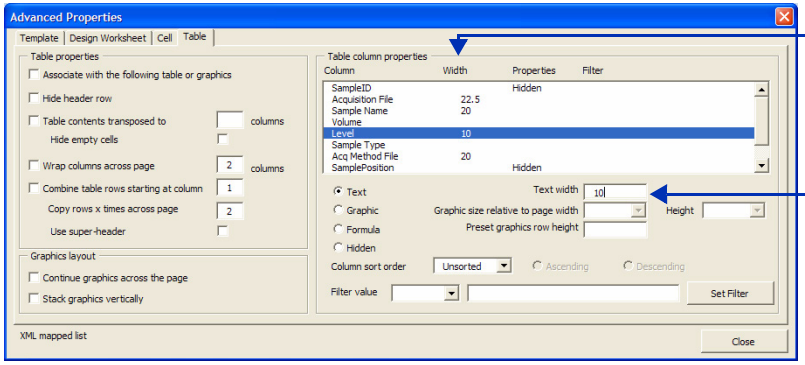


Figure 31 Selecting the **Level** column in Excel

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

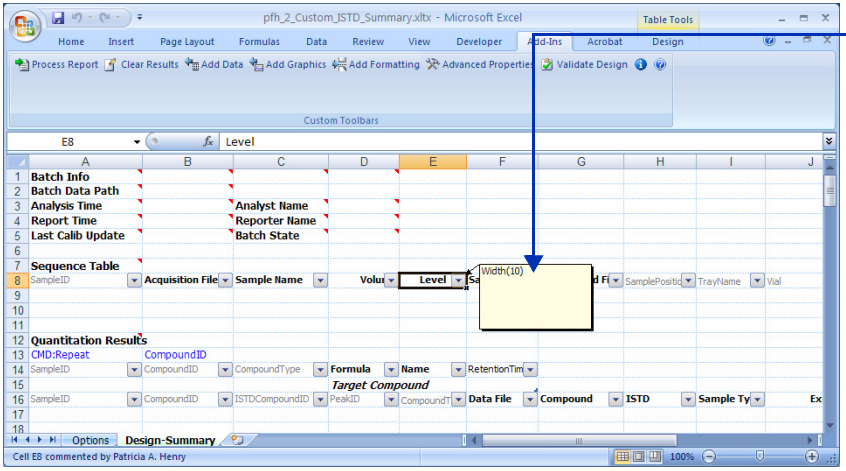
Step	Detailed Instructions	Comments
	c Click **Advanced Properties** in the Add-Ins tab in the Ribbon. **d** Type `10` in the **Text width** box. **e** Click **Close**. **f** Move the cursor over the **Level** column header to see the comment that has been added to this column.	• The Advanced Properties 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 32 Changing the width of the Level column



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 33 A **Width** comment has been added to the Level column

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

Step	Detailed Instructions	Comments
3 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Navigate to the *DrugsOfAbuse*\ *QuantReports**DrugsOfAbuseDemo* folder. **d** Select *report.results.xml*. **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 Add-Ins tab in the Ribbon.

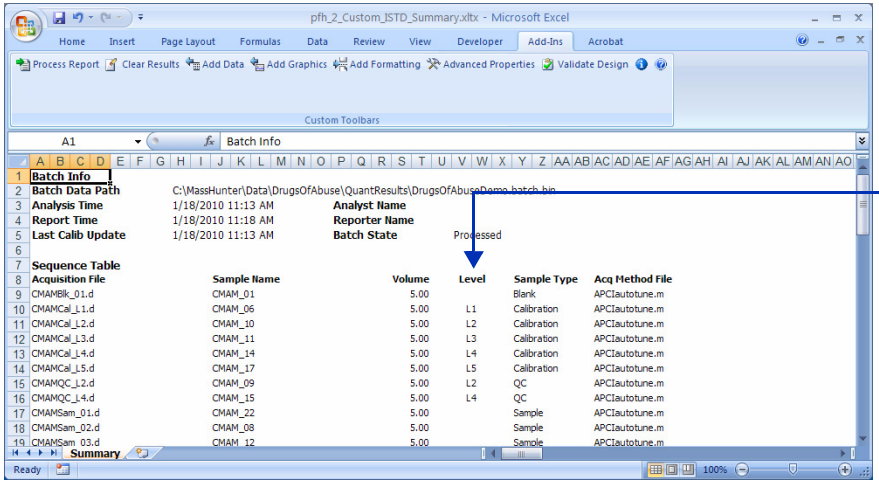


Figure 34 Verifying changes in the width of the column after using the Process Report command

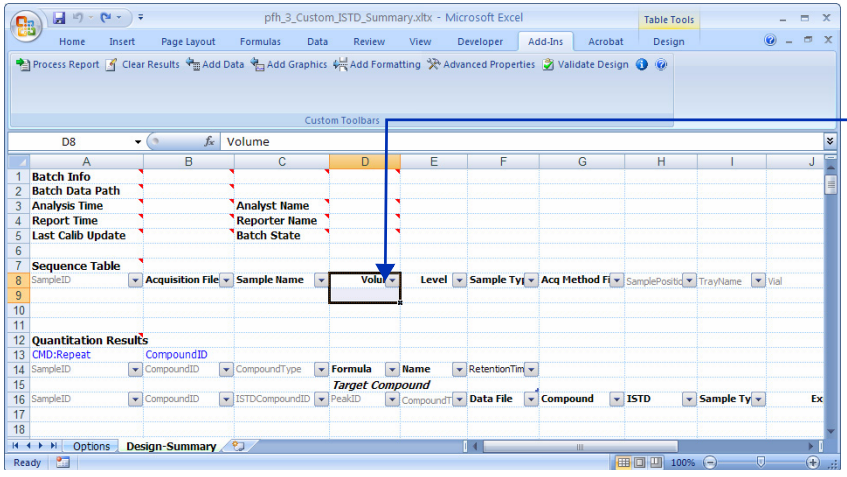
4 Save the changes to the template *iii*_3_Custom_ISTD_Summary.xltx. • You have to clear the results first.	**a** Click **Clear Results** in the Add-Ins tab in the Ribbon. **b** Click the **Microsoft Office Button** and then click **Save As** and click **Other Formats**. **c** In the Save As dialog box, type iii_3_Custom_ISTD_Summary.xltx. **d** Verify the folder selected in **Save in** is correct. **e** Click **Save**.	• The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**. • If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *MassHunter*\ *Report Templates**Quant**en-US*\ *Letter**ISTD**Parts* folder.

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\Letter\ISTD\ *iii*_3_Custom_ISTD_Summary.xltx.	• Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, *iii*_3_Custom_ISTD_Summary.xltx, 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 on the cell containing the word **Volume**. 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 on this cell in the Sequence Table.

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

Figure 35 Selecting the **Volume** column in the Sequence Table

Task 4. Move a column in a Quantitative Analysis table

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. Only 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.

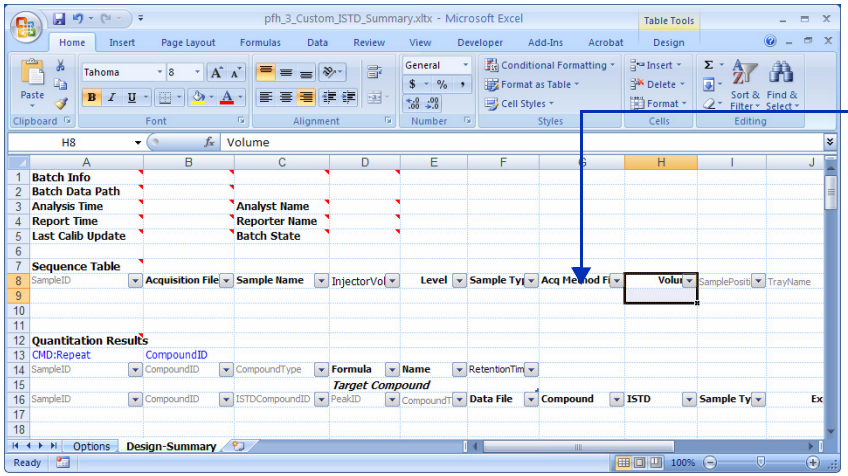


Figure 36 Moving the **Volume** column to the end of the table

Task 4. Move a column in a Quantitative Analysis table

Step	Detailed Instructions	Comments
3 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Navigate to the *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 **Volume**.	• The Process Report command is part of the MassHunter toolbar in the Add-Ins tab in the Ribbon.

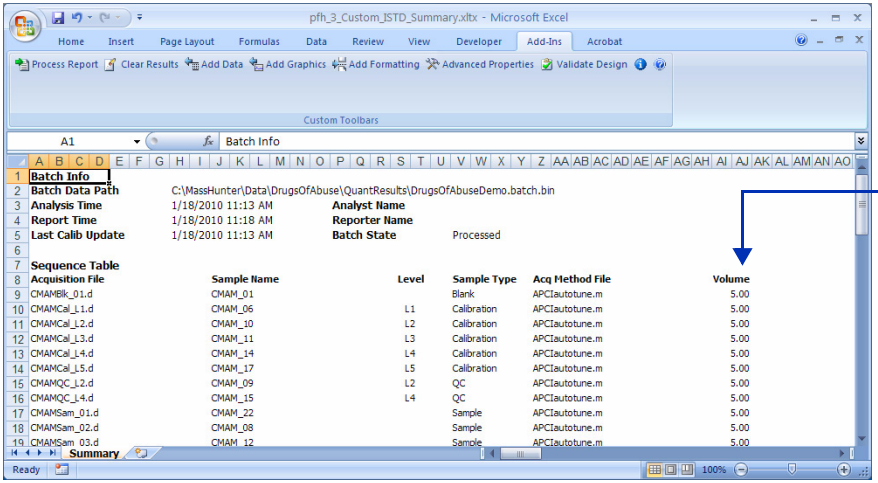


Figure 37 Verifying changes in the column header after using the Process Report command

Task 4. Move a column in a Quantitative Analysis table

Step	Detailed Instructions	Comments
4 Save the changes to the template *iii*_4_Custom_ISTD_Summary.xltx. • You have to clear the results first.	**a** Click **Clear Results** in the Add-Ins 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_Custom_ISTD_Summary.xltx. **d** Verify the folder selected in **Save in** is correct. **e** Click **Save**.	• The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**. • If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Parts* folder.

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\Letter\ISTD\ *iii*_4_Custom_ISTD_Summary.xltx.	**a** Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, iii_4_Custom_ISTD_Summary.xltx., 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 on 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 53.

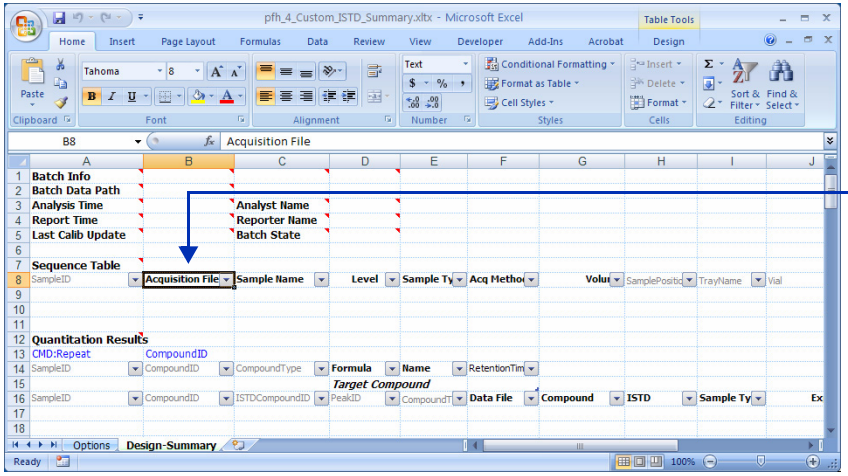
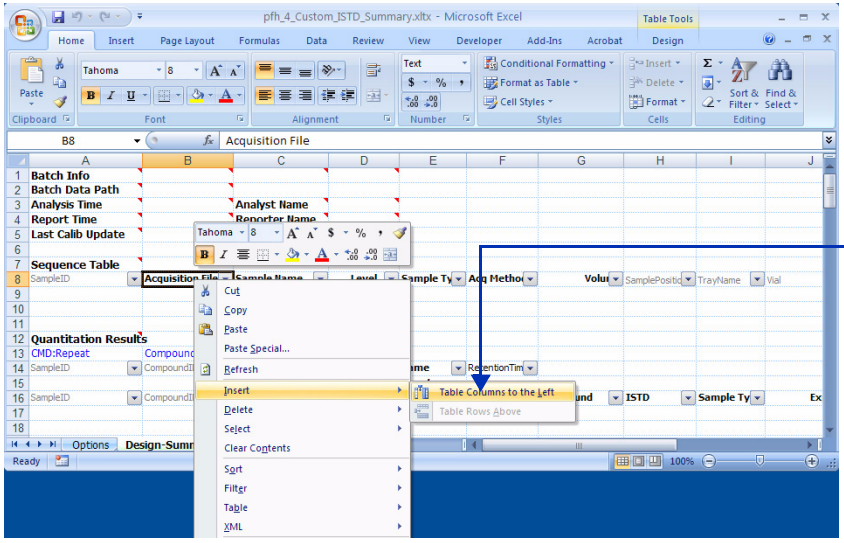


Figure 38 Selecting the Acquisition File cell in Excel

Task 5. Add a column to a Quantitative Analysis table

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 39 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 53 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

Step	Detailed Instructions	Comments

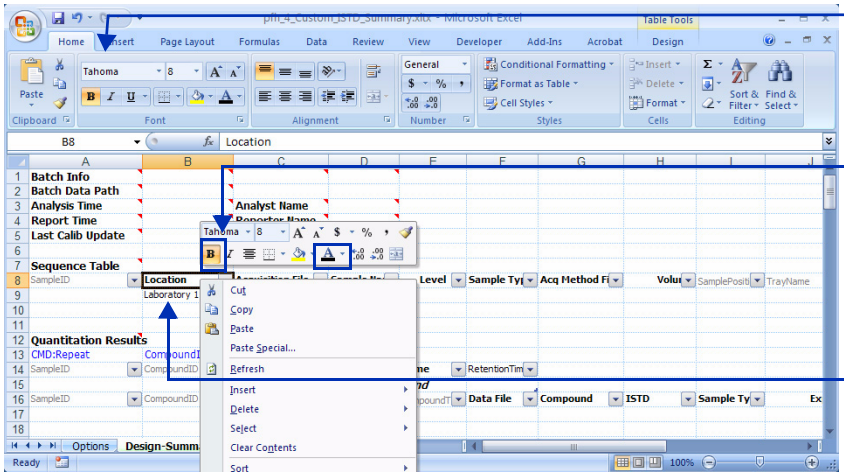


Figure 40 Change the format of the **Location** column header.

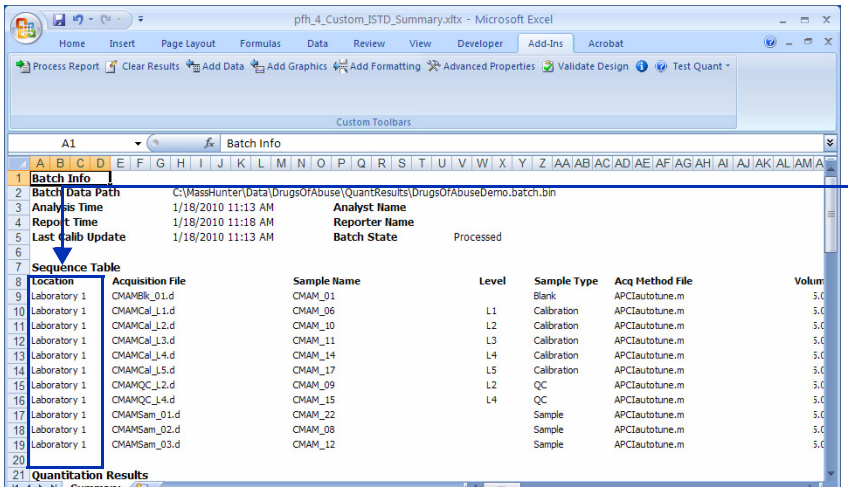
3 Test the changes to the template.

a Click **Process Report**.
b Click the **Browse** button.
c Navigate to the *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 Add-Ins tab in the Ribbon.

Task 5. Add a column to a Quantitative Analysis table

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 41 Verifying a new column is added to the table

4 Save the changes to the template *iii*_5_Custom_ISTD_Summary.xltx.

- You have to clear the results first.

a Click **Clear Results** in the Add-Ins 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.xltx.

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

e Click **Save**.

- The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**.
- If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Parts* folder.

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\Letter\ISTD\ *iii*_5_Custom_ISTD_Summary.xltx.	**f** Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, *iii*_5_Custom_ISTD_Summary.xltx., 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 the **Microsoft Office Button** and then click **Excel Options**. **b** In the Excel Options dialog box, mark the **Show Developer tab in the Ribbon** check box. **c** Click **OK**.

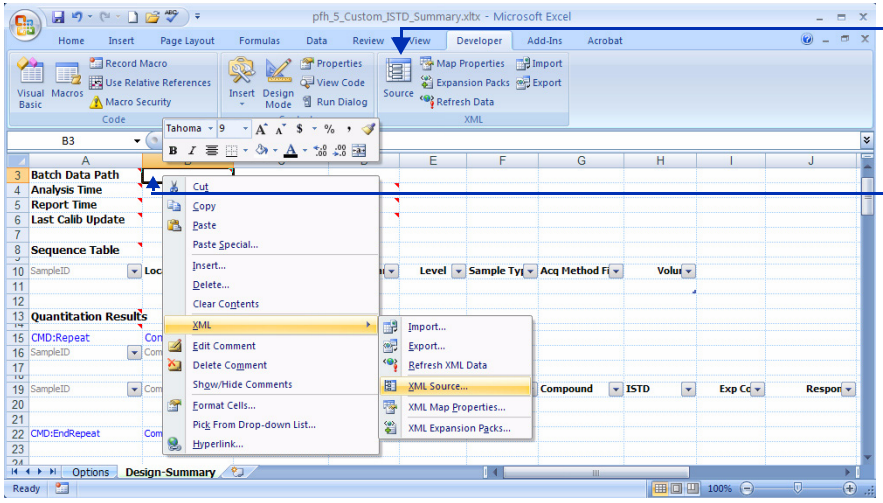
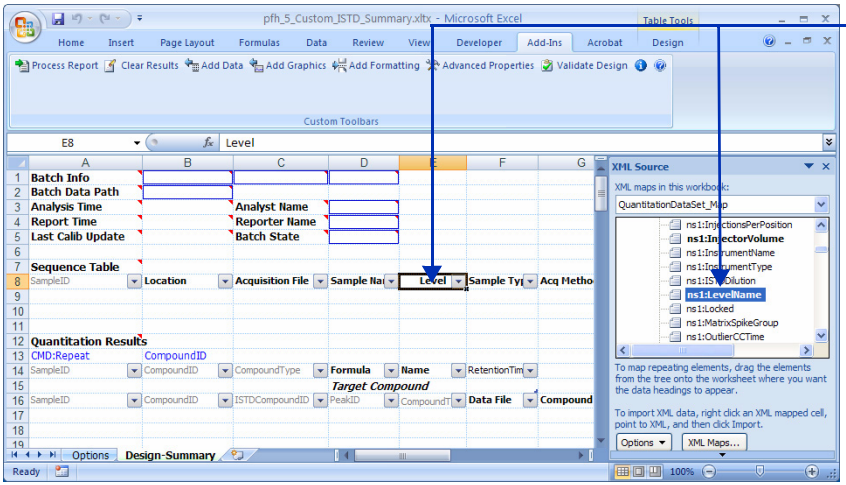


Figure 42 Displaying the XML Source task pane in Excel

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

Step	Detailed Instructions	Comments
3 Add the column **Barcode** to the end of the Sequence Table. • Hint: click on 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 on the Level column, the element ns1:LevelName in the XML Source window is highlighted.

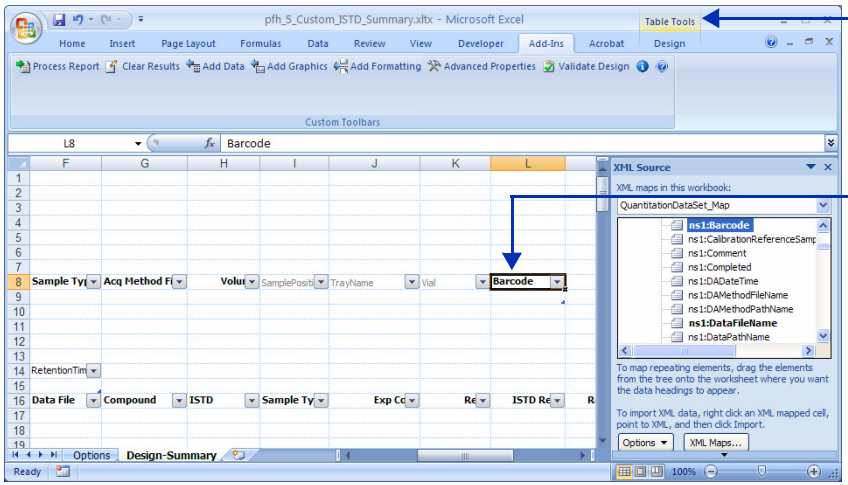
"ns1:" is part of the syntax of the element in the XML source window. Every item in the XML Source window starts with "ns1:".

Figure 43 Selecting the Level column in Excel

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 **Volume** 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.

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

Step	Detailed Instructions	Comments



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 on 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 44 Adding the **Barcode** column to the end of the Sequence Table

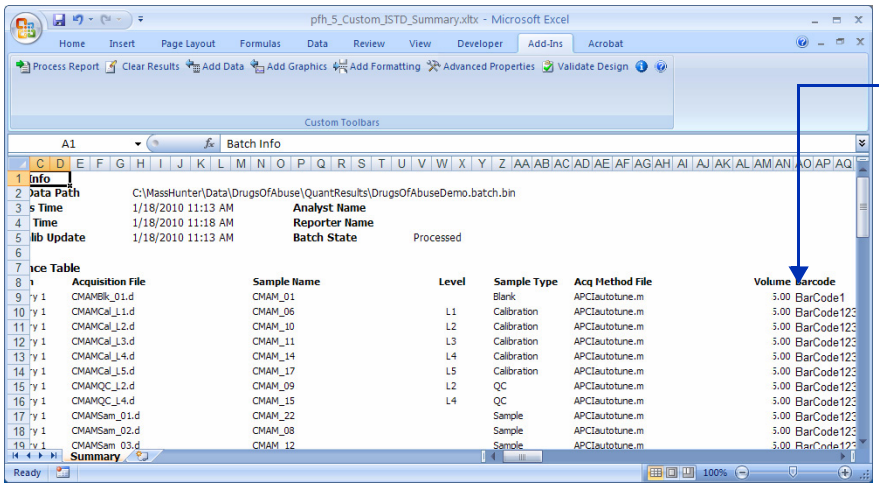
4 Test the changes to the template.

a Click **Process Report**.
b Click the **Browse** button.
c Navigate to the *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 Add-Ins tab in the Ribbon.

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

Step	Detailed Instructions	Comments



The last column in the Sequence Table is now the Barcode column.

Figure 45 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.xltx.

- You have to clear the results first.

a Click **Clear Results** in the Add-Ins 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*_6_Custom_ISTD_Summary.xltx.

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

e Click **Save**.

- The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**.
- If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Parts* folder.

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.

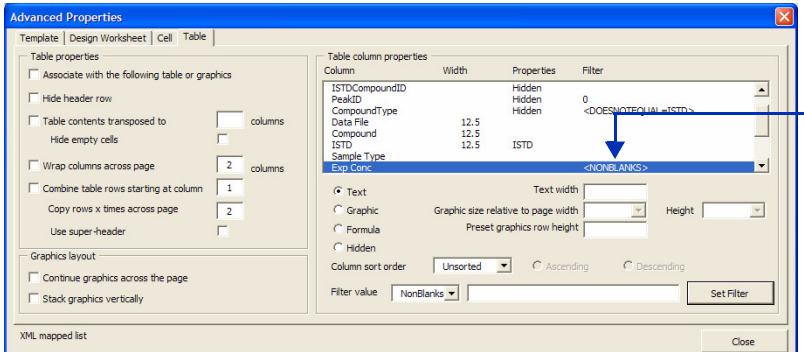
It is simpler to drag the new element to the end of the table.

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\Letter\ISTD\ *iii*_6_Custom_ISTD_Summary.xltx.	• Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, *iii*_6_Custom_ISTD_Summary.xltx, 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 the tenth (10th) column in the table. **c** Click **Advanced Properties**. **d** 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 Add-Ins tab in the Ribbon.



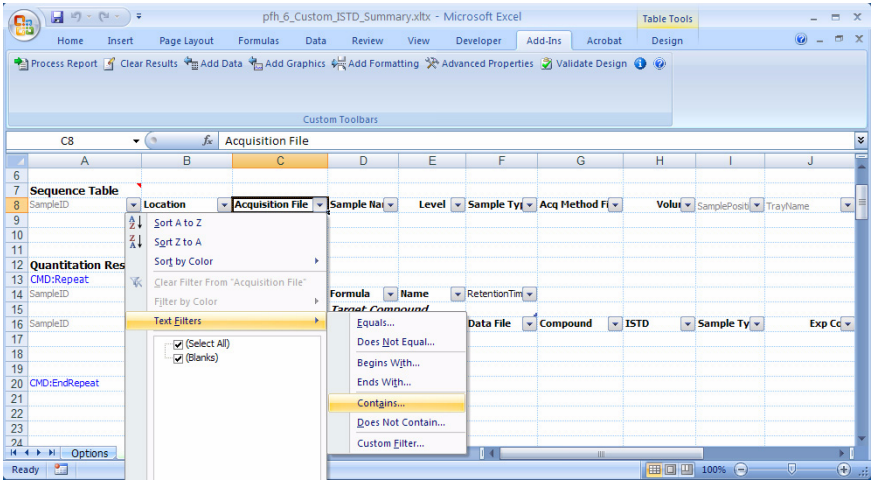
Select NonBlanks as the Filter Value and then click Set Filter.

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

Figure 46 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

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 on the arrow in the cell labeled **Acquisition File**. This column is the third column in the table. **c** Click **Text Filters > Contains**. The Custom Auto Filter dialog box is opened.	• A filter allows you to only include a row in the table if it passes the filter.



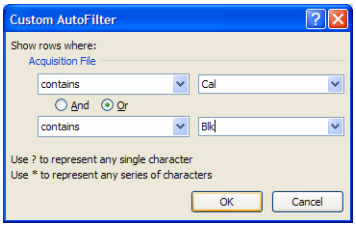
Click on the arrow in the Acquisition File column and click Text Filters > Contains.

Figure 47 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**.

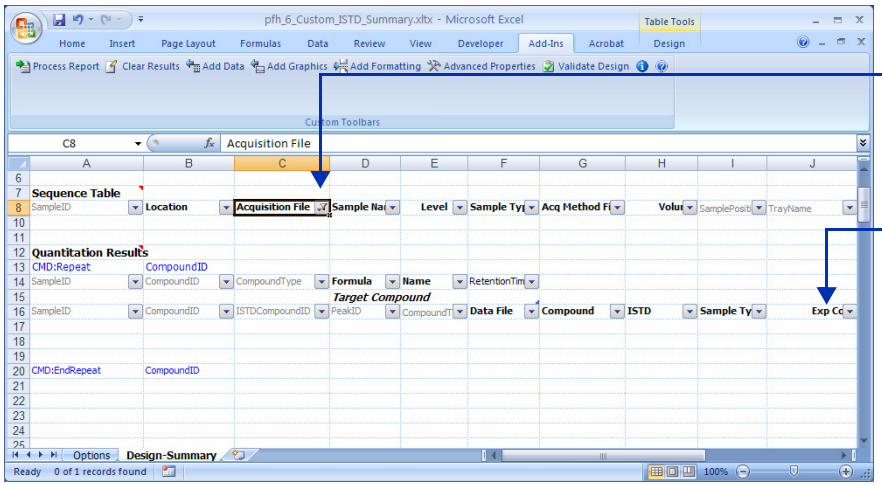
Task 7. Add a filter to a table in a Quantitative Analysis template

Step	Detailed Instructions	Comments



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

Figure 48 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 49 A filter is added to the **Acquisition File** column

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

Step	Detailed Instructions	Comments
4 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Navigate to the *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 Add-Ins tab in the Ribbon.

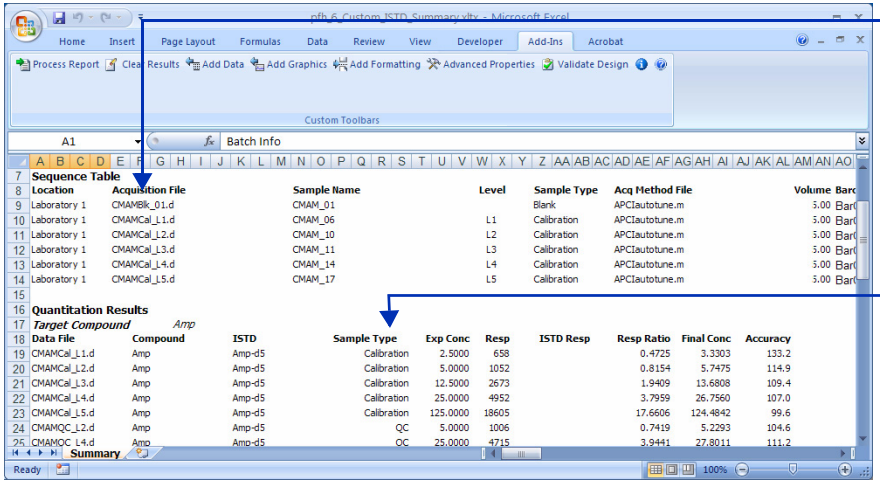


Figure 50 Verifying changes in the rows that are included in the filtered tables

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

Step	Detailed Instructions	Comments
5 Save the changes to the template *iii*_7_Custom_ISTD_Summary.xltx • You have to clear the results first.	**a** Click **Clear Results** in the Add-Ins 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*_7_Custom_ISTD_Summary.xltx. **d** Verify the folder selected in **Save in** is correct. **e** Click **Save**.	• The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**. • If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *MassHunter**Report Templates*\Quant**en-US**Letter*\ISTD**Parts* folder.

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

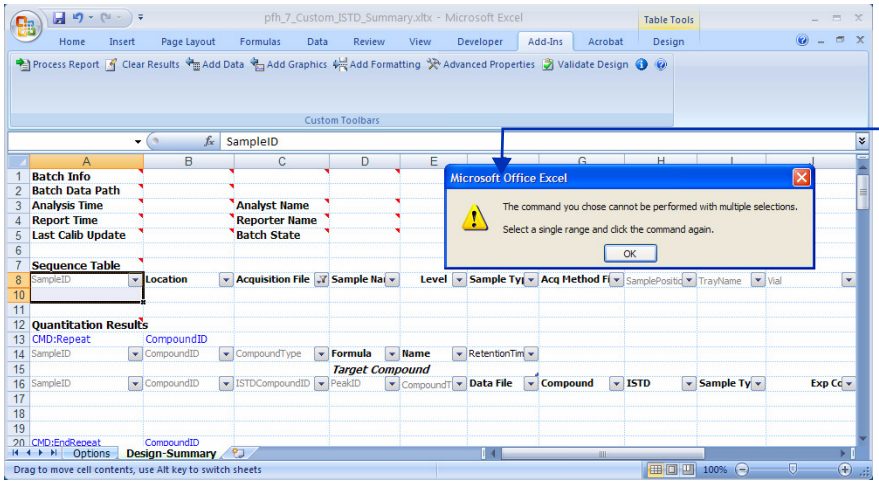
You can add a filter to a column in a table in two different ways. If you use the Advanced Properties dialog box to add a filter, you can still easily move and delete a column. However, if you use Excel features to add a filter to a table, you have to remove the filter before you can move or delete a 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\Letter\ISTD\ *iii*_7_Custom_ISTD_Summary.xltx.	• Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, *iii*_7_Custom_ISTD_Summary.xltx, 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 Volume 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 **Volume** and the cell beneath it**.** This column is the eighth (8th) column in the table. **c** Right-click the **Volume** column and try to click **Delete > Table Columns**. You cannot because this command is grayed out. **d** Click only the cell labeled **Volume**. **e** Right-click the Volume 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 the eighth (8th) column 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 select a location between two columns to move the column to. 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

Step	Detailed Instructions	Comments



If you try to move the Barcode column, Excel shows you this error or a similar error.

Figure 51 A filter is added to the **Acquisition File** column

f Click the column labeled **Acquisition File.** This column is the eighth (8th) column in the table.

g Click on the arrow in the cell labeled **Acquisition File**. This column is the third column in the table.

h Click **Text Filters > Contains**. The Custom Auto Filter dialog box is opened.

i Write down the filter. This filter is "contains Cal or Blk".

j Click **Cancel**.

k Click on the arrow in the cell labeled **Acquisition File**. This column is the third column in the table.

l Click **Clear Filter From "Acquisition File"**.

- Moving a column in a filtered table is a four step process:

a Write down 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

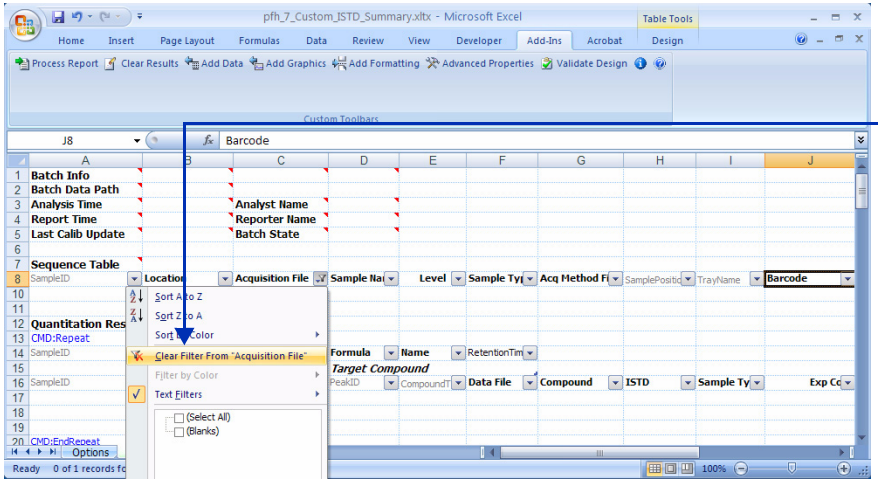
Step	Detailed Instructions	Comments
		**Remove the filter from the column.**

Figure 52 The filter is removed from the **Acquisition File** column

e Move the **Barcode** column directly after the Acquisition File column.

f Click on the arrow in the cell labeled **Acquisition File**. This column is the third column in the table.

g Click **Text Filters > Contains**. The Custom Auto Filter dialog box is opened.

h Type `Cal` in the first text field.

i Click **Or**.

j Select **contains** in the second box.

k Type Blk in the second text field.

l Click **OK**.

- Follow the instructions in "Task 4. Move a column in a table" on page 62 to move the **Barcode** column.
- Follow the instructions in "Task 7. Add a filter to a table" on page 74 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

Step	Detailed Instructions	Comments

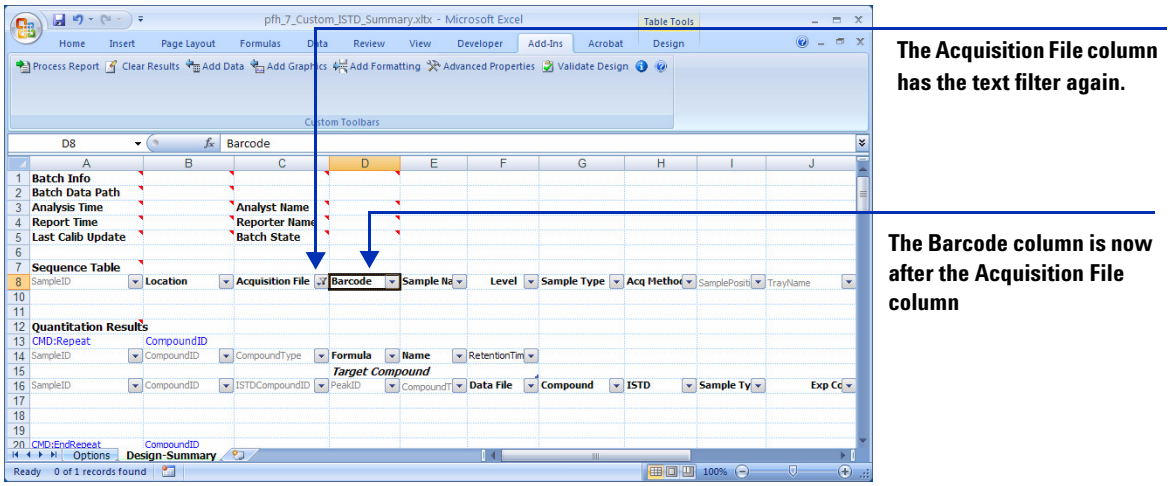


Figure 53 The Barcode column is moved and the filter has been added again

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 the thirteenth (13th) column 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 the twelfth (12th) column 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 62 to move the **Final Conc** column.

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

Step	Detailed Instructions	Comments

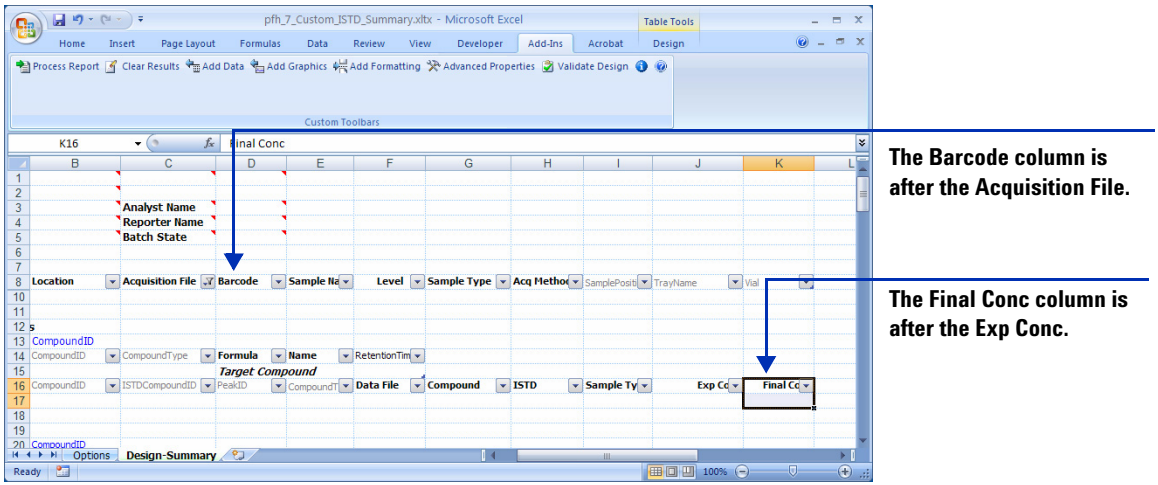
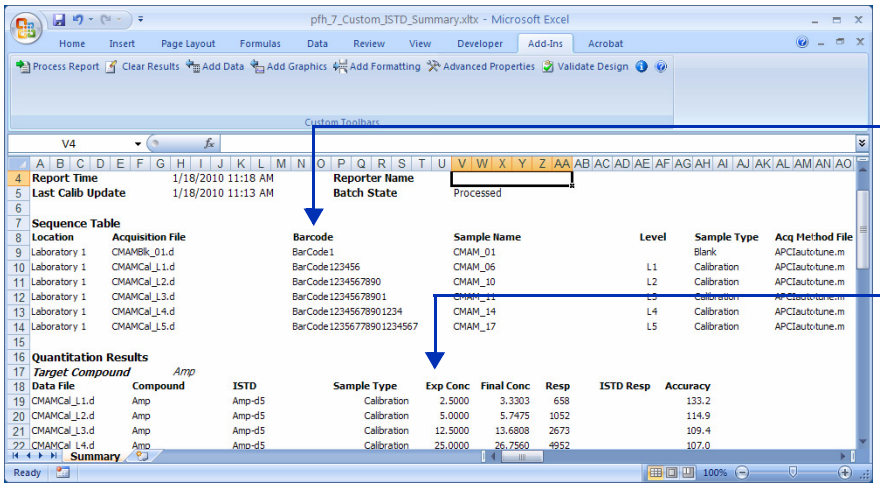


Figure 54 The **Barcode** column and the **Final Conc** column are moved

6 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Navigate to the *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 Add-Ins tab in the Ribbon.

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

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 55 Verifying that columns are moved in both filtered tables

7 Save the changes to the template *iii*_8_Custom_ISTD_Summary.xltx.

- You have to clear the results first.

a Click **Clear Results** in the Add-Ins 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*_8_Custom_ISTD_Summary.xltx.

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

e Click **Save**.

- The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**.
- If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Parts* folder.

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 Add-Ins 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.

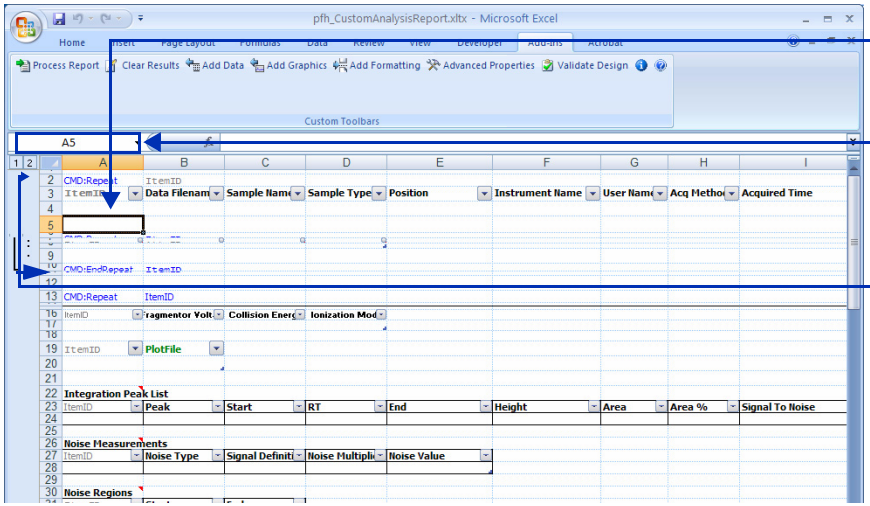
When you add a table to a template using the Add Data commands, a new XML map is added automatically. If you remove this table from the template in the future, make sure to also delete the XML map that was created. Reports print more quickly when you have fewer XML maps. You can delete unused XML maps 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.xltx**.	**a** Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 32 to open the template, *iii*_CustomAnalysisReport.xltx, 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 on 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

Step	Detailed Instructions	Comments



Click on this cell in the template.

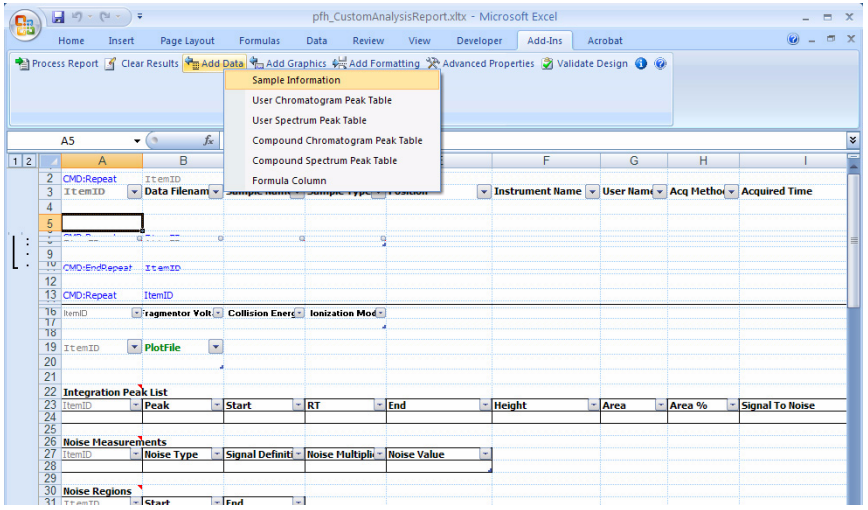
The current position in the template is shown here.

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 56 Selecting the **first cell** in row 9

c Click **Add Data > Sample Information** in the Add-Ins tab in the Ribbon.

- Extra rows are automatically added to the template for the new table.



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 57 Add a second Sample Information table.

Task 1. Add a table to a Qualitative Analysis template

Step	Detailed Instructions	Comments

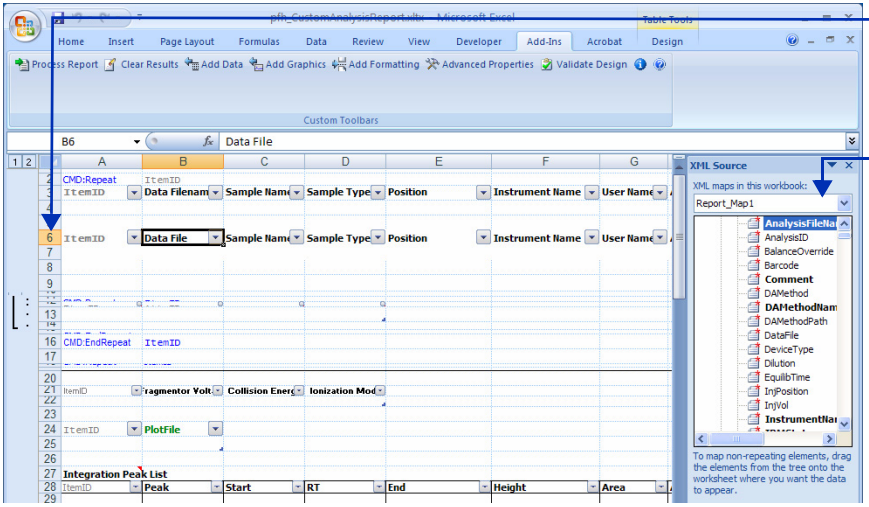
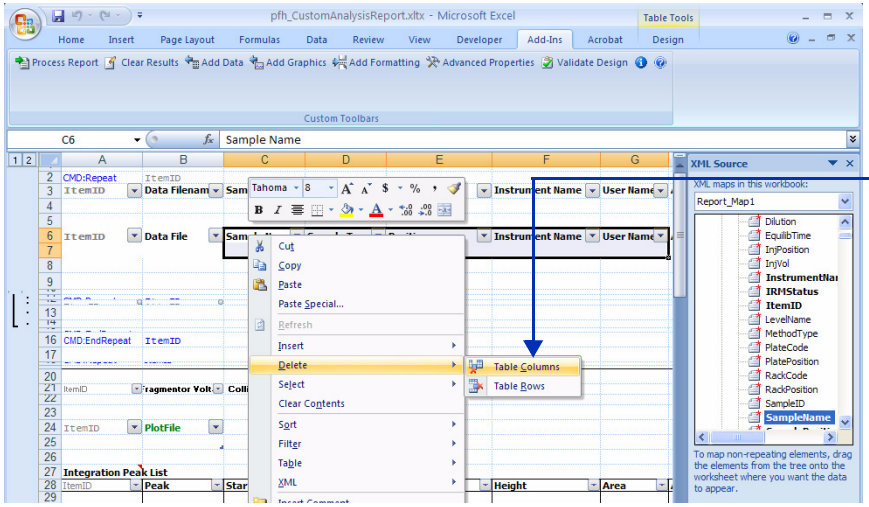


Figure 58 Add a second Sample Information table.

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 on the **Data Filename** column in the first table. The XML map is Report_Map. **b** Click on 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.
4 Change the second table to include only the following columns: • ItemID • Data File • Injector Volume • Dilution	**a** Click on 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.	• 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 56 to remove the columns.

Task 1. Add a table to a Qualitative Analysis template

Step	Detailed Instructions	Comments



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 59 Delete multiple columns in the second Sample Information table.

c Click the **Data File** column in the second table.

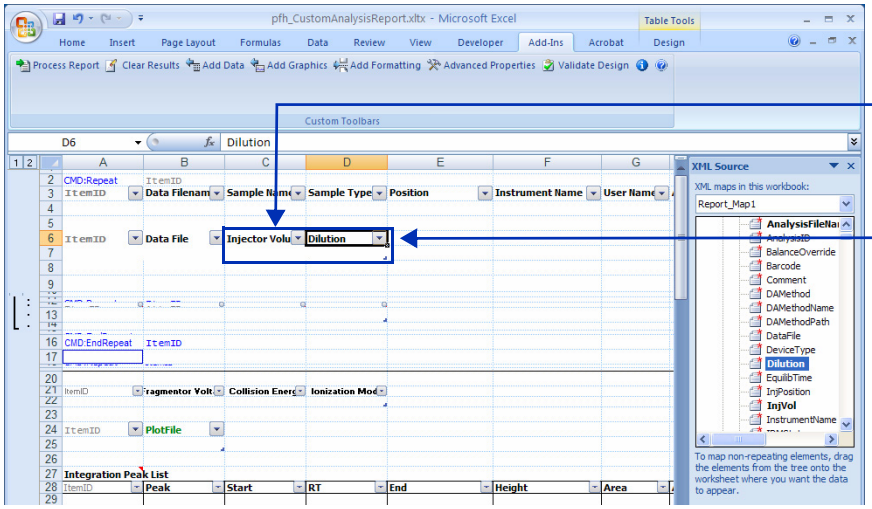
d Add the mapped columns, **InjVol and Dilution**.

e Rename the **InjVol** column to **Injector Volume**.

- You click on 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 70 to add the columns.
- Follow the instructions in "Task 1. Rename a column header in a table" on page 53 to rename the columns.

Task 1. Add a table to a Qualitative Analysis template

Step	Detailed Instructions	Comments



The Injector Volume and Dilution columns are added to the second table.

You can change the formatting for each column using standard Excel features in the Home tab.

Figure 60 The **Injector Volume** and **Dilution** columns are added to the second table

5 Test the changes to the template.

a Click **Process Report**.
b Click the **Browse** button.
c Navigate 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 Add-Ins tab in the Ribbon.

Task 1. Add a table to a Qualitative Analysis template

Step	Detailed Instructions	Comments

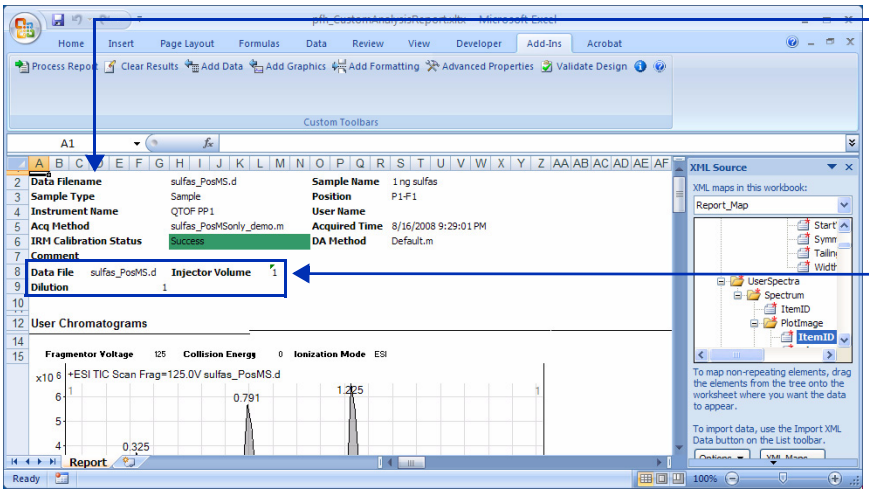


Figure 61 Verifying a new Sample Information table is added to the template

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.xltx.

a Click **Clear Results** in the Add-Ins 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.xltx.

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

e Click **Save**.

- The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**.
- If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *MassHunter*\ *Report Templates**Qual**en-US*\ *Letter* folder.

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 Add-Ins 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.

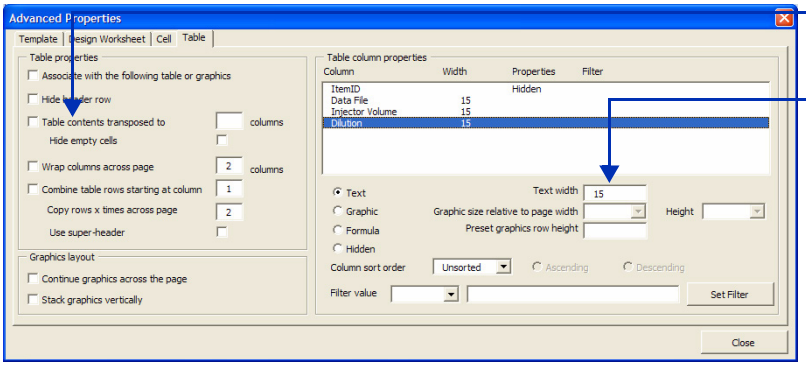
Another way to format a table is to hide the column headers. If you add a repeating section, you can turn on this feature to avoid repeating the column headers throughout the report.

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.xltx**.	**a** Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 32 to open the template, *iii*_1_CustomAnalysisReport.xltx, 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 on a column in the second table. **b** Click **Advanced Properties** which is part of the MassHunter toolbar in the Add-Ins 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

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 62 Changing table properties in the Advanced Properties dialog box

3 Format the first table.
- Hide the header row.

a Click on 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.

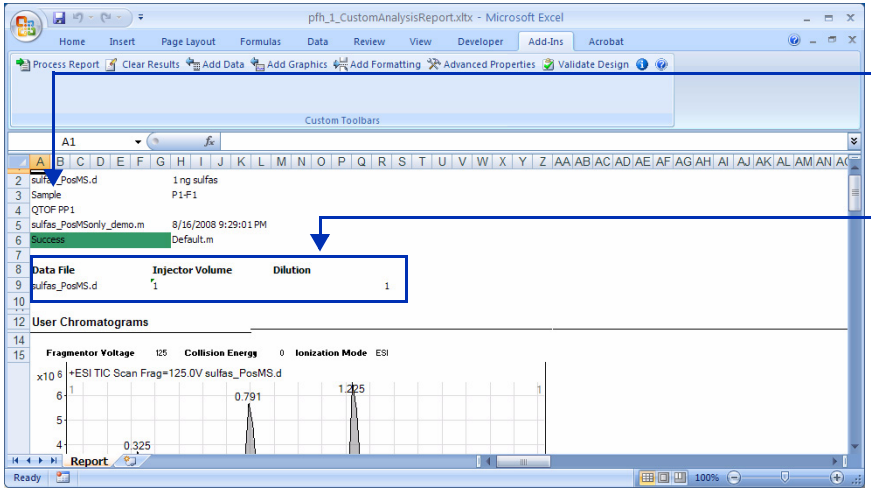
4 Test the changes to the template.

a Click **Process Report**.
b Click the **Browse** button.
c Navigate 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 Add-Ins tab in the Ribbon.

Task 2. Format a table in a Qualitative Analysis template

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 63 Verifying a new Sample Information table is added to the template

5 Save the changes to the template, *iii*_2_CustomAnalysisReport.xltx.

- You have to clear the results first.

a Click **Clear Results** in the Add-Ins 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.xltx, 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 (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**.
- If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *\MassHunter\Report Templates\Qual\en-US\Letter* folder.

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.xltx**, where *iii* are your initials.	**a** Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 32 to open the template, *iii*_2_CustomAnalysisReport.xltx, 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 on the cell containing the words **End**. This column is the fifth column in the table. **c** Click **Add Data > Formula Column** in the Add-Ins tab in the Ribbon. **d** Follow the instructions in "Task 1. Rename a column header in a table" on page 53 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

Step	Detailed Instructions	Comments

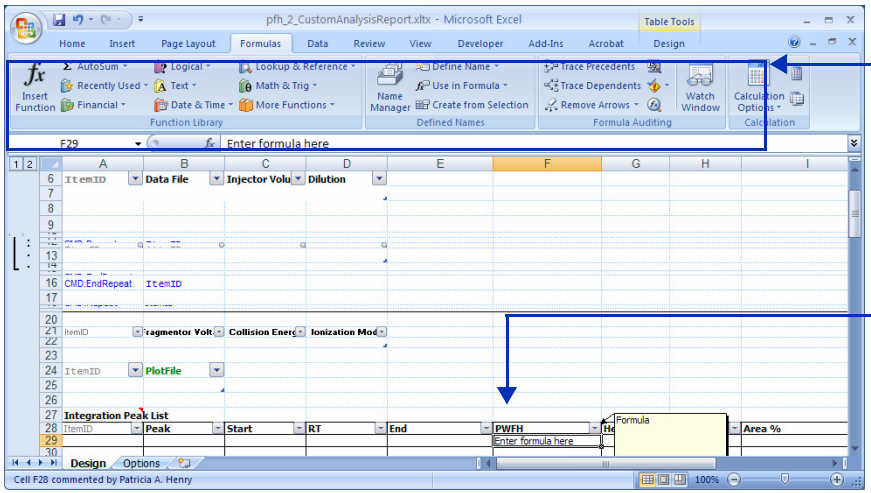


Figure 64 Add a formula column to the right of the **End** column.

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.

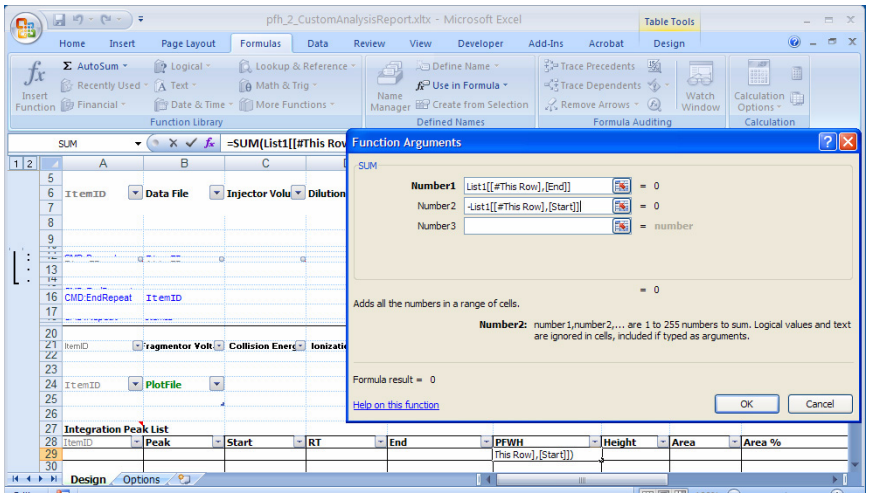
o Click the cell in the **Start** column that is in the same row as this formula. The reference to this cell is added after the "-".

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.

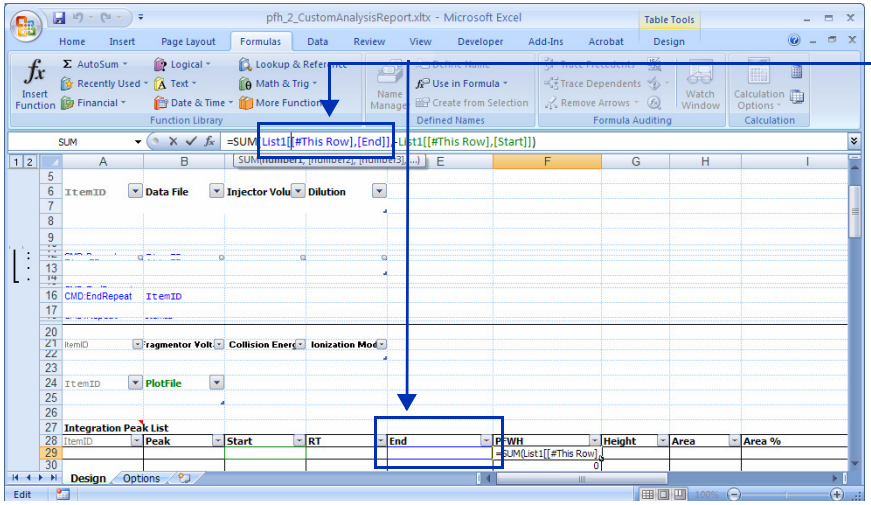
Task 3. Add a formula column to a Qualitative Analysis table

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 65 Using the Insert Function tool to add a formula to the RT Window column.

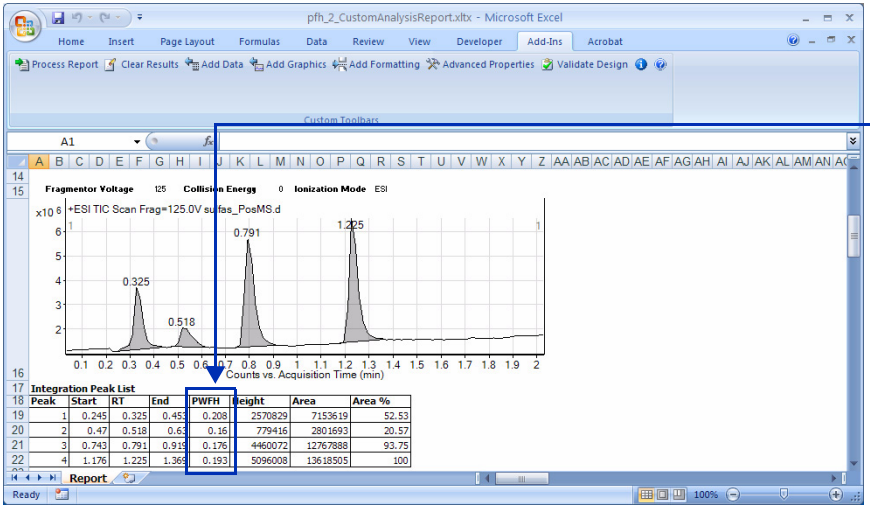


A formula starts with the equal sign. This formula is a sum of the two items listed. The blue part of the formula refers to the value in the End column. It is color-coded to match the outline of the cell in the Integration Peak List table. The green part of the formula refers to the value in the Start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

Figure 66 The formula has been added to the Integration Peak List table.

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

Step	Detailed Instructions	Comments
3 Test the changes to the template.	**a** Click the **Add-Ins** tab in the Ribbon. **b** Click **Process Report**. **c** Click the **Browse** button. **d** Navigate 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 Add-Ins 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 67 Verifying the formula column in the Integration Peak List table.

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

Step	Detailed Instructions	Comments
4 Save the changes to the template, *iii*_3_CustomAnalysisReport.xltx, where *iii* are your initials.	**a** Click **Clear Results** in the Add-Ins 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.xltx, 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 (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**. • If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *MassHunter**Report Templates**Qual**en-US**Letter* folder.

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

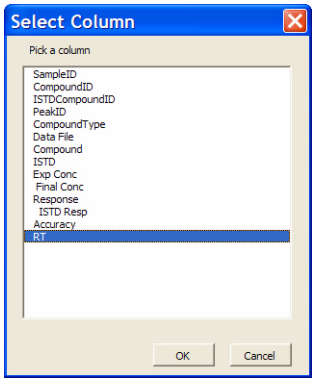
In the Quantitative Analysis program, a compound can be an internal standard (ISTD). You can include information about the internal standard in the same row in table as the related compound by adding an ISTD column.

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\Letter\ISTD\Parts*iii*_8_Custom_ISTD_Summary.xltx template.	**a** Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, *iii*_8_Custom_ISTD_Summary.xltx., 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 70 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 53 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 to

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

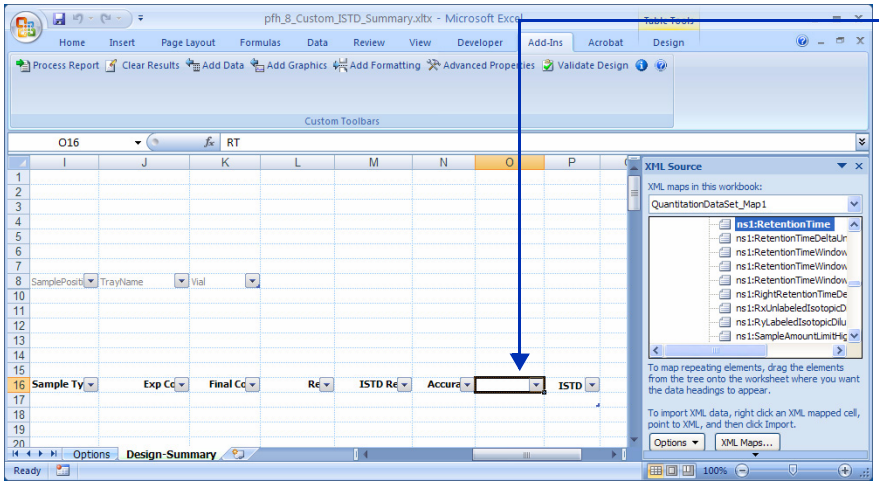
Step	Detailed Instructions	Comments



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 in order 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 68 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 on this column, you can see the Column Header in the Formula Bar.

Figure 69 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

Step	Detailed Instructions	Comments
3 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Navigate to the *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 Add-Ins tab in the Ribbon.

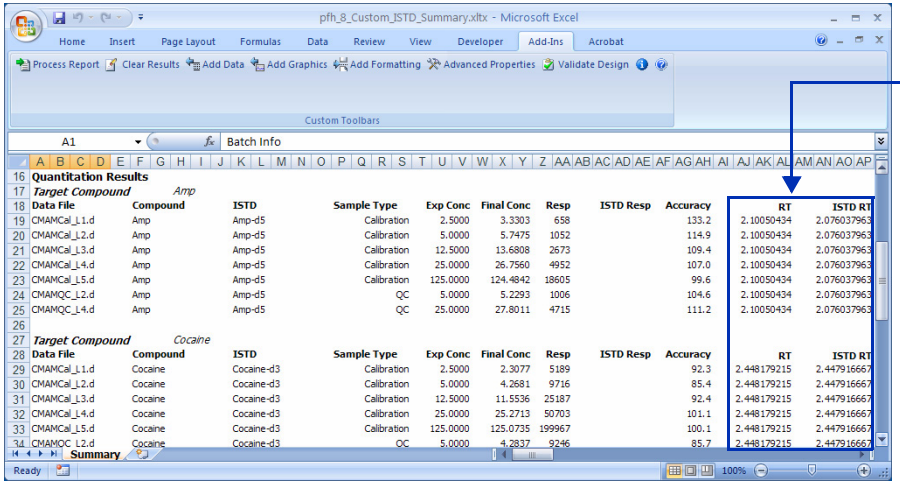


Figure 70 Verifying the RT and ISTD RT columns are added to the end of the table

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

Step	Detailed Instructions	Comments
4 Save the changes to the template, *iii*_9_Custom_ISTD_Summary.xltx. • You have to clear the results first.	**a** Click **Clear Results** in the Add-Ins 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*_9_Custom_ISTD_Summary.xltx. **d** Verify the folder selected in **Save in** is correct. **e** Click **Save**.	• The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**. • If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *MassHunter**Report Templates*\Quant**en-US**Letter*\ISTD**Parts* folder.

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.xltx**, where *iii* are your initials.	**a** Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 32 to open the template, *iii*_3_CustomAnalysisReport.xltx, 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 70 for instructions on adding a mapped column to a table.

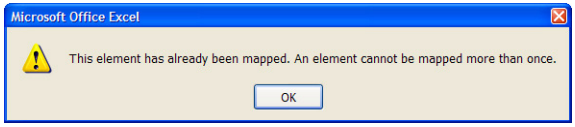
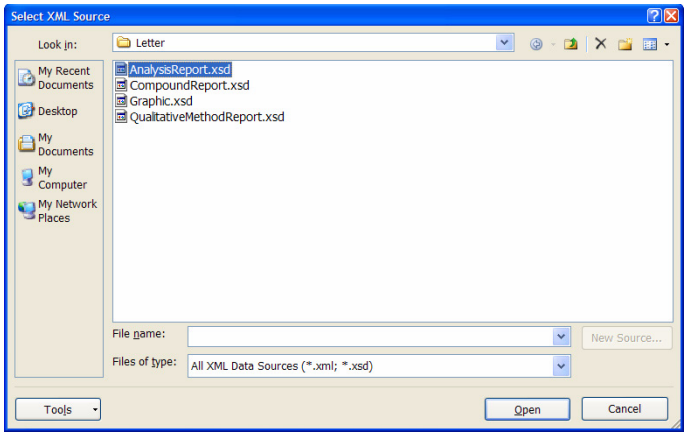


Figure 71 The error that is shown if you try to map a column two times.

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

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** Navigate 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

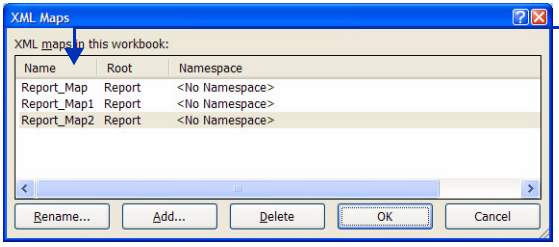
CompoundReport.xsd - Compound report

Graphic.xsd - Graphic report

QualitativeMethodReport.xsd - Qualitative Analysis Method Report

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

Figure 72 Add another map file.



Report_Map - original map file

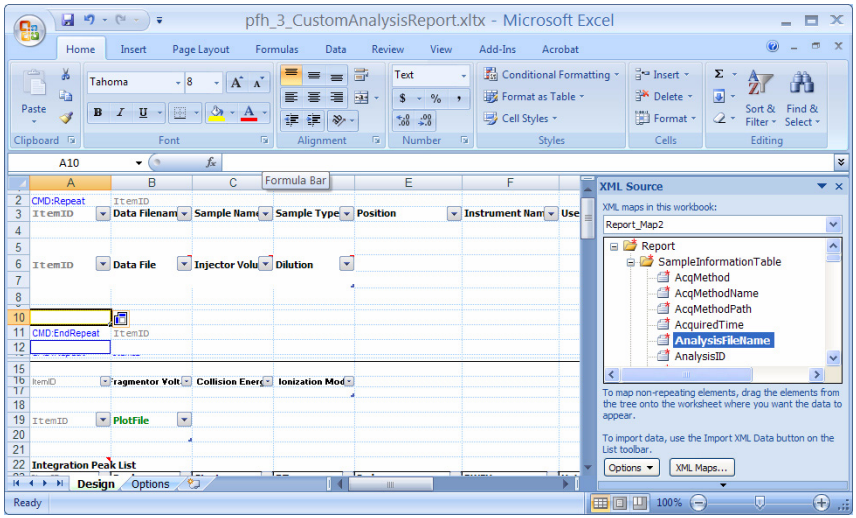
Report_Map1 - automatically added in Task 1 when the table was added

Report_Map2 - added manually in this task

Figure 73 Three XML maps are available in this template.

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

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.	



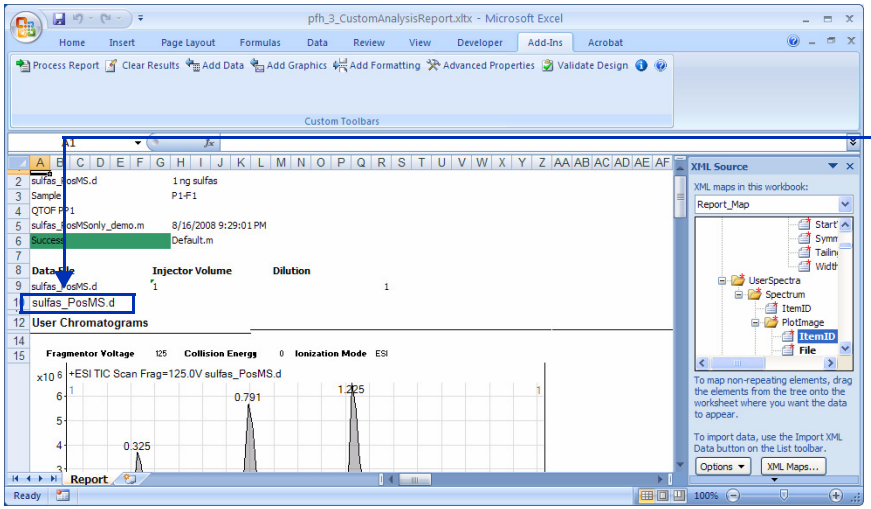
The AnalysisFileName is added to the first column in row 10. Because this cell is not part of a table, the column header is not automatically added above the value.

Figure 74 Add the AnalysisFileName item.

3 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Navigate 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 again.	• The **Process Report** command is part of the MassHunter toolbar in the Add-Ins tab in the Ribbon.

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

Step	Detailed Instructions	Comments



The AnalysisFileName is added after the second Sample Information table.

Figure 75 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.xltx, where *iii* are your initials.

a Click **Clear Results** in the Add-Ins 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.xltx.

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

e Click **Save**.

- The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**.
- If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *MassHunter**Report Templates*\Qual*\en-US**Letter* folder.

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:

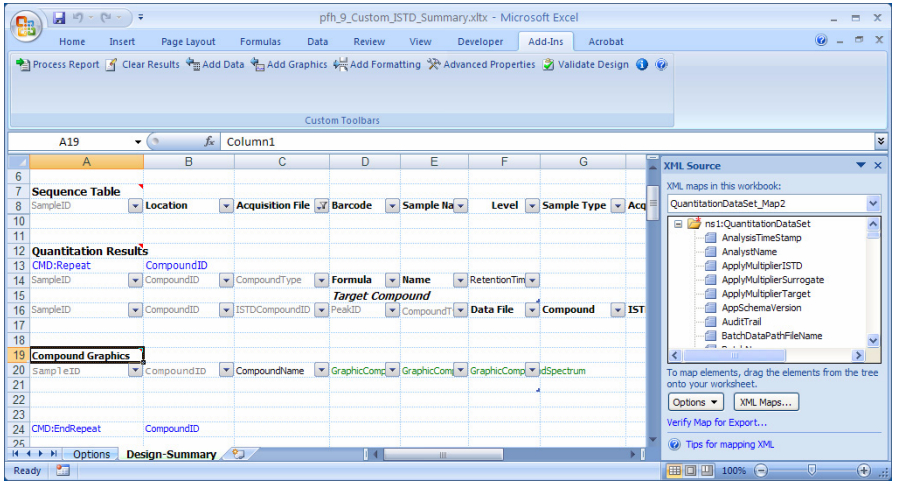
- Steps – Use these general instructions to proceed on your own to explore the program.
- Detailed Instructions – Use these if you need help or prefer to use a step-by-step learning process.
- Comments – Read these to learn tips and additional information about each step in the exercise.

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\Letter\ISTD\Parts*iii*_9_Custom_ISTD_Summary.xltx template.	**a** Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, *iii*_9_Custom_ISTD_Summary.xltx., 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 127 for an explanation of repeating sections. • Three different graphics are added in the Compound Graphics table.



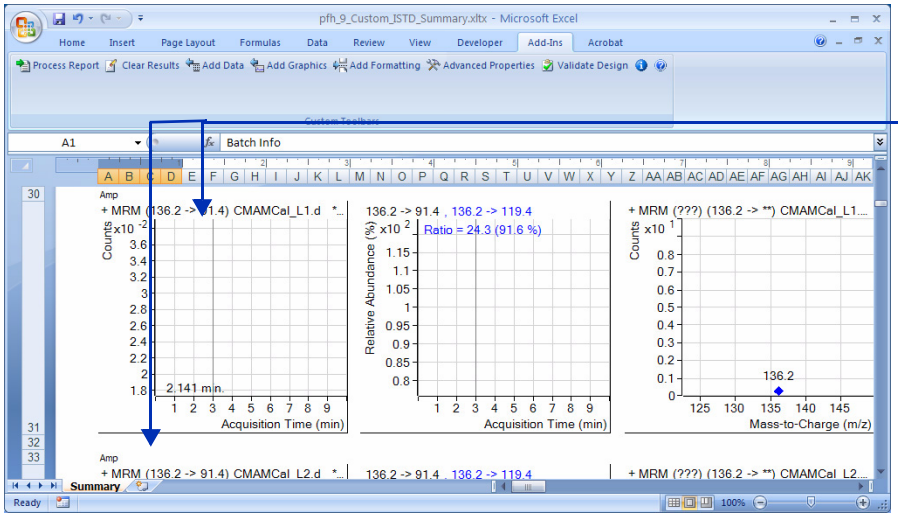
You can quickly find any graphics in the template because they are shown in green in the template.

The graphics are included in the CompoundID repeating section.

Figure 76 Select the **RT** column.

Task 1. Add graphics to a Quantitative Analysis template

Step	Detailed Instructions	Comments
3 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Navigate to the *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 Add-Ins 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 77 The compound graphics are added after the Target Compound table

Task 1. Add graphics to a Quantitative Analysis template

Step	Detailed Instructions	Comments
4 Save the changes to the template, *iii*_10_Custom_ISTD_ Summary.xltx. • You have to clear the results first.	**a** Click **Clear Results** in the Add-Ins 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*_10_Custom_ISTD_Summary.xltx. **d** Verify the folder selected in **Save in** is correct. **e** Click **Save**.	• The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**. • If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *MassHunter*\ *Report Templates**Quant**en-US*\ *Letter**ISTD**Parts* folder.

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.

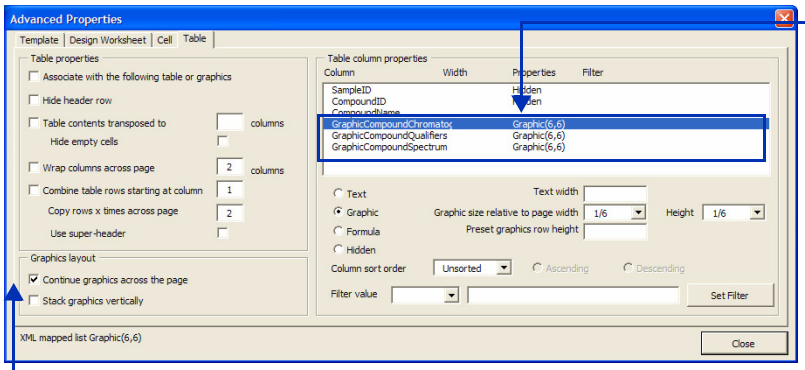
You can also mark whether or not to print graphics side-by-side. Normally, only graphics that are in the same row of the table are printed side-by-side. However, you can specify that graphics from different rows are printed side-by-side.

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\Letter\ISTD\Parts*iii*_10_Custom_ISTD_Summary.xltx template.	**a** Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, *iii*_10_Custom_ISTD_Summary.xltx., where "*iii*" are your initials.	• If you do not have the iii_10_Custom_ISTD_Summary.xltx 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 Add-Ins 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

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.

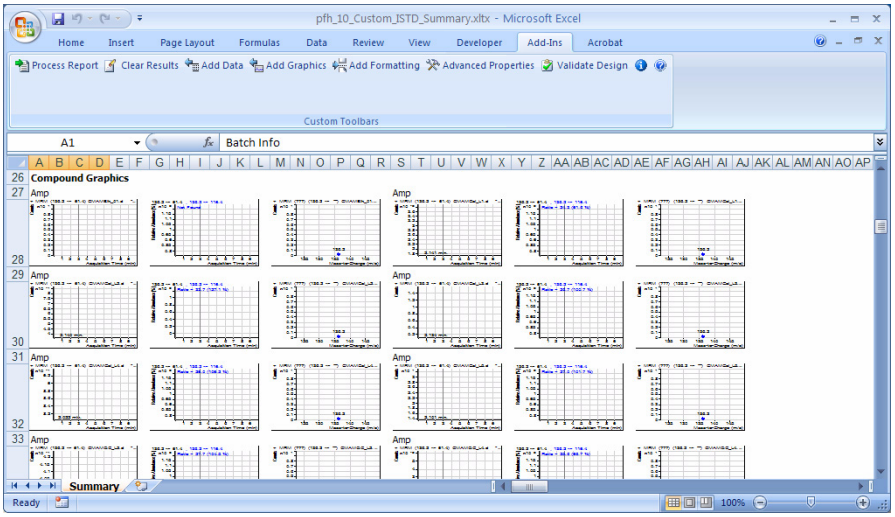
The Stack graphics vertically check box changes how the graphics are organized on the page. If this check box is cleared, then the related graphics are printed side-by-side. If this check box is marked, then related graphics are printed on consecutive rows.

Figure 78 Select the RT column.

3 Test the changes to the template.	**a** Click **Process Report**. **b** Click the **Browse** button. **c** Navigate to the *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 Add-Ins tab in the Ribbon.

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

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

Figure 79 Graphics are printed side-by-side when you mark **Continue graphics across the page**.

4 Save the changes to the template, *iii*_11_Custom_ISTD_Summary.xltx.

- You have to clear the results first.

a Click **Clear Results** in the Add-Ins 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*_11_Custom_ISTD_Summary.xltx.

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

e Click **Save**.

- The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**.
- If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *\MassHunter\Report Templates\Quant\en-US\Letter\ISTD\Parts* folder.

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.

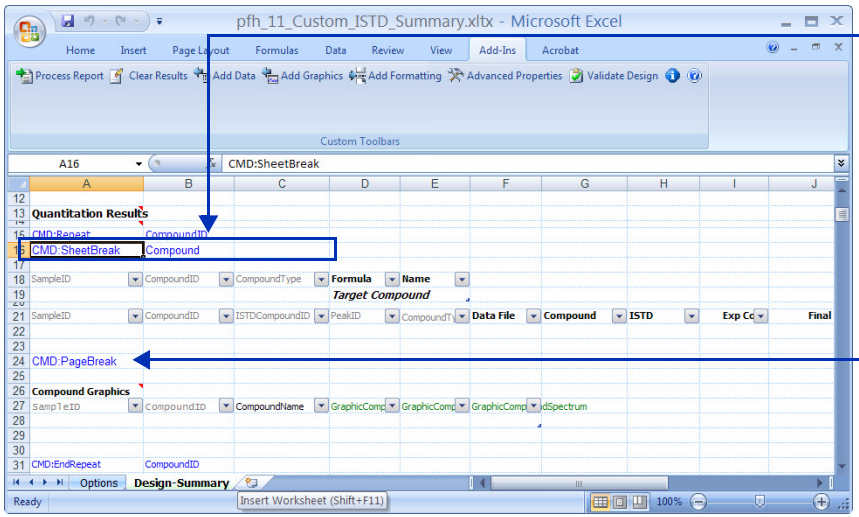
A sheet break is similar to a page break; the report automatically puts the next information in the report at the beginning of a new page. It also places the information on a new worksheet. When you add a sheet break, you can select an item that is already part of the template to label the new worksheet. 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 34 or "Task 5. Customize the footer of the Quantitative Analysis template" on page 44 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\Letter\ISTD\Parts*iii*_11_Custom_ISTD_Summary.xltx template.	**a** Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, *iii*_11_Custom_ISTD_Summary.xltx., 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 Add-Ins 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.
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 Add-Ins tab in the Ribbon.	• A page break only starts a new page. It does not change the worksheet label.

Task 1. Add a page break and a sheet break

Step	Detailed Instructions	Comments



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 80 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 hand 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 View tab.
h Click the **Add-Ins** tab.

- The footer also contains the Sheet Name in the left hand section.

Task 1. Add a page break and a sheet break

Step	Detailed Instructions	Comments
5 Test the changes to the template.	**a** Click the **Add-Ins** tab. **b** Click **Process Report**. **c** Click the **Browse** button. **d** Navigate to the *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 Add-Ins tab in the Ribbon.

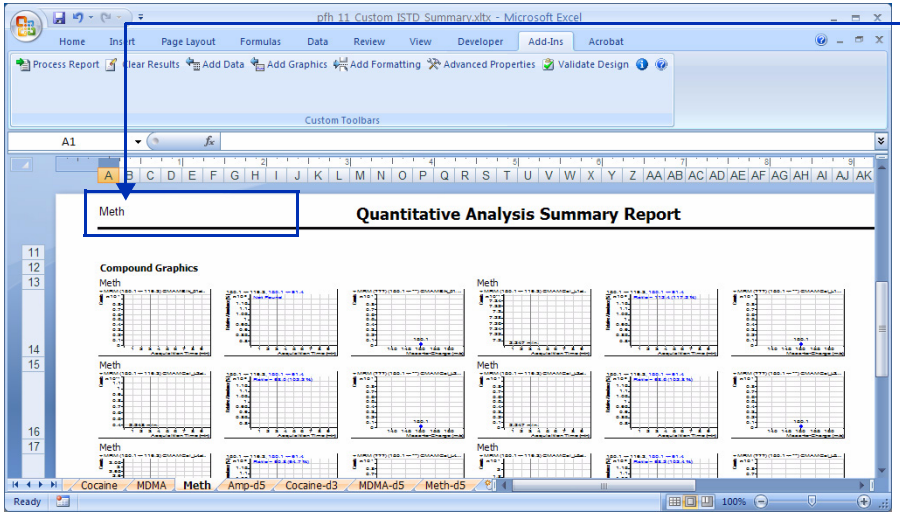


Figure 81 The Compound Graphics are printed at the start of the page. The worksheets are labeled with the compound name.

Task 1. Add a page break and a sheet break

Step	Detailed Instructions	Comments
6 Save the changes to the template, *iii*_12_Custom_ISTD_ Summary.xltx. • You have to clear the results first.	**a** Click **Clear Results** in the Add-Ins 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*_12_Custom_ISTD_Summary.xltx. **d** Verify the folder selected in **Save in** is correct. **e** Click **Save**.	• The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**. • If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *\MassHunter\ Report Templates\Quant\en-US\ Letter\ISTD\Parts* folder.

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.

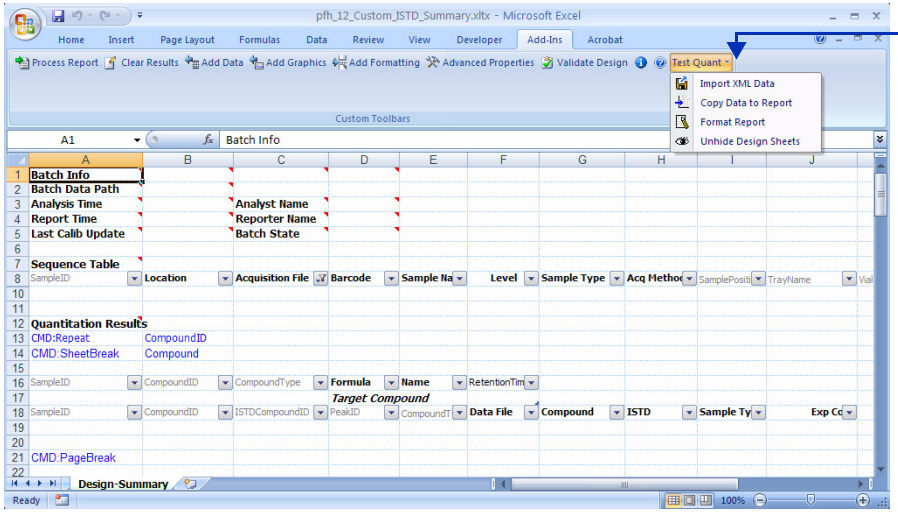
If you click **Unhide Design Sheets**, you can view the Design worksheets at the same time as the final report. The Design worksheets are hidden after the Format Report step.

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** Navigate 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

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\Letter\ISTD\Parts*iii*_12_Custom_ISTD_Summary.xltx template.	**a** Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, *iii*_12_Custom_ISTD_Summary.xltx., where "*iii*" are your initials.	• If you do not have the *iii*_12_Custom_ISTD_Summary.xltx template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the **Familiarization Templates** folder.

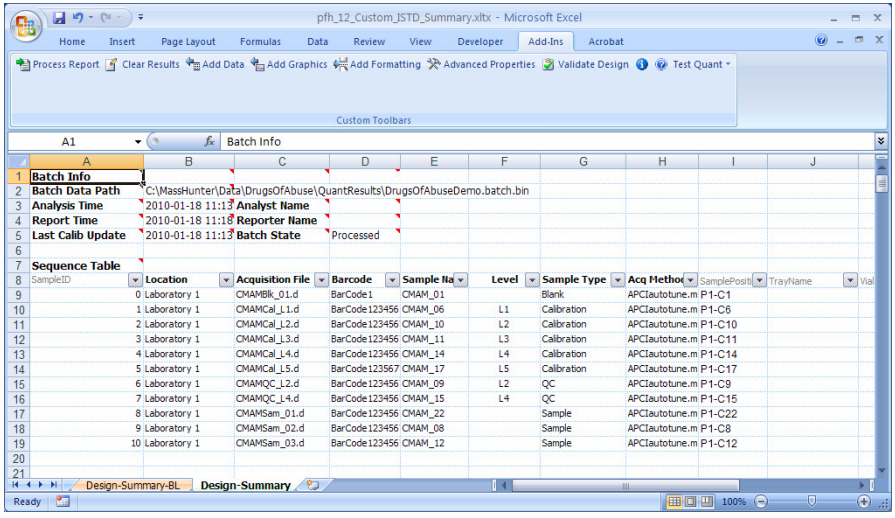


When you enable Test Mode, a new menu is added to the MassHunter Reporting toolbar. These commands allow you to step through processing the report which can help you determine the cause of a problem in the template.

Figure 82 The Test Mode menu.

Task 2. Use Test mode

Step	Detailed Instructions	Comments
5 Test the steps in the Test Mode menu.	**a** Click **Test Quant > Import XML Data.** **b** Click the **Browse** button. **c** Navigate to the *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 Add-Ins 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.

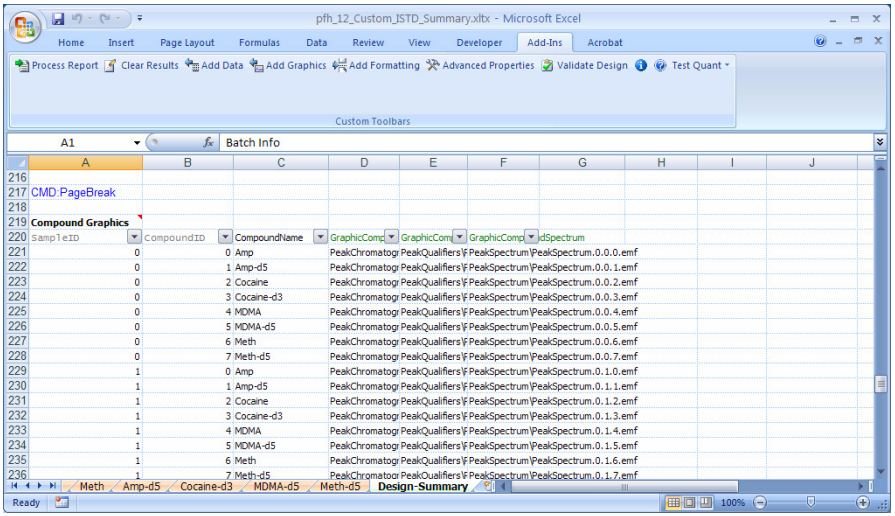


After the first step, the data is added to the template, but it is not filtered or copied to the report worksheets or formatted.

Figure 83 After the **Test Quant > Import XML Data** step

Task 2. Use Test mode

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

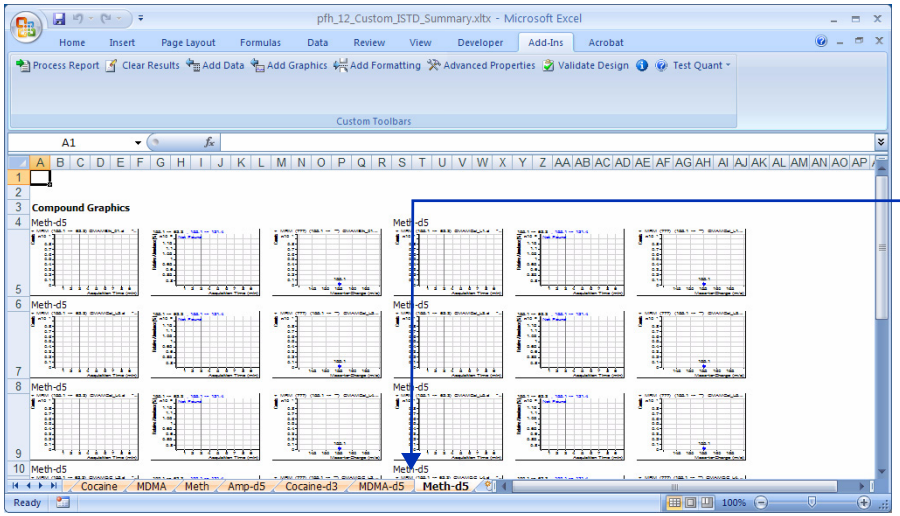


After the second step, the data is placed onto the appropriate worksheet and it is filtered, but it is not formatted. Also, the graphics are not included in the report yet.

Figure 84 After the **Test Quant > Copy Data to Report** step

Task 2. Use Test mode

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 85 After the **Test Quant > Format Quant** step

6 Clear the results and close Excel.	**a** Click **Clear Results** in the Add-Ins 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 131, 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, we can instead group all of the information about each compound together.

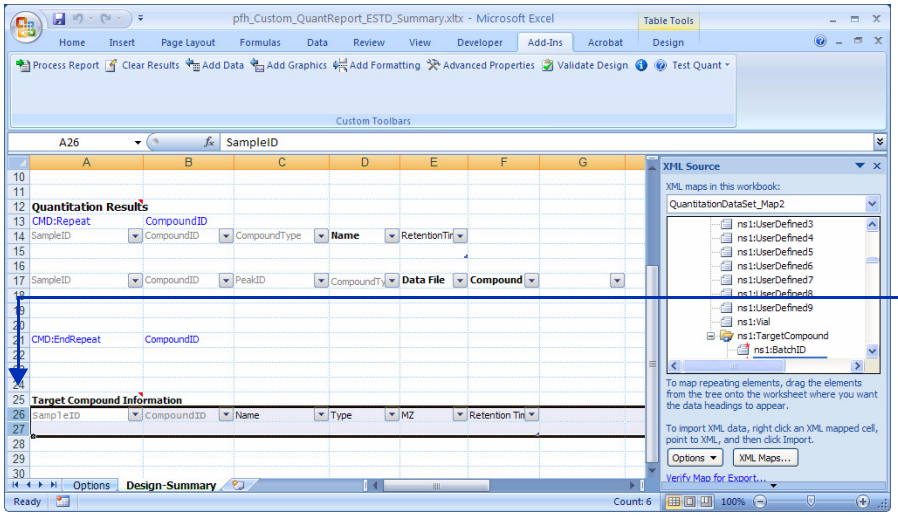
A repeating section is similar to the programming concept of a For/Next loop. **CMD:Repeat** is equivalent to "For each item in the Column Selected repeat the following lines". **CMD:EndRepeat** is equivalent to "Next" or the end of the lines to repeat.

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.xltx*.	**a** Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, *iii*_Custom_QuantReport_ESTD_Summary.xltx, where "*iii*" are your initials.	• Make a copy of the QuantReport_ESTD_Summary_B_04_00.xltx template and rename it to *iii*_Custom_QuantReport_ESTD_Summary.xltx, 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 Add-Ins tab in the Ribbon. The Target Compound Information table is added at the end of the report. **c** Select rows 26 to 27. Click the row number 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** button in the shortcut menu to change the font.

Task 3. Add a single repeating section

Step	Detailed Instructions	Comments



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

Figure 86 Adding a single repeating section.

d Click **Add Formatting > Repeating Section** in the Add-Ins tab in the Ribbon.

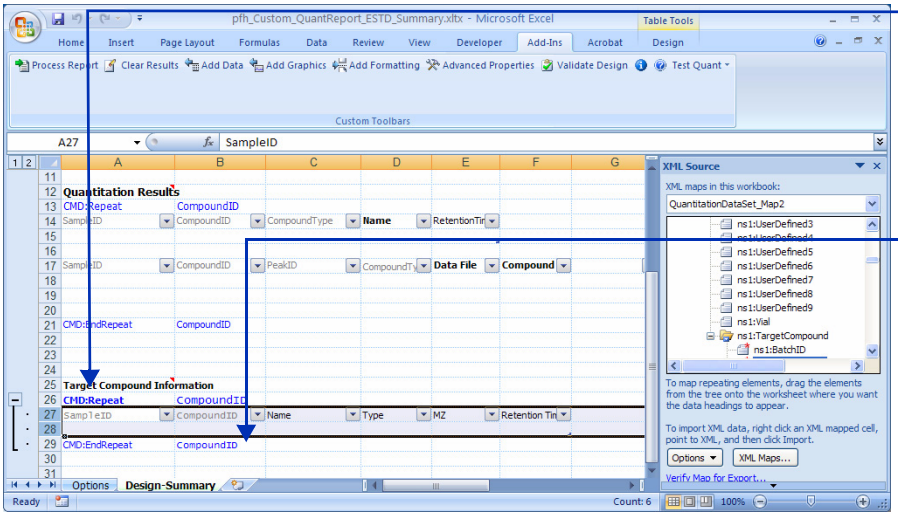
e In the Select Column dialog box, select **CompoundID**.

f Click **OK**.

- Usually, you repeat using one of the ID columns.
- In order 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

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

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 87 The repeating section is added around the Target Compound Information table

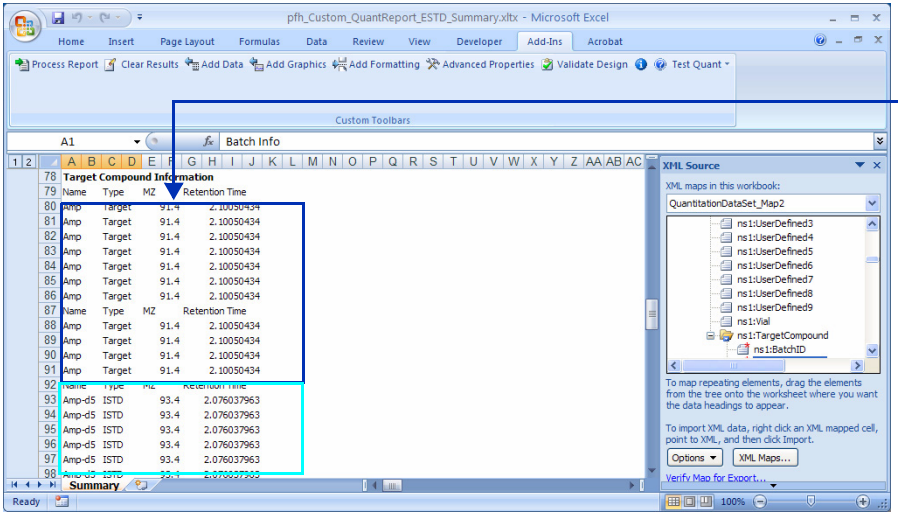
3 Test the changes to the template.

a Click **Process Report**.
b Click the **Browse** button.
c Navigate to the *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

Step	Detailed Instructions	Comments



The rows about each compound are grouped together.

Figure 88 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 Add-Ins 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_Custom_QuantReport_ESTD_Summary.xltx.

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

e Click **Save**.

- The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**.
- If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *\MassHunter\Report Templates\Quant\en-US\Letter\ESTD\Parts* folder.

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 127, 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

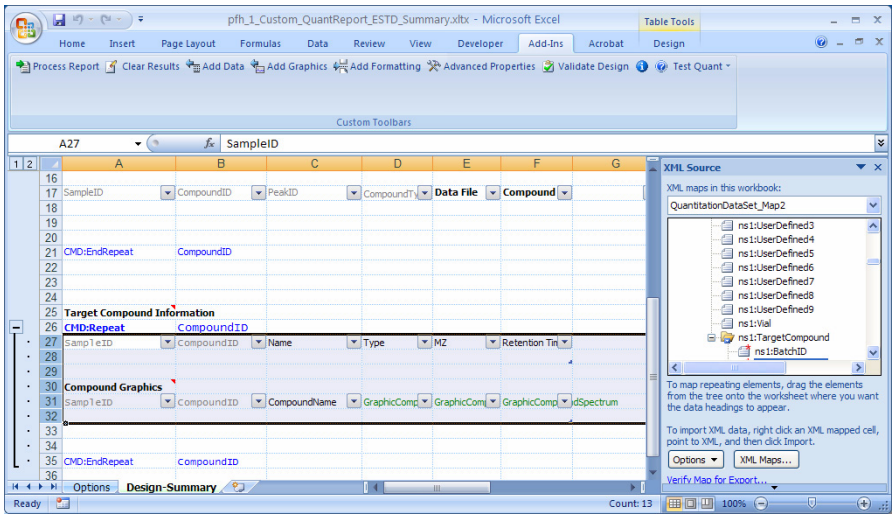
    Rows in the template
  - CMD:EndRepeat Item2
- CMD:EndRepeat Item1

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.xltx*.	**a** Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, *iii*_1_Custom_QuantReport_ESTD_Summary.xltx., where "*iii*" are your initials.	• If you do not have the iii_1_Custom_QuantReport_ESTD_Summary.xltx 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 Add-Ins tab in the Ribbon. **e** Select rows 27 to 32. Click the row number 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

Step	Detailed Instructions	Comments



Rows 27 through 32 are selected. The CMD:Repeat row and the CMD:EndRepeat rows are not selected.

Figure 89 Selecting both tables inside of the Repeating Section

f Click **Add Formatting > Repeating Section** in the Add-Ins 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

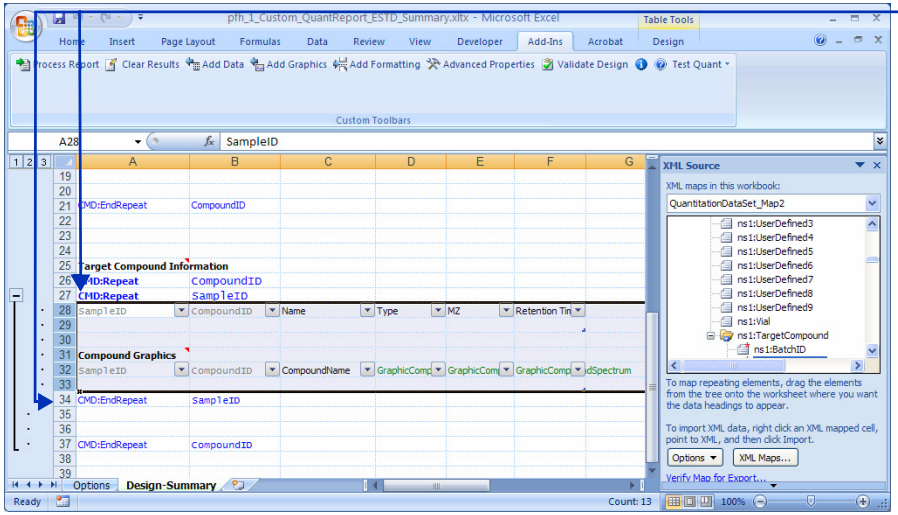
Step	Detailed Instructions	Comments
		**The command CMD:Repeat is added before the selected rows, and the command CMD:EndRepeat is added after the selected rows. Both of these commands are between the original CMD:Repeat CompoundID and CMD:EndRepeat CompoundID rows.**

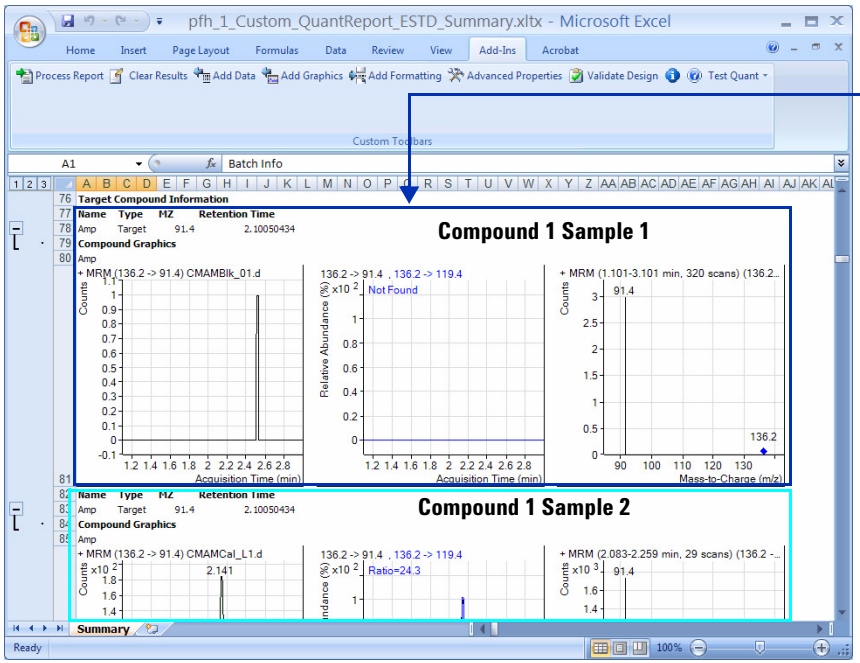
Figure 90 An inner repeating section is added which includes both tables

3 Test the changes to the template.

a Click **Process Report**.
b Click the **Browse** button.
c Navigate to the *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

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 91 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 Add-Ins 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_Custom_QuantReport_ESTD_Summary.xltx.

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

e Click **Save**.

- The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**.
- If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *\MassHunter\Report Templates\Quant\en-US\Letter\ESTD\Parts* folder.

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.

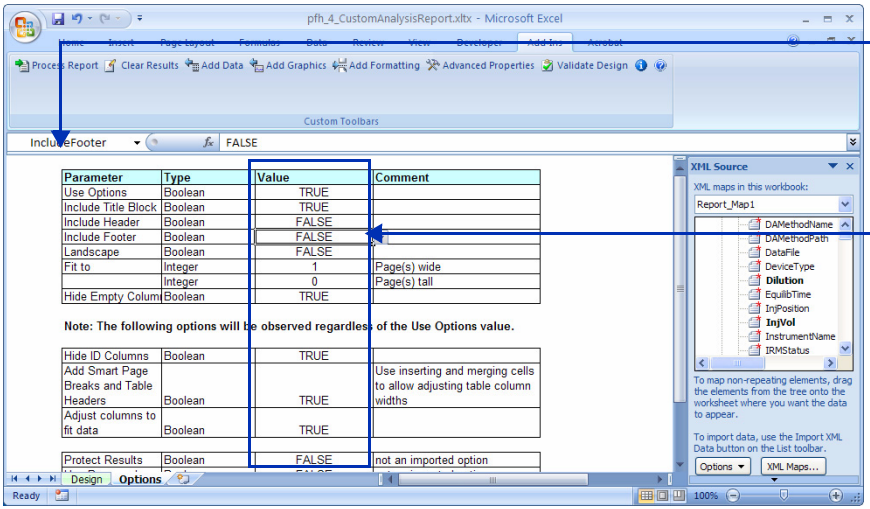
Two options that affect the speed of report generation are **Add Smart Page Breaks** and **Adjust Columns to Fit Data**. These options are needed for proper formatting of a report. However, if you are only interested in creating output for a LIMS system, you may choose to set both off these options to **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.xltx**, where *iii* are your initials.	**a** Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 32 to open the template, *iii*_4_CustomAnalysisReport.xltx, 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

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

Figure 92 Change the values in the Options worksheet

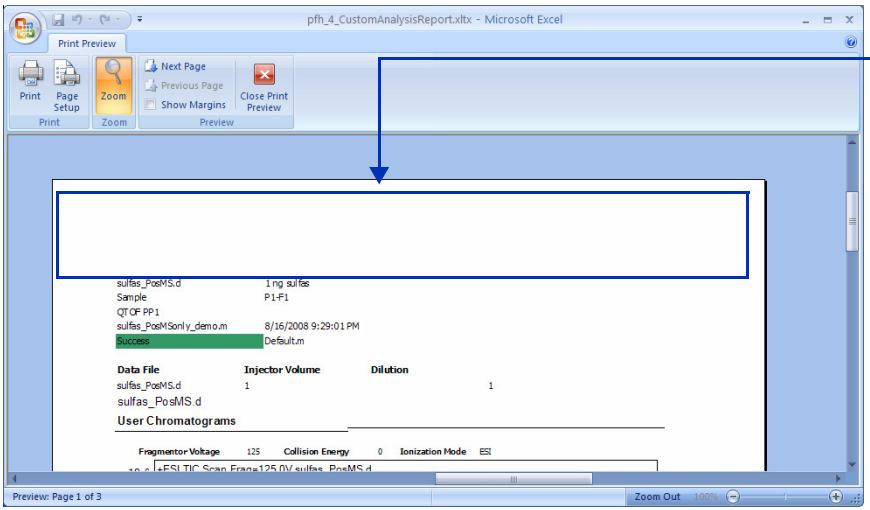
3 Test the changes to the template.

a Click **Process Report**.
b Click the **Browse** button.
c Navigate 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 Add-Ins tab in the Ribbon.

Task 5. Change values on the Options worksheet

Step	Detailed Instructions	Comments



The header and the footer are not included in the

The Qualitative Analysis program lets you set several of these options in the user interface. The values that you set here in the template are overridden by the values in the Qualitative Analysis user interface when you print from the Qualitative Analysis programs.

Figure 93 Verifying that the header and footer are not shown

4 Save the template to *iii*_5_CustomAnalysisReport.xltx, where *iii* are your initials.
- You have to clear the results first.

a Click **Clear Results** in the Add-Ins 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_CustomAnalysisReport.xltx.
d Verify the folder selected in **Save in** is correct.
e Click **Save**.

- The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**.
- If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *\MassHunter\Report Templates\Qual\en-US\Letter* folder.
- 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.xltx**, where *iii* are your initials.	**a** Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 32 to open the template, *iii*_5_CustomAnalysisReport.xltx, 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 Add-Ins tab in the Ribbon. **d** Click the Formulas tab. **e** Click **Insert Function**. **f** In the Insert 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.

Task 6. Add a formula using the IF function

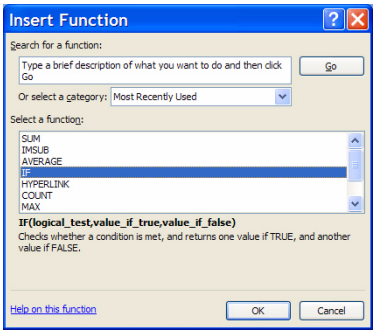
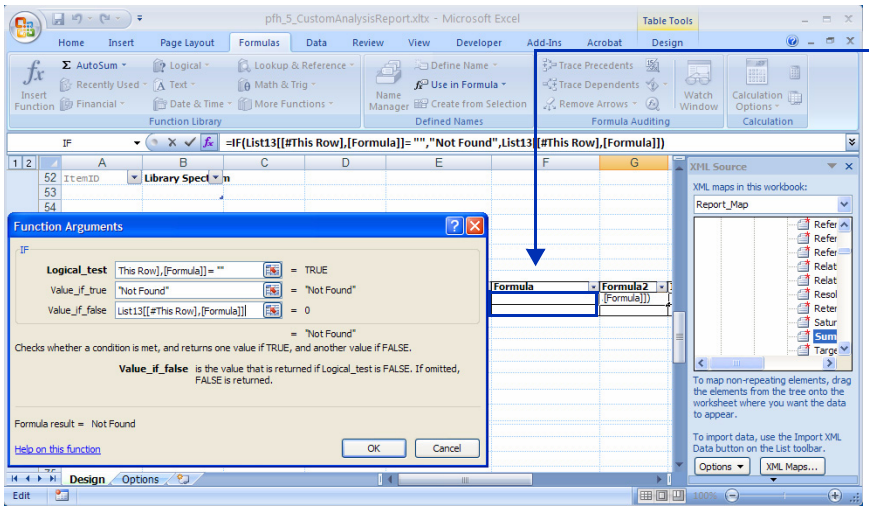
Step	Detailed Instructions	Comments
	**Select the IF function and click OK.**	

Figure 94 Select the **IF** function

	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**.	• 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

Step	Detailed Instructions	Comments



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 95 Enter the formula using the Function Arguments dialog box

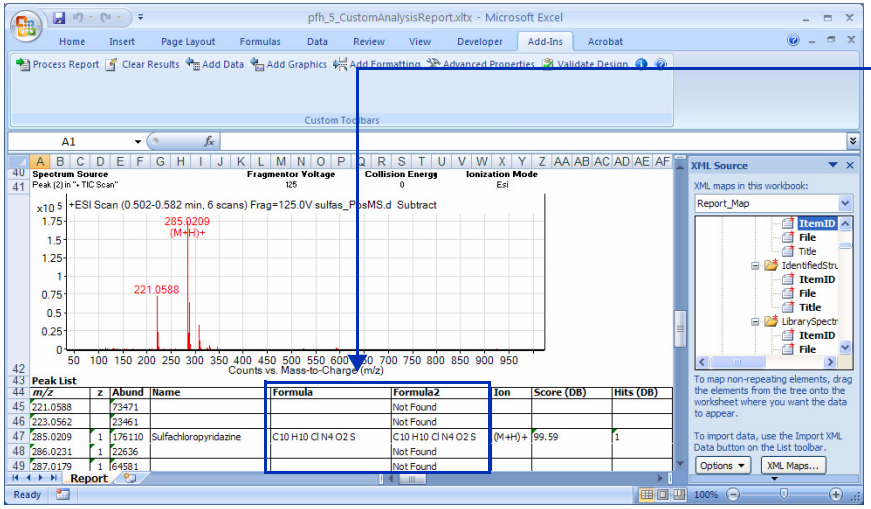
3 Test the changes to the template.

a Click **Process Report**.
b Click the **Browse** button.
c Navigate 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 Add-Ins 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

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 96 The empty cells in the Formula column are replaced with "Not Found" in the Formula2 column

4 Save the template to *iii*_6_CustomAnalysisReport.xltx, where *iii* are your initials.

- You have to clear the results first.

a Click **Clear Results** in the Add-Ins 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*_6_CustomAnalysisReport.xltx.

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

e Click **Save**.

- The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**.
- If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *MassHunter*\ *Report Templates**Qual**en-US*\ *Letter* folder.

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.

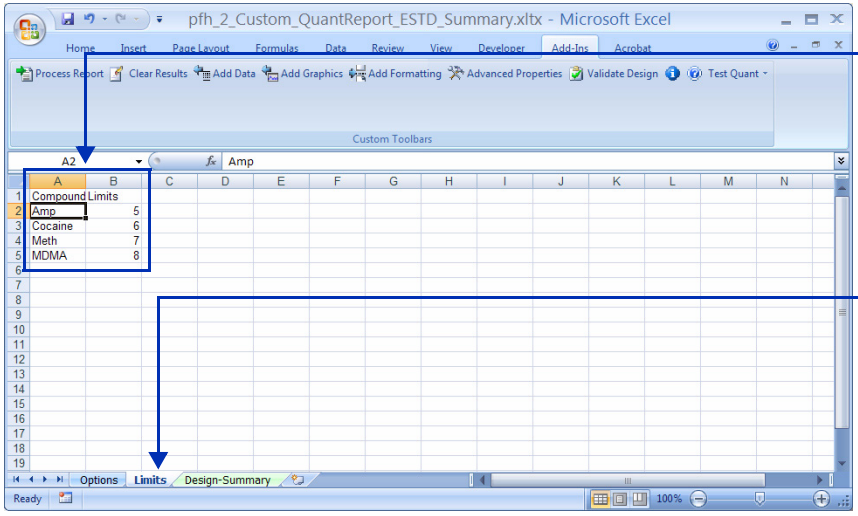
The VLOOKUP function does slow down processing of the report, so you want to make the VLOOKUP range as small as possible.

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.xltx.	**a** Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, *iii*_2_Custom_QuantReport_ESTD_Summary.xltx., where "*iii*" are your initials.	• If you do not have the iii_2_Custom_QuantReport_ESTD_Summary.xltx 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

Step	Detailed Instructions	Comments



The Compounds and Limits are added to the worksheet.

The name of the worksheet is changed to Limits.

Figure 97 Adding the new worksheet and renaming it Limits

k Click **Advanced Properties** in the Add-Ins tab in the Ribbon.

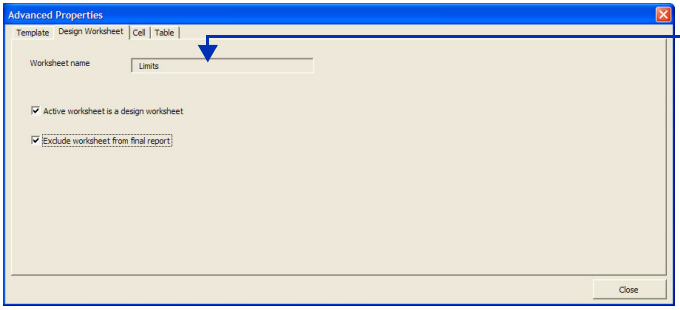
l Click the **Design Worksheet** tab.

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.

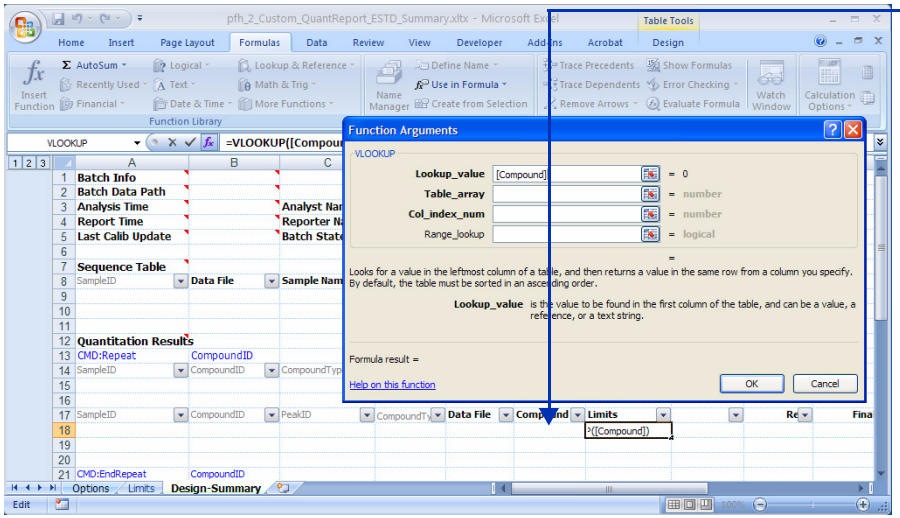


The name of the worksheet is shown in this dialog box, but you cannot edit it in this tab.

Figure 98 Mark both check boxes in this dialog box

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

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.

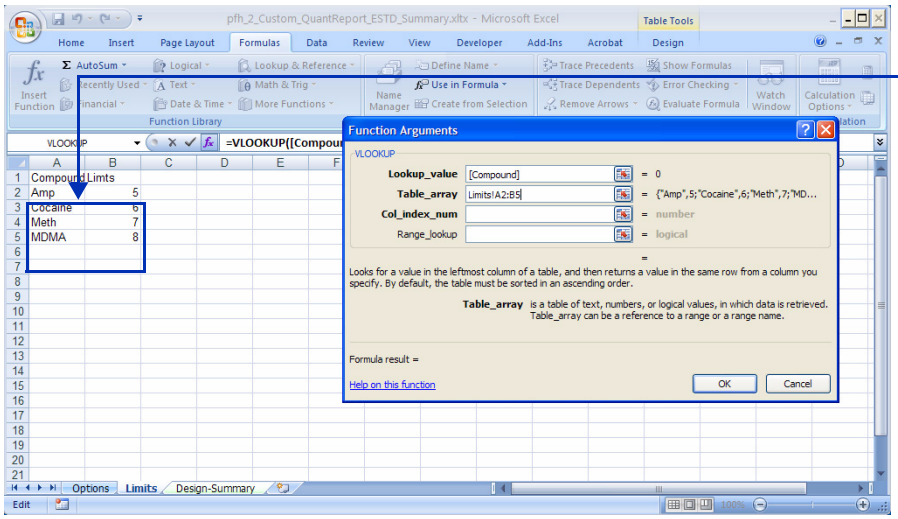


The Lookup_value is the value that you want to look up in the Limits worksheet. So, you click on the cell in the Compound column that contains the results. Do not click on the column header.

Figure 99 Add the Lookup_value to the Function Arguments dialog box

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

Step	Detailed Instructions	Comments
	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.



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

Figure 100 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

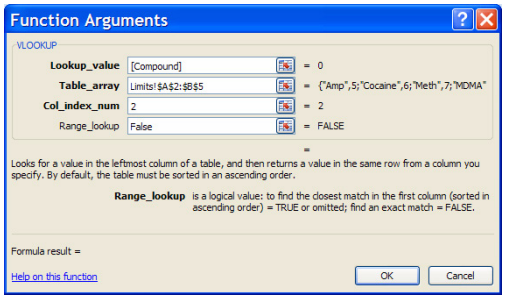
Step	Detailed Instructions	Comments
		**Select the area containing the compound names and limits. You do not include the column headers.**

Figure 101 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

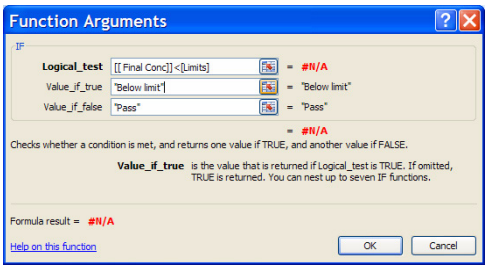
Step	Detailed Instructions	Comments
		**The quotation marks are automatically added when you leave the field.**

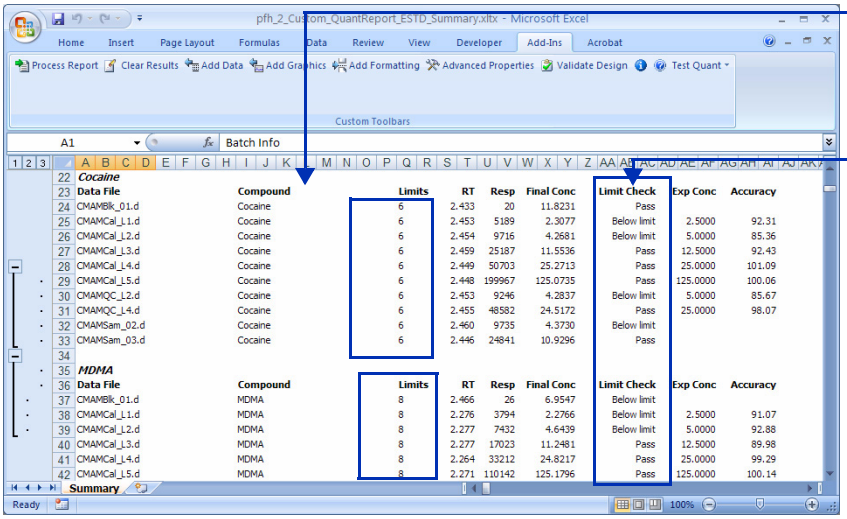
Figure 102 Adding the formula to see if the Final Concentration is above the limits from the VLOOKUP function

5 Test the changes to the template.

a Click **Process Report**.
b Click the **Browse** button.
c Navigate to the *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

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 103 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 Add-Ins 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_Custom_QuantReport_ESTD_Summary.xltx.

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

e Click **Save**.

- The **Save as type** is **Excel Template (*.xltx)** for most reports. If the report you are modifying has the extension .XLT, then the **Save as type** selection is **Excel 97-2003 Template (*.xlt)**.
- If you change the **Save as type**, the folder is automatically changed to the Microsoft *Templates* folder. Navigate to the *\MassHunter\Report Templates\Quant\en-US\Letter\ESTD\Parts* folder.

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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 2007 or Microsoft Excel 2010.

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