

# Agilent MassHunter Workstation Software Reporting

# **Familiarization Guide**



# Notices

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# **Software Revision**

If you have comments about this guide, please send an e-mail to feedback\_lcms@agilent.com.

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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.

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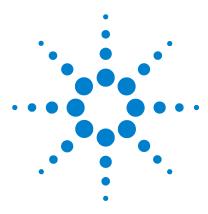
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# Exercise 1 Creating Reports

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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.

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# Task 1. Open the Qualitative Analysis program

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

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Task 1. Open the	Uuamanve Anai	vsis program		Die Gala mes
		,		p.0

Steps	Detailed Instructions	Comments	
<ol> <li>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.</li> </ol>	<ul> <li>a Double-click the Agilent MassHunter Qualitative Analysis icon, . The system displays the Open Data Files dialog box.</li> <li>b Go to the folder \MassHunter\Data or the folder where the example files are located.</li> </ul>	<ul> <li>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.</li> <li>You can get help for any window, dialog box, or tab by pressing the F1 key when that window is active.</li> </ul>	

- Make sure that **Use current method** is clicked.
- Make sure that the check box for Run 'File Open' actions from selected method is clear.

0 D-1 5"	£0		
Open Data File Look in	ExampleDat	taFiles 💌 🗢	<u>ک ک</u>
My Recent Documents Desktop My Documents	Casulfas_high_ Int sulfas_PosAu Int sulfas_PosM Int sulfas_PosM	utoMSMS.d S.d	
My Network Places	Filenames : Files of type :	" sulfas_PosAutoMSMS.d" " sulfas_PosN Data Files (".d)	IS.d"  Open Cancel Help
Options C Load worlds C Load results Use current Load result Run File O selected m	method method data pen' actions from	Sample Information Sample Name : User Name : Sample Position : Description :	

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

Task 1. Open the Qualitative Analysis program

Steps	Detailed Instructions	Comments
	<ul> <li>c Press and hold the Shift key while you click sulfas_PosAutoMSMS, sulfas_PosMS.d and sulfas-PosTargetedMSMS.d.</li> <li>d Click Open. All three data files are displayed in Data Navigator, and 3 chromatograms are displayed in the Chromatogram Results window.</li> </ul>	<ul> <li>If you press the Ctrl key instead, you can pick files which are not directly next to each other in the list.</li> <li>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.</li> </ul>

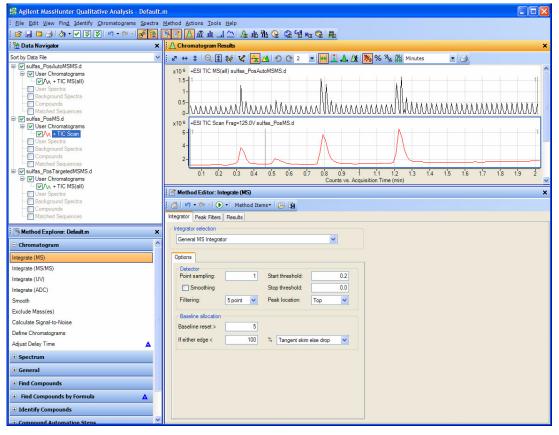
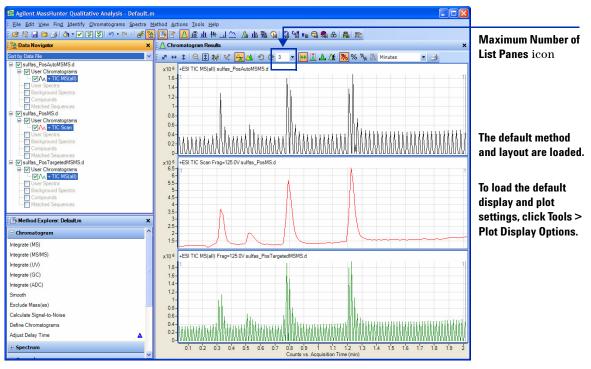


Figure 2 Qualitative Analysis main window

Task 1. Open the Qualitative Analysis program

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

Steps	Detailed Instructions	Comments	
<ul> <li>2 Return the main window to its default workflow, General. The default method and layout are loaded.</li> <li>Make sure you can see all three chromatograms.</li> </ul>	<ul> <li>a If necessary, click Tools &gt; Configure for Workflow &gt; General.</li> <li>b Click the down arrow next to the Maximum Number of List Panes icon in the Chromatogram Results Toolbar, and select 3.</li> </ul>	<ul> <li>The display and plot settings will remain the same even after you switch to the General workflow. These settings differ depending or your specific situation.</li> <li>You can change the layout by clicking the View &gt; Window Layouts &gt; Load Layout command.</li> </ul>	





# 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.

Steps	Detailed Instructions	Comments	
<b>1</b> Save the intermediate report files.	<ul> <li>a Click Tools &gt; Intermediate Report Files.</li> <li>b Mark the Keep intermediate report directories check box.</li> <li>c Click OK.</li> </ul>	your report templates, remember to	
<ul> <li>2 Change the analysis report selections:</li> <li>Mark the check boxes for the chromatograms, spectra or tables you want to print.</li> <li>Clear the check boxes for the chromatograms, spectra or tables you do not want to print.</li> </ul>	<ul> <li>a In Method Explorer, click General &gt; Analysis Report.</li> <li>b Mark the check boxes for any additional sections you want to print.</li> <li>c Clear any chromatogram and spectra choices you do not want to print.</li> </ul>	• After you have finished customizing your report templates, remember to clear the <b>Keep intermediate report</b>	

# Task 2. Print an analysis report

Task 2. Print an analysis report

### Task 2. Print an analysis report (continued)

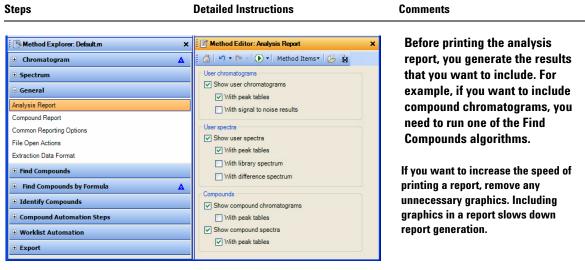


Figure 4 Analysis Report section in the Method Editor

3	Select the template to use when	а
	printing this report.	

- 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 2. Print an analysis report

Steps	Detailed Instructions	Comments
Method Explorer: Default.m	K Method Editor: Common Reporting Options	×
🗉 Chromatogram	🗄 🔄 🕶 🕶 🕑 🔹 Method Items 🕶 📴	
Spectrum	Templates Options	
🖻 General	General	Mark this check box if you do
Analysis Report Compound Report	Page orientation:            Page orientation:              • O Portrait               Landscape            Image: Hide empty columns in tables              • O Landscape               • O Landscape	not want to include empty columns in any table in the
Common Reporting Options	Show sample information	
File Open Actions	Peak table limits (include all peaks unless limits are specified)	report.
Extraction Data Format	Chromatogram peaks 10 largest peaks per table	
Find Compounds	Mass spectrum peaks 10 largest peaks per table	
Find by Auto MS/MS	Custom plot limits (autoscaled unless limits are specified)	
Find by Targeted MS/MS	User Chromatograms 2.000-10.000 min	You can specify the plot limits to
Find by Molecular Feature	Compound chromatograms min	
Find Compounds by Formula	MS spectra 100.0000-1200.0000 m/z	use in the report for each type of
Identify Compounds	MS/MS spectra m/z	graphic.
Compound Automation Steps	Deconvoluted spectra 15000.00-35000.00 Da	
Worklist Automation	UV spectra 240-330 nm	
Export		

# Task 2. Print an analysis report (continued)

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

# 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.

Step	Detailed Instructions	
<b>1</b> Save the intermediate report files.	<ul> <li>a Click Tools &gt; Intermediate Report Files.</li> <li>b Mark the Keep intermediate report directories check box.</li> <li>c Click OK.</li> </ul>	<ul> <li>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.</li> <li>After you have finished customizing your report templates, remember to clear the Keep intermediate report directories check box.</li> </ul>
<ul> <li>2 Change the compound report selections:</li> <li>Run one of the Find Compounds algorithms</li> <li>Mark the check boxes for the chromatograms, spectra or tables you want to print.</li> <li>Clear the check boxes for the chromatograms, spectra or tables you do not want to print.</li> </ul>	Click <b>File &gt; Open Data File</b> to load a data file. Click one of the commands in the <b>Find</b> menu to find compounds. In Method Explorer, click <b>General &gt;</b> <b>Compound Report</b> . Mark the check boxes for any additional sections you want to print. Clear any chromatogram and spectra choices you do not want to print.	<ul> <li>Only sections that are marked in the Compound Report tab are included in the report.</li> <li>A section in a report is only included if: <ul> <li>You mark the check box in this section.</li> <li>The results are available in the Qualitative Analysis program. For example, if you have not found compounds, then the compound table cannot be included.</li> <li>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</li> </ul> </li> </ul>

are customizing a template.

Task 3. Print a compound report

#### Task 3. Print a compound report

Step	Detailed Instructions	Comments
Method Explore: Default.m × Chromatogram A	Image: Second Report       Image: Second Repor	× To increase the speed of creating a
Spectrum General Analysis Report Compound Report Common Reporting Options File Open Actions Extraction Data Format File Gen Actions Extraction Data Format Find Compounds Find Compounds General Automation Extraction Export Export Export	Compounds  Compound set Sort by: Retention time Sort order: Increasing  Exclude details for unidentified compounds  Commatograms Show user chromatogram(s)  Show compound chromatogram(s)  Compound spectrum Show MS spectrum Show MS spectrum Show MS spectrum Compound spectrum (zoomed in on special peaks) Compound spectrum (zoomed in on special peaks) Compound spectrum Show MS spectrum Compound spectrum Show MSMS spectrum Compound spectrum Show MSMS spectrum Show MSMS spectrum Show MSMS peak table Compound spectrum Show MSMS spectrum Show difference spectrum	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.

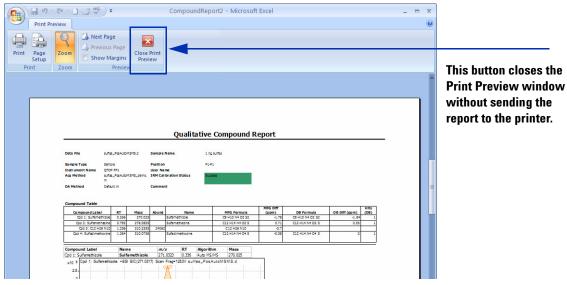
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- e Verify the settings on this tab.
- The report templates that are shipped with the software are separated into two folders. One folder contains reports that are formatted to print on Letter size paper. The other folder contains reports that will print on A4 size paper.
- Several different compound report templates are available in each folder.

Task 3. Print a compound report

#### Task 3. Print a compound report

Step	Detailed Instructions	Comments
<ul> <li>Print the report.</li> <li>Preview the report.</li> </ul>	<ul> <li>a Click the arrow in the  icon and select Print Compound Report to print the report.</li> <li>b In the Print Compound Report dialog box, click All results.</li> <li>c Mark Print report.</li> <li>d Mark Print preview.</li> <li>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.</li> <li>f Click OK.</li> </ul>	<ul> <li>You also can print a compound report by doing any of the following</li> <li>Right-click the Compound Report section in the Method Editor, and click Print Compound Report.</li> <li>Click File &gt; Print &gt; Compound Report.</li> <li>Click Generate Analysis Report in the Actions menu.</li> <li>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.</li> </ul>





- 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

S	tep	Detailed Instructions	Comments
1	Save the intermediate report files.	<ul> <li>a Click Tools &gt; Intermediate Report Files.</li> <li>b Mark the Keep intermediate report directories check box.</li> <li>c Click OK.</li> </ul>	<ul> <li>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.</li> <li>After you have finished customizing your report templates, remember to clear the Keep intermediate report directories check box.</li> </ul>
2	<ul> <li>Select the folder to use when printing this report.</li> <li>You can select the folder to use.</li> <li>A graphic report always uses either the template graphic.xltx or graphicfullpage.xltx.</li> </ul>	<ul> <li>a In Method Explorer, click General &gt; Common Reporting Options.</li> <li>b Verify that the correct Report template folder is selected.</li> </ul>	• 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.	<ul> <li>a Right-click the Chromatogram Results window and click Print.</li> <li>b In the Print dialog box, click All chromatograms.</li> <li>c Clear the One chromatogram per page check box.</li> <li>d Select the Printer name.</li> <li>e Mark the Print Preview check box.</li> <li>f Click the Options tab.</li> <li>g Review the settings.</li> <li>h Click OK.</li> </ul>	<ul> <li>You can only print a graphic if a graphic is currently showing in the Qualitative Analysis program.</li> <li>You can print a graphics report from any of the graphics windows including:         <ul> <li>Chromatogram Results window</li> <li>Spectrum Preview window</li> <li>MS Spectrum Results window</li> <li>Deconvolution Results window</li> <li>UV Spectrum Results window</li> <li>If the <b>One chromatogram per page</b> check box is marked, then the graphicfullpage.xltx template is used.</li> </ul> </li> </ul>

Task 4. Generate a graphics report

# Task 3. Print a graphics report

Step D	etailed Instructions	Comments
Print	Print	
A Pint Options     Report contents     All chromatogram(s)     Only highlighted chromatogram(s)     Only visible chromatogram(s)     Only visible chromatogram(s)     One chromatogram per page     Report destination     Printer name: Adobe PDF     Yint Preview      OK Cance	Print Options Contents V Include header V Include footer	Orientation Portrait Landscape OK Cancel

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

Print Previ	ew Alter Page Close Print Show Margins Close Print Preview	Graphic1 - Microsoft Excel	_ = x @	
Print	Zoom Preview	ualitative Plot Window Report		This button closes the Print Preview window without sending the report to the printer.
Preview. Page 1 of 1	x10 s +ESI TIC Scan Frag=125.0V	DE 07 08 09 11 11 12 13 14 15 16 17 18 19 2 Counts acquisiton Time (min) suttas_PoeMS.d	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	

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.

1

Task 5. Open a batch in the Quantitative Analysis program

# 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
<ol> <li>Open the Quantitative Analysis program and then open a batch file.</li> <li>Select either the default batch or the batch you created if you did the exercises in the Quantitative Analysis Familiarization Guide.</li> </ol>	<ul> <li>a Double-click the Agilent MassHunter Quantitative Analysis (QQQ) icon</li> <li>b Click File &gt; Open Batch.</li> <li>c Navigate to the folder \ Your Directory \DrugsOfAbuse\.</li> <li>d Select a batch. You can select either DrugsOfAbuseDemo.batch.xml of <i>iii_Test_01.</i></li> <li>e Click Open.</li> </ul>	<ul> <li>You can also start the program by clicking Programs &gt; Agilent &gt; MassHunter Workstation &gt; Quantitative Analysis (QQQ) from the Start menu.</li> <li>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.</li> <li>You can get help for any window, dialog box, or tab by pressing the F</li> </ul>

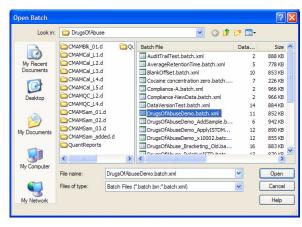


Figure 10 Open a batch file

key when that window is active.

Task 5. Open a batch in the Quantitative Analysis program

	Task 5. Open the Quantitative Analysis program (conti	nued)
--	---	-------

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

	gilent	t MassHunte	er Quantitative A	Analysis - E	)rugs()	fAbuse - pfh_Repor	t_01										
File	Edit	View Analyz	e Method Update	e Report To	ols He	lp											
Ð		🖬 i 📭 i 🗘	Analyze Batch	🕜 🤅 Layo	out: 🕎		Restore Def	ault Lay	out								
atch	n Table	e															
Sa	mple:	1 J. S	ample Type: <all></all>		Compou	ind: 💓 Amp		-	🔿 IST	D:	Amp-d5				1	2	8
	_		San	nple	_		Amp Met_			_	Amp Result	is		Qualif	ier	Amp-d5	5 (IST.
(1)	7	7 Name	Data File	Туре	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	RT	Resp
Ĭ	)	Blank-1	CMAMBIk 01.d	Blank		5/12/2006 1:48 PM				Пİ							
Г	8	Calib-L1	CMAMCal_L1.d	Cal	L1	5/12/2006 1:51 PM	2.5000	2.141	658		3.3187	3.3187	132.7	24.3		2.129	139
	\$	Calib-L2	CMAMCal_L2.d	Cal	L2	5/12/2006 1:54 PM	5.0000	2.140	1059		5.7493	5.7493	115.0	33.5		2.128	129
L		Calib-L3	CMAMCal_L3.d	Cal	L3	5/12/2006 1:57 PM	12.5000	2.134	2673		13.6808	13.6808	109.4	26.7		2.121	137
L		Calib-L4	CMAMCal_L4.d	Cal	L4	5/12/2006 2:00 PM	25.0000	2.022	4952		26.7561	26.7561	107.0	29.1		1.990	130
L		Calib-L5	CMAMCal_L5.d	Cal	L5	5/12/2006 2:03 PM	125.0000	2.101	18605		124.4844	124.4844	99.6	27.0		2.076	105
L	_	QC-L2	CMAMQC_L2.d	QC	L2	5/12/2006 2:06 PM	5.0000	2.142	1006		5.2293	5.2293	104.6	27.7		2.131	135
L	_	QC-L4	CMAMQC_L4.d	QC	L4	5/12/2006 2:09 PM	25.0000	2.135	4716		27.8039	27.8039	111.2	25.6		2.121	119
•		Sample-1	CMAMSam_01.d	Sample	_	5/12/2006 2:12 PM		0.4.10	4004	님	1 0077	1 0077		00.0	님	0.400	
L	_	Sample-2	CMAMSam_02.d CMAMSam 03.d	Sample Sample	_	5/12/2006 2:15 PM 5/12/2006 2:18 PM		2.143	1004 2590		4.8977	4.8977		30.9 25.3	Н	2.130	144
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np Z	↔ M (136 0 <sup>2</sup> 8-	‡ <u>&amp;</u> 🛣	AMCal_L4.d		Ш Ш		Close Amp - 5	↔ Levels, 1 y = 7 R <sup>2</sup> 6-	5 Levels	Use	ed, 5 Points, 5			Weig	ht: N	L. V	IST
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mp Z	↔ M (136 0 <sup>2</sup> 8-	‡ <u>&amp;</u> 🛣	AMCal_L4.d		ş ılı		Close Amp - 5	↔ \$ Levels, 1 y = 7 R^2 6-	5 Levels	Use	ed, 5 Points, 5			Weig	ht: N		ISTI
np Z	↔ M (136 0 <sup>2</sup> 8- 7-	‡ <u>&amp;</u> 🛣	AMCal_L4.d		<u>ş</u> TF		Close Amp - 5 Sa x10 Gds 1. 4 4 4 1. 1. 1.	↔ \$ Levels, 1 y = 7 R^2 6-	5 Levels	Use	ed, 5 Points, 5			Weig	ht: N		IST
np Z	↔ M (136 0 <sup>2</sup> 8- 7- 6-	‡ <u>&amp;</u> 🛣	AMCal_L4.d		<u>ş</u> ılı <u>ş</u>		Close Amp - 5 Sa x10 Gds 1. 4 4 4 1. 1. 1.	↔ Levels, 1 y = 7 - R^2	5 Levels	Use	ed, 5 Points, 5			Weig	ht: N	• •	IST
np Z	↔ M (136 0 <sup>2</sup> 8- 7- 6- 5- 4-	‡ <u>&amp;</u> 🛣	AMCal_L4.d		± ⊥IT ₹		Close Amp - 5 38 x10 505 1.1 - - - - - - - - - - - - - - - - - -	↔ Levels, 1 - y = 7 R^2	5 Levels	Use	ed, 5 Points, 5			Weig	ht: N		IST
mp Z	↔ M (136 0 <sup>2</sup> 8 7 6 5 5 4 3	‡ <u>&amp;</u> 🛣	AMCal_L4.d		j ⊥T T		Close Amp - 5 38 x10 10 44 1. 24 1. 24 1. 20 0. 0. 0.	↔ \$ Levels, 1 y = 7 R^2 6- 4- 2- 1- 8- 6-	5 Levels	Use	ed, 5 Points, 5			Weig	ht: N		IST
mp Z	↔ M (136 0 <sup>2</sup> 8- 7- 6- 5- 4-	‡ <u>&amp;</u> 🛣	AMCal_L4.d		L II E		Close Amp - 5 38 x10 505 1.1 - - - - - - - - - - - - - - - - - -	↔ \$ Levels, 1 y = 7 R^2 6- 4- 2- 1- 8- 6-	5 Levels	Use	ed, 5 Points, 5			Weig	ht: N	L	ISTI
mp Z	↔ M (136 0 <sup>2</sup> 8 7 6 5 5 4 3	‡ <u>&amp;</u> 🛣	AMCal_L4.d				Close Amp - 5 38 x10 10 44 1. 24 1. 24 1. 20 0. 0. 0.	↔ \$ Levels. 1 y = 7 R^2 6- 1 - 8- 6- 4 -	5 Levels	Use	ed, 5 Points, 5			Weig	ht: N		ISTI
mp 2	↔ M (136 0 <sup>2</sup> 8- 7- 6- 5- 4- 3- 2-	‡ <u>&amp;</u> 🛣	AMCal_L4.d				Close Amp - 5 ss x10 ds 1. dc 1. extra tree 0. 0. 0. 0. 0.	↔ \$ Levels. 1 y = 7 R^2 6- 1 - 8- 6- 4 -	5 Levels	Use	ed, 5 Points, 5			Weig	ht: N		ISTI
mp 2	↔ M (136 0 <sup>2</sup> 8- 7- 6- 5- 4- 3- 2- 1-	‡ <u>&amp;</u> 🛣	AMCal_L4.d				Close Amp - 5 ss x10 ds 1. dc 1. extra tree 0. 0. 0. 0. 0.	↔ \$ Levels. 1 y = 7 R^2 6- 4- 2- 1- 8- 6- 4- 2- 1- 2- 2- 1- 2- 2- 1- 2- 1- 2- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 1- 2- 1- 1- 2- 1- 1- 2- 1- 1- 1- 2- 1- 1- 1- 1- 1- 1- 1- 1- 1- 1	5 Levels	2480	sd, 5 Points, 5	Points Used	1.2 QCs	Weig	ht: N		ISTI
mp 2	↔ M (136 0 <sup>2</sup> 8 7 6 5 4 3 2 2 1 0	\$ <u>A</u> <u>⊼</u> 2->91.4) CM	AMCal_L4.d 2.	022 min.			Close Amp - 5 39 x10 50 11 49 1. 41 12 49 12 49 12 40 40 40 40 40 40 40 40 40 40 40 40 40	↔ \$ Levels. 1 y = 7 R^2 6- 4- 2- 1- 8- 6- 4- 2- 1- 2- 2- 1- 2- 2- 1- 2- 1- 2- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 1- 2- 1- 1- 2- 1- 1- 2- 1- 1- 1- 2- 1- 1- 1- 1- 1- 1- 1- 1- 1- 1	5 Levels	2480	ed, 5 Points, 5	Points Used	1.2 QCs	1.8	2 2	22 2	4 2
mp NRI	↔ M (136 0 <sup>2</sup> 8 7 6 5 4 3 2 2 1 0	\$ <u>A</u> <u>⊼</u> 2->91.4) CM	AMCal_L4.d 2.	022 min.			Close Amp - 5 § x10 6 0. 0. 0. 0. 0. 0. 0. 0. 0.	↔ \$ Levels. 1 y = 7 R^2 6- 4- 2- 1- 8- 6- 4- 2- 1- 2- 2- 1- 2- 2- 1- 2- 1- 2- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 2- 1- 1- 2- 1- 1- 2- 1- 1- 2- 1- 1- 1- 2- 1- 1- 1- 1- 1- 1- 1- 1- 1- 1	5 Levels (0935 * x = 0.99942	2480	sd, 5 Points, 5	Points Used	1.2 QCs	1.8	2 2		4 2

Figure 11 Quantitative Analysis program after analyzing batch

Task 6. Generate quantitation reports using the standard dialog box

# 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.

Steps	Detailed Instructions	Comments
<ol> <li>If necessary, open the batch file <i>iii_Report_01.batch.xml</i>.</li> <li>If the batch is already open, skip to step 2.</li> </ol>	<ul> <li>a To start the Quantitative Analysis program, click the Quantitative Analysis (QQQ) icon on your Desktop.</li> <li>b Click Open Batch and the toolbar to display the Open Batch dialog box.</li> <li>c Navigate to \Your Directory \DrugsOfAbuse and select iii_Test_01.batch.xml.</li> <li>d Click Open.</li> </ul>	<ul> <li>You can also start the program by clicking Programs &gt; Agilent &gt; MassHunter Workstation &gt; Quantitative Analysis (QQQ) from the Start menu.</li> <li>If the default layout is not shown, click Restore Default Layout on the toolbar before opening the batch. Restore <u>D</u>efault Layout</li> </ul>
<ul> <li>2 Select report options.</li> <li>The first template is Quantreport_ISTD_ResultsSum mary_B_04_00.xltx</li> <li>The Reports folder should be \ Your Directory\ DrugsofAbuse\QuantReports.</li> <li>The default filename is <i>iii_Test_01</i>, where "<i>iii</i>" are your initials.</li> </ul>	<ul> <li>a Click Report &gt; Generate. The system displays the standard Report dialog box.</li> <li>b Click</li></ul>	<ul> <li>You can only add one report at a time using the standard Report dialog box.</li> <li>The report is automatically printed to the default printer.</li> </ul>

Task 6. Generate quantitation reports using the standard dialog box

Task 6. Generate quantitation reports using the standard dialog box

#### Steps **Detailed Instructions** Comments Report X Template file: t Templates\Quant\en-US\A4\ISTD\Results\QuantReport\_ISTD\_ResultsSummary\_B\_04\_00xttx Report folder: C:\MassHunter\Data\DrugsOfAbuse\QuantReports\pfh\_Report\_01 Batch report Single sample report for selected samples Start Queue Viewer Advanced... OK Cancel **3** Generate the report. a Click OK in the Report dialog box to • One job is added to the queue. The • View the status of the report generate the report. reports are printed in the order generation in the Task Queue **b** Click **Report > Queue Viewer** to requested. You can see the status of Viewer. monitor the report generation process. the reports in the Queue Viewer The system displays the Task Queue program. Viewer program. c Watch the progress of the report in the Status column.

#### Task 6. Generate quantitation reports using the standard dialog box

Task 6. Generate quantitation reports using the standard dialog box

eps	Detailed Instructions		Comments
	🗿 Agilent MassHunter Quantitative Analysis - Task Queu	e Viewer	
	File Service Tasks Action Help		
	) 🗈 🛛 🛃 🕅 🖉		
	Name Creation Time	Status	Completion
	₩DugsOfAbuse_pfh_Report_01.20100209.100204.p 2/9/2010 104	12:04 AM Process.	
	<		>
	<b>3</b> ]		Connected;
	Agilent MassHunter Quantitative Analysis - Task Queur      File Service Tasks Action Help      Our DELX C*	) Viewer	
	File     Service     Tasks     Action     Help       Image:	Status	Connected ,;;
	File     Service     Tasks     Action     Help       Image:	Status	Connected ,;;
	File     Service     Tasks     Action     Help       Image:	Status	Connected ,;;

# Task 6. Generate quantitation reports using the standard dialog box

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

# 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.

Steps	Detailed Instructions	Comments
<ol> <li>If necessary, open the batch file <i>iii</i>_<b>Report_01.batch.xml</b>.</li> <li>If the batch is already open, skip to step 2.</li> </ol>	<ul> <li>a To start the Quantitative Analysis program, click the Quantitative Analysis (QQQ) icon on your Desktop.</li> <li>b Click Open Batch and an on the toolbar to display the Open Batch dialog box.</li> <li>c Navigate to \ Your Directory \ DrugsOfAbuse and select iii_Test_01.batch.xml.</li> <li>d Click Open.</li> </ul>	<ul> <li>You can also start the program by clicking Programs &gt; Agilent &gt; MassHunter Workstation &gt; Quantitative Analysis (QQQ) from the Start menu.</li> <li>If the default layout is not shown, click Restore Default Layout on the toolbar before opening the batch.</li> <li>Restore Default Layout</li> </ul>
<ul> <li>2 Start to generate a report using the advanced Report dialog boxes.</li> <li>The destination directory should be \ Your Directory \ DrugsofAbuse \ QuantReports.</li> <li>The default filename is iii_Test_01, where "iii" are your initials.</li> </ul>	<ul> <li>a Click Report &gt; Generate. The system displays the standard Report dialog box.</li> <li>b Click Advanced.</li> <li>c Click Generate report results file.</li> </ul>	<ul> <li>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.</li> <li>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.</li> </ul>

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

Steps	<b>Detailed Instructions</b>	Comme
	Report	
	Report results file Choose to generate report results file or use existing file. Choo report results file is generated.	se batch file from which the
	Generate report results file     Choose a batch file from which the report results file is general     Batch file:     Batch file:     Differ:     Differ:	
	Use existing report results file/report graphics files     Report folder:     C:\MassHunter\Data\DrugsOfAbuse\QuantReports\pfh_Report	_01-2 Brgwse
	Queue Viewer <back next=""></back>	Enish Cancel

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

- **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.

Report graphics files	
	, and specify graphics options. Tum off when you know do not use graphics files. Tuming off will reduce report
Generate graphics files	
Instrument type determining nume	eric formats in graphics files
	-
Load graphics settings file	
	Browse
Load fixed graphics file	Browse
Load fixed graphics file	Biowse
Load fixed graphics file	Edt Browse
Load fixed graphics file	Edt Browse

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

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

Steps	Detailed Instructions	Comments		
<ul> <li>Add two templates.</li> <li>The first template is Quantreport_ISTD_ResultsSum mary_B_04_00.xltx</li> <li>The second template is QuantReport_ISTD_ ResultsByCompound_FAST_B_ 04_00.xltx.</li> <li>Make sure the report name is <i>TemplateName</i> xlsx, where <i>TemplateName</i> is the exact name of the template.</li> </ul>	<ul> <li>a Click Add under Reports. The system displays the Open dialog box.</li> <li>b Navigate to the Letter\ISTD\Results folder.</li> <li>c Select <ul> <li>Quantreport_ISTD_ResultsSummary_</li> <li>B_03_01.xltx and click Open.</li> <li>The program adds the template to the Template field in the Reports pane.</li> <li>d In the Report File Name column in the Reports table, verify that the template is</li> <li>QuantReport_ISTD_Results_B_03_01</li> <li>.xlsx.</li> <li>e Select a printer for this report.</li> <li>f Click Add under Reports. The system displays the Open dialog box.</li> <li>g Select</li> <li>Quantreport_ISTD_ResultsByCompound_FAST_B_04_00.xltx. Click Open.</li> <li>h Verify that the template is</li> <li>QuantReport_ISTD_Results_B_03_01</li> <li>.xlsx.</li> </ul> </li> </ul>	<ul> <li>Note that the <b>B_03_01</b> designatio corresponds to the Quantitative Analysis software release, which will change over time. Therefore, the report file names may change correspondingly.</li> <li>If you want to print to A4 paper, navigate to the A4 folder.</li> <li>Templates are separated into the following folders: <ul> <li>ESTD</li> <li>ISTD</li> <li>LIMS</li> <li>Method</li> <li>misc</li> <li>Outliers - this folder contains several folders for the different types of outliers.</li> <li>UnknownsAnalysis</li> </ul> </li> </ul>		
	Click Next			

j Click Next.

Report Reports Choose template files, report file names, printers, and publish formats	The Report File Name is filled in automatically.
Template Report File Name Printer Publish Format	
C:\MassHunter\Rep_mary_B_04_00.xltx 🛄 QuantReport_IB_04_00.xlsx Adobe PDF 🛛 🗹 None> 💌	
C:\MassHunter\Rep.FAST_B_04_00.xttxQuantReport_IB_04_00.xtsx Addbe PDF V None> V	You select a printer for each template.
Add     Bemove       Queue Viewer     Stack       Next >     Brigh       Cancel	

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

<b>T</b>   7	<u> </u>						D (	11 I.	1
IASK /.	Generate (	quantitation	reports	usina	the	advanced	Report	gialog	poxes

Steps	Detailed Instructions	Comments
5 Specify which samples and compounds to include in the report.	<ul> <li>a Click Batch report.</li> <li>b Mark All samples.</li> <li>c Mark All compounds.</li> </ul>	<ul> <li>You can create a separate report for each sample by clicking Single sample report.</li> </ul>
<ul> <li>Select the Batch report option</li> </ul>	l.	

- Select All samples.
- Select All compounds.

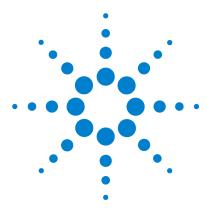
eport			×
Samples/Compounds			
Choose report mode, samp	es and compounds.		
Report mode:			
<ul> <li>Batch report</li> </ul>	O Single sample report		
Samples:			
All samples	Choose samples		
Compounds:			
All compounds	Choose compounds		
Queue Viewer		< <u>Back</u> Next > Einish Cancel	1
			<u>ر</u>

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.

🕟 💷 🔯 🗙 🝽			
Name	Creation Time	Status	Completion
DrugsOfAbuse_pfh_Report_01.20100209.100204.d	2/9/2010 10:02:04 AM	Done	2/9/2010 10:03:11 AM
DrugsOfAbuse pfh Report 01.20100209.111821.p	2/9/2010 11:18:21 AM	Process	
- 10			
			>

d Close the Task Queue Viewer program.



Agilent MassHunter Workstation Software Reporting Familiarization Guide

# **Exercise 2 Customizing a template**

Task 1. Open a Qualitative Analysis template 32

Task 2. Customize the footer of the Qualitative Analysis template 34

Task 3. Use the new template in the Qualitative Analysis program 39

Task 4. Open a Quantitative Analysis template 42

 Task 5. Customize the footer of the Quantitative Analysis template
 44

Task 6. Use the new template in the Quantitative Analysis program 48

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.

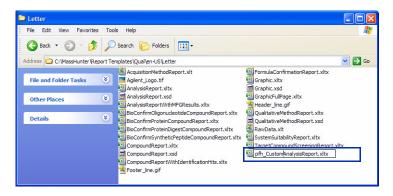


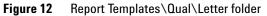
# Task 1. Open a Qualitative Analysis template

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

Task 1. Open a Qualitative Analysis template	Task 1. Or	oen a Qualita	ative Analys	is template
--	------------	---------------	--------------	-------------

Step	Detailed Instructions	Comments	
<ol> <li>Make a copy of the AnalysisReport.xltx file and rename the file iii_CustomAnalysisReport.xltx</li> </ol>	<ul> <li>a Open the Windows Explorer program.</li> <li>b Navigate to the <i>Report Templates</i> \ <i>Qual</i> folder in the folder where you installed the data.</li> <li>c Navigate to the <i>Letter</i> or A4 folder</li> <li>d Right-click the <i>AnalysisReport.xltx</i> file and click Copy.</li> <li>e Click Edit &gt; Paste to add a copy of the report template to the current folder.</li> <li>f Right-click the new file, Copy of AnalysisReport.xltx and click Rename.</li> <li>g Type <i>iii CustomAnalysisReport.xltx</i>.</li> </ul>	<ul> <li>You do the same steps to open a Quantitative Analysis template.</li> <li>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.</li> </ul>	





- **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.

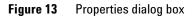
 If a template is read-only, you cannot save any changes to the template.

# Customizing a template 2

Task 1. Open a Qualitative Analysis template

Step	Detailed Instructions	Comments
	pfh_CustomAnalysisReport.xltx Properties         General       RoboSource         pfh_CustomAnalysisReport.xltx         Type of file:       Mcrosoft Office Excel Template         Opens with:       Mcrosoft Office Excel       Change         Location:       C:MassHurter/Report Templates/Qual/en-USV         Size:       55.2 KB (55.58 bytes)         Size on disk:       56.0 KB (57.344 bytes)         Created:       Today, February 08, 2010, 9:41:03 AM         Modified:       Tuesday, May 19, 2009, 5:08:28 AM         Accessed:       Today, February 08, 2010, 9:41:32 AM         Attributes:       Read-only       Hidden         Advanced       OK       Cancel       Appl	Clear the Read-only check box.

# Task 1. Open a Qualitative Analysis template



- **3** Open the template.
- Right-click the new file and click **Open**.

Task 2. Customize the footer of the Qualitative Analysis template

# 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	<b>Qualitative Anal</b>	vsis template
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Step		<b>Detailed Instruct</b>	ions	Comments		
Switch to the Page L • Switch to the Desi if necessary.		Views group in Ribbon. You ca Layout icon (	yout in the Workbook in the View tab in the in also click the Page ) at the bottom of the to switch to the Page	<ul> <li>In the Page Layout view, the Header and Footer are visible.</li> <li>The Header is printed at the top of each page and the footer is printed at the bottom of each page.</li> <li>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.</li> </ul>		
Norma Page Custom Views V Norma Layout Full Screen Workbook Views	Pin_customunaliysiste Formulas Data Revi Ruler ♥ Formula Bar Gridlines ♥ Headings Message Bar Show/Hide	View Developer Ac	d-Ins Acrobat @ . r Window I II	Click this button to switch to th Page Layout view.		
E57 • 6 fx	B C	D	E F	× *		
44	vetrum ▼ Difference Sp( ▼ rum					
- 47 (Framily) - 48 - 49 - 50 - 51 - 52 ItenID - 53 - 54 - 55 (M0:EndRepeat	temID	x	s Formula	This template has three different sheets. Make sure that the design worksheet is visible.		
56 57 59 CMD:Repeat 60 CompoundIII 61 1 1 1 1 1 1 1 1 1 1 1 1 1						
57         CMD:Repeat           59         CMD:Repeat           60         CompoundII           61         Integration Pe           63         CompoundID           64         CompoundID	ItemID ItemID PlotFile aR List ItemID Start	× RT × End	× Hegnt ×	You can also click this button to		
57         CMD.Repeat           59         CMD.Repeat           60         CompoundII           61         Integration Pe           63         CompoundID           64         CompoundID	ItemID It	× RT × End	Printed at: 9:59 AM on: 2/8/2010	You can also click this button to switch to the Page Layout view		

Figure 14 Switching to the Page Layout view in Excel

#### Customizing a template 2

Task 2. Customize the footer of the Qualitative Analysis template

Task 2. Customize the footer of the C	Qualitative Analysis template
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Step	Detailed Instructions	Comments		
<ul> <li>2 Change the footer.</li> <li>Add the worksheet name to the left section of the footer.</li> </ul>	<ul> <li>a Scroll to the bottom of the design page in Excel.</li> <li>b Click the left section of the footer. A text section appears containing the text &amp;[Picture].</li> <li>c Click at the end of this text to add something to this section.</li> <li>d Type a space.</li> <li>e Click Sheet Name in the Header &amp; Footer Elements group in the Design tab. The text &amp;[Tab] is added. &amp;[Tab] is the name of the tab or worksheet.</li> </ul>	<ul> <li>Excel has different keywords in the header or footer that refer to different pieces of information:</li> <li>&amp;[Page] = the page number</li> <li>&amp;[Pages] = the total number of pages</li> <li>&amp;[Date] = the date the report was created</li> <li>&amp;[Time] = the time the report was created</li> <li>&amp;[File] = the name of the Excel template file</li> <li>&amp;[Picture] = the picture that you selected</li> </ul>		

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.

Home Inse	rt Page Layout F	mulas Data	Review	View	Develop	er Ad	dd-Ins	Acrobat	Design	0 -	
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- 64											
67	CompoundID	ItemID 🔽	Spectrum	-							
	&[Picture] &[Ta	b]			Page 1 of	f 5		Printe	d at: 10:18 AM on: 2	/8/2010	
-	Footer										
Design	Options / 😏				4						

Figure 15 The Header and Footer Design Tab in Excel

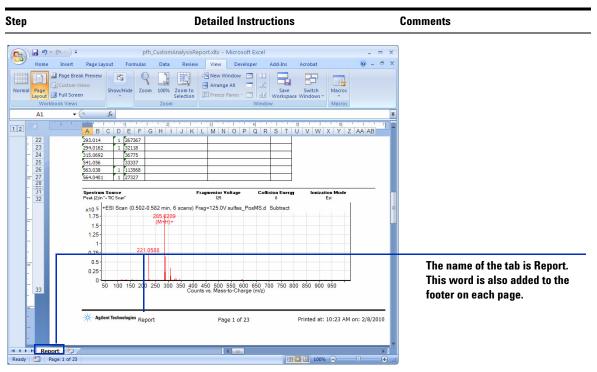
# 2 Customizing a template

Task 2. Customize the footer of the Qualitative Analysis template

# Task 2. Customize the footer of the Qualitative Analysis template

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

Task 2. Customize the footer of the Qualitative Analysis template



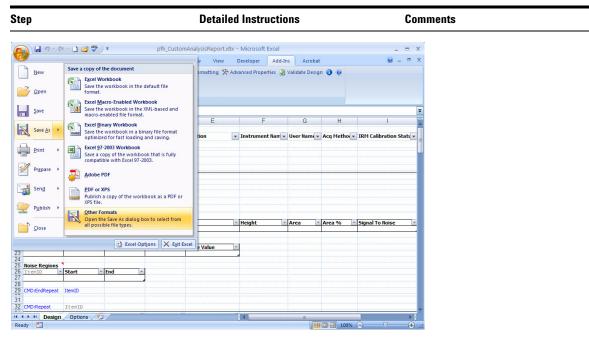
#### Task 2. Customize the footer of the Qualitative Analysis template

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



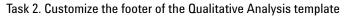


Figure 17 The Save As menu in the Microsoft Office button menu

### 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.

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.	<ul> <li>Follow the instructions in "Task 1. Open the Qualitative Analysis program" on page 10.</li> </ul>		
2	Change the template that is used for the analysis report.	<ul> <li>a In Method Explorer, click General &gt; Common Reporting Options.</li> <li>b Select the template iii_CustomAnalysisReport.xltx as the Analysis report template, where iii are your initials.</li> <li>c Clear any chromatogram and spectra choices you do not want to print.</li> </ul>	<ul> <li>The new report template is automatically found and included in the list of possible analysis report templates when the Qualitative Analysis program is started.</li> <li>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:</li> <li>a Click the button next to the Report template folder.</li> <li>b Click OK. Do not change the folder that is selected.</li> </ul>	

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

Steps	Detailed Instructions	Comments
Method Explorer: Default.m	X Method Editor: Common Reporting Options	×
Chromatogram	🛕 🔄 🔊 🕶 🖓 🔹 💽 🔹 Method Items 🔹 🕞 🙀	
🗄 Spectrum	A Templates Options	
🗉 General	Report template folder	
Analysis Report	C:\MassHunter\Report Templates\Qual\en-US\Letter	
Compound Report	Report templates	
Common Reporting Options	Analysis report template :	You select the new report template
File Open Actions	pfh_CustomAnalysisReport.xbx	for the Analysis report here.
Extraction Data Format	Compound report template:	for the Analysis report here.
Find Compounds	Compound Report xitx	
Find Compounds by Formula	Qualitative method report template :	
Identify Compounds	Qualitative Method Report xltx	
Compound Automation Steps	Acquisition method report template :	
Worklist Automation	AcquisitionMethodReport.xtt	
+ Export		

**3** Select the template to use when **a** In Method

- a In Method Explorer, click General > • The report templates that are printing this report. **Common Reporting Options.** shipped with the software are **b** Verify that the correct **Report template** separated into two folders. One folder is selected. folder contains reports that are c Verify that the correct Analysis report formatted to print on Letter size template is being used. paper. The other folder contains d Click the **Options** tab. reports that will print on A4 size e Verify the settings on this tab. 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.	<ul> <li>You can interactively print the report in multiple ways:         <ul> <li>From the main menu, click File &gt; Print &gt; Analysis Report.</li> <li>From the main toolbar, click the Printer icon.</li> <li>Click the Print Analysis Report icon,</li> <li>Click the Print Analysis Report icon,</li> <li>in the Method Editor toolbar.</li> </ul> </li> <li>Right-click the Analysis Report section in the Method Editor, and click Print Analysis Report.</li> <li>From the data file shortcut menu in the Data Navigator, click Print Analysis Report.</li> <li>Click Generate Analysis Report in the Actions menu.</li> </ul>	The Run icon <b>N</b> 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. Use the new template in the Qualitative Analysis program

Task 4. Open a Quantitative Analysis template

# Task 4. Open a Quantitative Analysis template

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

Task 4. Open a Quantita	tive Analysis template
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Step	Detailed Instructions	Comments	
1 Make a copy of the QuantReport_ISTD_Summary_B_0 4_00.xltx file and rename the file iii_Custom_ISTD_Summary.xltx	<ul> <li>a Open the Windows Explorer program</li> <li>b Open the <i>Report Templates</i>\<i>Quant</i>\ <i>en-US</i> folder in the folder where you installed the data.</li> <li>c Navigate to the <i>Letter</i> or <i>A4</i> folder.</li> <li>d Navigate to the <i>ISTD/Parts</i> folder.</li> <li>e Right-click the <i>QuantReport_ISTD_Summary_B_04_00.xltx</i> file and click Copy.</li> <li>f Click Edit &gt; Paste to add a copy of the report template to the current folder.</li> <li>g Right-click the new file, <i>Copy of QuantReport_ISTD_Summary_B_04_0 0.xltx</i>, and click Rename.</li> <li>h Type <i>iii_Custom_ISTD_Summary.xltx</i>.</li> </ul>	<ul> <li>You do the same steps to open a Qualitative Analysis template.</li> <li>In the Report Templates\Quant\ en-US\Letter or A4 folder, the templates are separated into additional folders, including <i>ESTD</i> and <i>ISTD</i>.</li> </ul>	
	► Parts File Edit View Favorites Tools Help Constant Parts Tools Help Constant Parts Tools Help Constant Parts Tools Help		
	Address C (MassHunter/Report Templates/Quant/en-US/Letter/ISTD/Parts		
		Size Type	

QuantReport\_ISTD\_Calibration\_FAST\_B\_04\_00.xltx

QuantReport\_ISTD\_Complete\_B\_04\_00.xltx QuantReport\_ISTD\_Complete\_FAST\_B\_04\_00.xltx

QuantReport\_ISTD\_Samples\_B\_04\_00.xitx QuantReport\_ISTD\_Samples\_FAST\_B\_04\_00.xitx

QuantReport\_ISTD\_Summary\_B\_04\_00.xltx
QuantReport\_ISTD\_Summary\_FAST\_B\_04\_00.xltx

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.

Parts folder

c Click OK.

Details

Figure 19

 If a template is read-only, you cannot save any changes to the template.

35 KB Microsoft Offic...

81 KB Microsoft Offic...

82 KB Microsoft Offic...

44 KB Microsoft Offic... 52 KB Microsoft Offic...

38 KB Microsoft Offic... 36 KB Microsoft Offic...

MassHunter\Report Templates\Quant\en-US\Letter\ISTD\

Task 4. Open a Quantitative Analysis template

Step	Detailed Instructions	Comments
	General       Security       Summary         Image: Security       Summary         Image: Security       Summary         Type of file:       Microsoft Office Excel Template         Opens with:       Image: Microsoft Office Excel Template         Location:       C:MassHunter/Report Templates/Quart/Letter         Size:       33 4 KB (34.206 bytes)         Size on disk:       36 0 KB (36.864 bytes)         Created:       Today, October 15, 2008, 11:16 00 AM         Modified:       Saturday, September 06, 2008, 5:27:24 PM	2 X VS
	Accessed: Today_Oddaber 15.2008.11.16.00 AM Attributes: Read-only Hidden Advanced	box. This check box may already be clear.

#### Task 4. Open a Quantitative Analysis template

Figure 20 Properties dialog box

**3** Open the template.

• Right-click the new file and click **Open**.

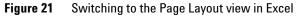
Task 5. Customize the footer of the Quantitative Analysis template

### 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 templat	Task 5.	Change the	e footer of the	Quantitative	Analysis template
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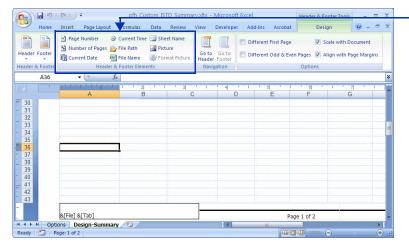
tep	Detailed Instructions	Comments
Switch to the Page Layout view.	a Click <b>Page Layout</b> in the Workbook Views group in the View tab in the Ribbon. You can also click the <b>Page</b> <b>Layout</b> icon ( ) at the bottom of the Excel program to switch to the Page Layout view.	<ul> <li>In the Page Layout view, the Header and Footer are visible.</li> <li>The Header is printed at the top of each page and the footer is printed at the bottom of each page.</li> <li>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.</li> </ul>
		Click this button to switch to the Page Layout view.
24           26           27           28           29           30           51           33           34           35		This template has two different sheets. Make sure that the Design Summary worksheet is visible.
<sup>20</sup> 37		

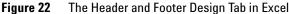


Task 5. Customize the footer of the Quantitative Analysis template

Task 5. Change the footer of the	Quantitative Analysis template
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Step	Detailed Instructions	Comments	
<ul> <li>2 Change the footer.</li> <li>Add the worksheet name to the left section of the footer.</li> </ul>	<ul> <li>a Scroll to the bottom of the design page in Excel.</li> <li>b Click the left section of the footer. A text section appears containing the text &amp;[File].</li> <li>c Click at the end of this text to add something to this section.</li> <li>d Type a space.</li> <li>e Click Sheet Name in the Header &amp; Footer Elements group in the Design tab. The text &amp;[Tab] is added. &amp;[Tab] is the name of the tab or worksheet.</li> </ul>	<ul> <li>Excel has different keywords in the header or footer that refer to different pieces of information:</li> <li>&amp;[Page] = the page number</li> <li>&amp;[Pages] = the total number of pages</li> <li>&amp;[Date] = the date the report was created</li> <li>&amp;[Time] = the time the report was created</li> <li>&amp;[File] = the name of the Excel template file</li> <li>&amp;[Picture] = the picture that you selected when</li> </ul>	





- 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.

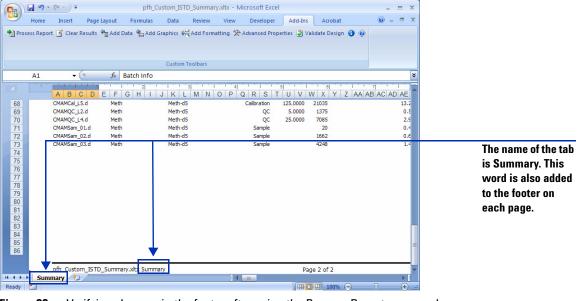
The Header & Footer Elements are shown in the Design tab when you click on one of the sections in the header or footer. You can click these buttons to quickly add these items to the header or footer.

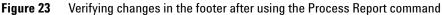
By default, the worksheet name in the template is Design-Summary. The worksheet name in the report is Summary. In a different exercise, you will learn how to change the worksheet name.

Task 5. Customize the footer of the Quantitative Analysis template

Task 5. Change the footer of the	Quantitative Analysis template
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<ul> <li>4 Test the changes to the template.</li> <li>a Click Process Report.</li> <li>b Click the Browse button.</li> <li>c Navigate to the DrugsOfAbuse \ QuantReports \DrugsOfAbuse Demo folder.</li> <li>d Select report.results.xml.</li> <li>e Click Open.</li> <li>f Click OK.</li> <li>g After the report is processed, click Page Layout in the Workbook Views group in the View tab in the Ribbon.</li> <li>h Scroll to the bottom of the page to see the change. The name of the tab is added after the Agilent logo.</li> <li>The Process Report command is part of the MassHunter toolbar in the Add-Ins tab in the Ribbon.</li> <li>You can only see the header and the footer in the Page Layout view.</li> </ul>	Step	Detailed Instructions	Comments
	<b>4</b> Test the changes to the template.	<ul> <li>b Click the Browse button.</li> <li>c Navigate to the DrugsOfAbuse\ QuantReports\DrugsOfAbuseDemo folder.</li> <li>d Select report.results.xml.</li> <li>e Click Open.</li> <li>f Click OK.</li> <li>g After the report is processed, click Page Layout in the Workbook Views group in the View tab in the Ribbon.</li> <li>h Scroll to the bottom of the page to see the change. The name of the tab is</li> </ul>	<ul><li>part of the MassHunter toolbar in the Add-Ins tab in the Ribbon.</li><li>You can only see the header and the</li></ul>





*Report Templates\Quant\en-US\ Letter\ISTD\Parts* folder.

Task 5. Customize the footer of the Quantitative Analysis template

Step	Detailed Instructions	Comments
<ul> <li>5 Save the changes to the template.</li> <li>You have to clear the results first.</li> <li>You can either save the template to the same name or to a new name.</li> </ul>	<ul> <li>a Click Clear Results in the Add-Ins tab in the Ribbon.</li> <li>b Click the Microsoft Office Button and then click Save.</li> <li>c (optional) To save to a different template name, click Save As and click Other Formats.</li> <li>d In the Save As dialog box, type a new File name,</li> <li>e Verify the folder selected in Save in is correct.</li> <li>f Click Save.</li> </ul>	<ul> <li>You can click Save As &gt; Other Formats if you want to change the name of the template.</li> <li>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).</li> <li>If you change the Save as type, the folder is automatically changed to the Microsoft Templates folder. Navigate to the \MassHunter\</li> </ul>

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Save As	Excel Binary Workbook Save the workbook in a binary file for optimized for fast loading and saving		F	G	H	1
Print	Excel 97-2003 Workbook Save a copy of the workbook that is f compatible with Excel 97-2003.	ully				
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Figure 24 The Save As menu in the Microsoft Office button menu

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

### 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.

Steps	Detailed Instructions	Comments		
<ol> <li>Open the Quantitative Analysis program and open a batch file.</li> <li>Select either the default batch or the batch you created if you did the exercises in the Quantitative Analysis Familiarization Guide.</li> <li>Analyze the batch, and inspect the results for each compound.</li> </ol>	• Follow the instructions in "Task 5. Open a batch in the Quantitative Analysis program" on page 22.	<ul> <li>If the Quantitative Analysis program is already running, you do not need to restart the program.</li> </ul>		
<ul> <li>2 Open the Report dialog box.</li> <li>Verify the default destination directory for reports is \Your Directory\DrugsofAbuse\QuantReports.</li> <li>The default filename is iii_Test_01, where "iii" are your initials.</li> </ul>	<ul> <li>a Click Report &gt; Generate. The system displays the standard Report dialog box.</li> <li>b Click</li></ul>	<ul> <li>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.</li> </ul>		

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

Steps	Detailed Instructions	Comments	
<ul> <li>3 Select the report template to use.</li> <li>Add the template, iii_Custom_ISTD_Summary.xltx.</li> <li>Make sure the report name is <i>iii_Custom_ISTD_Summary.xls</i>. By default, it is set to the name of the template.</li> </ul>	<ul> <li>a Click Add under Reports. The system displays the Open dialog box.</li> <li>b Navigate to the Letter \ISTD folder.</li> <li>c Select <ul> <li>iii_Custom_ISTD_Summary.xltx and click Open.</li> <li>The program adds the template to the Template field in the Reports pane.</li> </ul> </li> <li>d In the Report File Name column in the Reports table, verify that the template is iii_Custom_ISTD_Summary.xltx.</li> <li>e Mark the Start Queue Viewer check box.</li> </ul>	<ul> <li>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:</li> <li>Specify a different printer than the default printer</li> <li>Re-use existing graphics files</li> <li>Specify a different numeric format for graphics than the default format.</li> <li>Create a separate report for each sample.</li> <li>Include only some of the samples in the report.</li> <li>Include only some of the compounds in the report.</li> </ul>	

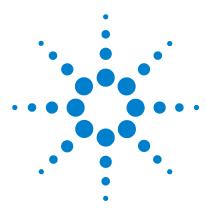
#### Task 6. Use the new template in the Quantitative Analysis program

#### 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.

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



Agilent MassHunter Workstation Software Reporting Familiarization Guide

# Exercise 3 Customizing a table

Task 1. Rename a column header in a table53Task 2. Delete a column from a table56Task 3. Change the width of a column in a table59Task 4. Move a column in a table62Task 5. Add a column to a table66Task 6. Add a mapped column to a table70Task 7. Add a filter to a table74Task 8. Move or delete a column in a filtered table79

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.



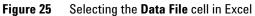
Each exercise is presented in a table with three columns:

- 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.

Open the Quantitative Analysis template \MassHunter\Report Templates\Quant\en-US\Letter\ ISTD\ <i>iii</i> Custom ISTD Summary.xltx	<ul> <li>Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the</li> </ul>	• If you did not do the previous task, example templates are available on
template, where " <i>iii</i> " are your initials.	template, iii_Custom_ISTD_Summary.xltx, where " <i>iii</i> " are your initials.	the Agilent Technologies MassHunter Reporting User Information DVD in the <b>Familiarization Templates</b> folder.
Change the name of the <b>Data File</b> column to <b>Acquisition File</b> .	<ul> <li>a Find the table labeled Sequence Table.</li> <li>b Click on the cell containing the words Data File. This column is the second column in the table.</li> </ul>	
	summary.xdx - Microsoft Excel Table Tools -	The contents of the current cell are shown here in the Formula bar.
Batch Info Batch Data Path Analysis Time Report Time Last Callb Update Sequence Table		Click on this cell in the Sequence Table.
I SampleID V Data File Sample Hame V Posit	ion Volut Level Sample Type Acq Metho( SamplePost	One of the column headers in a table in the Quantitation
G. (CH0:Repeat:         CompoundID         CompoundIType         Form           5         SampleID         CompoundID         CompoundIType         Form           5         SampleID         CompoundID         ISTDCompoundID         Freed           7         Press         SampleID         CompoundID         Freed	et Compound	Results section also is called Data File. Columns in different tables can have the
0 CMD:EndRepeat CompoundID 1 2 4 → H Options Design-Summary 2		same name.



Task 1. Rename a column header in a table

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

	De	tailed Instruc	tions		Comments
	C	can also click	sition File. in the Formula B e part of the name	ar to	• 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.
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4 Report Time Re	nalyst Name Leporter Name Latch State				
6 7 Sequence Table 8 SampleID  Acquisition File Sa 10	ample Name 💌 Position 💌	Volut v Level v	sample Type 💌 Acq Metho(	SamplePosit	
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#### 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. Rename a column header in a table

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🐴 Process Report 🥤 Clear	Results 🍓 Add Data 🐏 Add Gra	phics 👫 Add Formatting 💲	Advanced Pr	opertie	es 🛃 Validate D	esign 🚯 🔞		
		Custom Toolbars						
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2 Batch Data Path	C:\MassHunter\Data\DrugsC		ISUTADUSEDEN	io.Dati	cn.bin			
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CMAMCal_L2.d	CMAM_10 CMAM_11	P1-C11	5.00	L2 L3	Calibration	APCIautotune.m		
3 CMAMCal L4.d	CMAM_14	P1-C14	5.00	L4	Calibration	APCIautotune.m		
1 CMAMCal L5.d	CMAM 17	P1-C17	5.00	L5	Calibration	APCIautotune.m		
CMAMQC_L2.d	CMAM_09	P1-C9	5.00	L2	QC	APCIautotune.m		
6 CMAMQC_L4.d	CMAM_15	P1-C15	5.00	L4	QC	APCIautotune.m		
7 CMAMSam_01.d	CMAM_22	P1-C22	5.00		Sample	APCIautotune.m		
8 CMAMSam_02.d	CMAM_08	P1-C8	5.00		Sample	APCIautotune.m		
9 CMAMSam 03.d	CMAM 12	P1-C12	5.00		Sample	APCIautotune.m	¥	
Summary	1		14					
Ready 🛅						I I I I I I I I I I I I I I I I I I I	∍0	

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

Figure 27 Verifying changes in the column header after using the Process Report command

**igure 21** Vernying changes in the column header after using the rocess hepo

- 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.

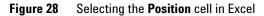
- The Save as type is Excel Template (\*.xltx) for most reports. If the report you are modifying has the extension .XLT, then the Save as type selection is Excel 97-2003 Template (\*.xlt).
- If you change the Save as type, the folder is automatically changed to the Microsoft *Templates* folder. Navigate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

Task 2. Delete a column from a table

# Task 2. Delete a column from a table

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

τε	ep			D	etailed l	nstructi	ons			Co	omments
	Open the Qu template \M Templates\( <i>iii_</i> 1_Custor	1assHunt ⊇uant∖Le	ter\Report etter\ISTD\		Open a templat templat iii_1_C	Quantita te" on pa te, ustom_l	ructions ative Ana age 42 to STD_Sur your initi	alysis o open th mmary.x	ıe		If you did not do the previous task, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the <b>Familiarization Templates</b> folder.
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Task 2. Delete a column from a table

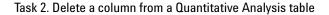
#### Task 2. Delete a column from a Quantitative Analysis table

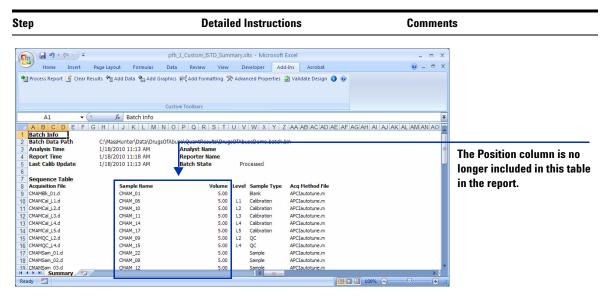
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Figure 29 Deleting the Position column

- **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 table





#### 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

### 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

	ep			D	etailed	Instruct	ions			Com	nents
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1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16	Process Report Clear  E8  A Batch Info Batch Data Path Analysis Time Report Time Last Calib Update Sequence Table SampleID  Quantitation Result CMD:Repeat SampleID  SampleID  V	Results Add	Data Add Graphic Cur Level C Analyst Name Reporter Name Batch State	s 4 Add Form tom Toolbars	E Level	F Sample Ty( •	G Acq Hethod F	H SamplePostic	TrayAlame V V	J	entire column in Excel does not change the width of the column in a table. Click on the Level column in
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17	E8   E8  A Batch Info Batch Data Path Analysis Time Last Calib Update Sequence Table SampleID  Quantitation Result CMD:Repeat SampleID  SempleID  CMD:Repeat CMD:Repe	r Results 4 Add	Add Graphic Cur Cur Cur Cur Canadyst Name Reporter Name Batch State Sample Name Sample Name	s 4 Add Form tom Toolbars	E Level	F Sample Ty(+ RetentionTim(+)	G Acq Hethod F	H SamplePostic		J E	entire column in Excel does not change the width of the column in a table. Click on the Level column in
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16	Process Report Clear E8 A Batch Info Batch Data Path Analysis Time Report Time Last Calib Update Sequence Table SampleID VIO.Repeat SampleID SampleID	r Results 4 Add	Add Graphic Cur Cur Cur Cur Canadyst Name Reporter Name Batch State Sample Name Sample Name	s 4 Add Form tom Toolbars	E Level	F Sample Ty(+ RetentionTim(+)	G Acq Hethod F	H SamplePostic		J E	entire column in Excel does not change the width of the column in a table. Click on the Level column in
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18	E8  E8 E8 E8 E8 EXCh Info Batch Info Batch Data Path Analysis Time Report Time Last Calib Update Sequence Table Quantitation Result CMD:Repeat SampleID SampleID SampleID	r Results 4 Add	Add Graphic Cur Cur Cur Cur Canadyst Name Reporter Name Batch State Sample Name Sample Name	s 4 Add Form tom Toolbars	E Level	F Sample Ty(+ RetentionTim(+)	G Acq Hethod F	H SamplePositic		J E	entire column in Excel does not change the width of the column in a table. Click on the Level column in

Figure 31 Selecting the Level column in Excel

Step

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

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

#### **Detailed Instructions**

- 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.

#### Comments

- 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.

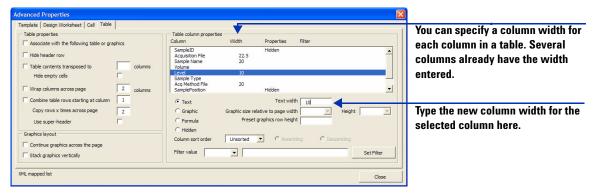
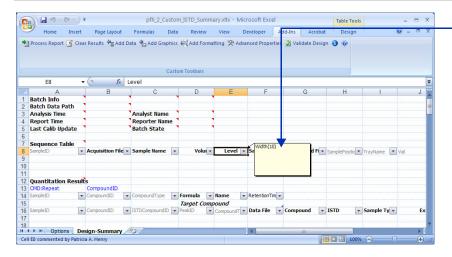


Figure 32 Changing the width of the Level column



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 table

Task 3.	Change tl	he width o	of a column	in a (	Quantitative	Analysis table

J	ep		Detaile	d Insti	ructions		Commer	its
;	Test the chan	ges to the template	<ul> <li>b Click</li> <li>c Navi</li> <li>Quan</li> <li>folde</li> <li>d Sele</li> <li>e Click</li> <li>f Click</li> </ul>	k the <b>B</b> igate t n <i>tRepo</i> er. ct <i>repo</i> k <b>Open</b> k <b>OK</b> . F	orts\Drug ort.result	utton. <i>igsOfAbuse\</i> <i>jsOfAbuseDemo</i> <i>s.xml.</i> equence Table. The	part o	rocess Report command is f the MassHunter toolbar in dd-Ins tab in the Ribbon.
	<b>••••</b> ••••••••••••••••••••••••••••••••	ofh	_2_Custom_ISTD_Summ	arv.xltx - M	licrosoft Excel		_ = ×	
1	100							
ſ	Home Insert	Page Layout Formulas Data Results 🖷 Add Data 🐏 Add Graphics		Develope Advanced Pro		Acrobat ate Design 🜒 🛞	0 - ª x	
	🐏 Process Report 🧃 Clear	Results Hadd Data Add Graphics					@ _ 5 X	
	Process Report 🔏 Clear	Results H Add Data Add Graphics	해 Toolbars	Advanced Pro	operties 🔰 Valid	ate Design 🔮 🧶	3	
	🐏 Process Report 🧃 Clear	Results H Add Data Add Graphics	H Add Formatting 🎌	Advanced Pro	operties 🖉 Valid		3	
	Al Clear A B C D E F 1 Batch Info 2 Batch Data Path 3 Analysis Time	Results hadd Data hadd Graphics Custo G H I J K L M N O C:\MassHunter\Data\DrugsOfAbu 1/18/2010 11:13 AM	4 <sup>™</sup> Add Formatting ≫ om Toolbars P Q R S T L use\QuantResults\Drugs( Analyst Name	Advanced Pro	operties 🖉 Valid	ate Design 🔮 🧶	3	The width of this column i
	A1 Clear A C C D E F Batch Info Batch Data Path Analysis Time 4 Report Time	Results Add Data Add Graphics Custo F Batch Info G H I J K L M N O C:\MassHunter\Data\DrugsOfAbu 1/18/2010 11:13 AM	Image: Add Formatting     Image: Add Formatting       Image: Add Formatting     Image: Add Formatting    <	Advanced Pro	X Y Z AAA	ate Design 🔮 🧶	3	The width of this column in
	Al Clear A B C D E F 1 Batch Info 2 Batch Data Path 3 Analysis Time	Results hadd Data hadd Graphics Custo G H I J K L M N O C:\MassHunter\Data\DrugsOfAbu 1/18/2010 11:13 AM	4 <sup>™</sup> Add Formatting ≫ om Toolbars P Q R S T L use\QuantResults\Drugs( Analyst Name	Advanced Pro	X Y Z AAA	ate Design 🔮 🧶	3	The width of this column i the table is slightly wider.
	A1 Clear A1 I AB C DE IF Batch Info 2 Batch Data Path 3 Analysis Time 4 Report Time 5 Last Calib Update 6	Results Add Data Add Graphics Custo F Batch Info G H I J K L M N O C:\MassHunter\Data\DrugsOfAbu 1/18/2010 11:13 AM	Image: Add Formatting     Image: Add Formatting       Image: Add Formatting     Image: Add Formatting    <	Advanced Pro	X Y Z AAA	ate Design 🔮 🧶	3	
	A1 Clear ABCDEF Batch Info Batch Data Path 3 Analysis Time 4 Report Time 5 Last Calib Update 6 7 Sequence Table	Custo Cu	H Add Formatting m Toolbars P Q R S T L use\QuantResults\Drugs( Analyst Name Reporter Name Batch State	Advanced Pro J V W S DfAbuseDem Processed	operties 🖉 Valid X   Y   Z   AA   A No batch bin	BIACIADIAEIAFIAGIAHIAI AJ A	3	
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	A1  Clear  A1  A1  A1  A1  A1  A1  A1  A1  A1  A	Custo Add Data ♣ Add Graphics Custo A Batch Info G H J J K L M N O C: (MassHunfer,(Data)Crugs0fAbu 1/18/2010 11:13 AM 1/18/2010 11:13 AM Sample Name CMAM_06 CMAM_06 CMAM_10 CMAM_10	High Add Formatting     High Add Formatting       Am Toolbars       P     Q       R     S       T     L       ScountResults/Drugs       Analyst Name       Reporter Name       Batch State       Scount       S.00       S.00       S.00       S.00       S.00       S.00	Advanced Pro J V W J DfAbuseDerr Processed Level L1 L2 L3	X Y Z AAA So batch bin Sample Type Blank Calibration Calibration	Aca Hethod File APCladotome.m APCladotome.m APCladotome.m APCladotome.m	3	
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	A1  A1 A1 A1 A1 A1 A1 A1 A1 A1 A1 A1 A1 A1	Results         ♣ Add Data         ♣ Add Graphics           Cust         Cust           ▲         Batch Info           G         H         J           K         Batch Info           C         HassHunter(Data)upgofAbu 1/18/2010 11:13 AM           1/18/2010 11:13 AM           Sample Hame           CMAM_01           CMAM_06           CMAM_11           CMAM_14           CMAM_17	H Add Formatting X am Toolbars P Q R S T L Use\QuantResults\Drugs Analyst Name Reporter Name Batch State Volume S.00 S.00 S.00 S.00 S.00 S.00 S.00 S.0	Advanced Pro J V W J OfAbuseDerr Processed Level L1 L2 L3 L4 L5	X Y Z AAA so batch bin Sample Type Blank Calibration Calibration Calibration	Acq hethod File Acq hethod File APClautobure.m APClautobure.m APClautobure.m APClautobure.m APClautobure.m APClautobure.m	3	
	A1 Clear A1 A1 A1 A1 A1 A1 A1 A1 A1 A1 A1	Add Data         Add Graphics           Custs         Custs           F         Batch Info           G         H         J           K         L         M           O         C:MassHunder(Data)DrugsOfAbu 1/18/2010 11:13 AM         1/18/2010 11:13 AM           1/18/2010 11:13 AM         CMAM_06           CMAM_06         CMAM_10           CMAM_11         CMAM_14           CMAM_05         CMAM_17	High Add Formatting       ★         Im Toolbars       P         Im Toolbars       P         Im Toolbars       Image: Source of the sourc	Advanced Pro J V W J OfAbuseDerr Processed Level L1 L2 L3 L4 L5 L2	Sample Type Blank Calibration Calibration Calibration Calibration Calibration Calibration Calibration Calibration Calibration Calibration	Acq Hethod File AC[AD]AE[AF]AG]AH AL AJ AF ACQLADDAE] ACCADDURE APCCantobure.m APCCantobure.m APCIantobure.m APCIantobure.m APCIantobure.m APCIantobure.m	3	
	A1	Results         ♣ Add Data         ♣ Add Graphic           Cust         Cust           ▲         Batch Info           G         H         J         K           J         K         L         M           C:         WassHunter(Data)         M         0           J/18/2010         11:13         AM         1/18/2010         11:13           J/18/2010         11:13         AM         1/18/2010         11:13           CMAM_010         CMAM_05         CMAM_10         CMAM_11           CMAM_11         CMAM_17         CMAM_09         CMAM_09	H Add Formatting X m Toolbars P Q R S T U use\QuantResults\DrugG Analyst Name Reporter Name Batch State Volume S.00	Advanced Pro J V W J OfAbuseDerr Processed Level L1 L2 L3 L4 L5	X Y Z AAA bo batch bin Sample Type Bink Calibration Calibration Calibration Calibration Calibration Calibration Calibration Calibration Calibration	Acq Method File Acq Method File APCIantoture.m APCIantoture.m APCIantoture.m APCIantoture.m APCIantoture.m APCIantoture.m APCIantoture.m APCIantoture.m APCIantoture.m	3	
	A1 Clear A1 A1 A1 A1 A1 A1 A1 A1 A1 A1 A1	Add Data         Add Graphics           Custs         Custs           F         Batch Info           G         H         J           K         L         M           O         C:MassHunder(Data)DrugsOfAbu 1/18/2010 11:13 AM           1/18/2010 11:13 AM           1/18/2010 11:13 AM           CMAM_06           CMAM_06           CMAM_10           CMAM_11           CMAM_14           CMAM_17           CMAM_06	High Add Formatting       ★         Im Toolbars       P         Im Toolbars       P         Im Toolbars       Image: Source of the sourc	Advanced Pro J V W J OfAbuseDerr Processed Level L1 L2 L3 L4 L5 L2	Sample Type Blank Calibration Calibration Calibration Calibration Calibration Calibration Calibration Calibration Calibration Calibration	Acq Hethod File AC[AD]AE[AF]AG]AH AL AJ AF ACQLADDAE] ACCADDURE APCCantobure.m APCCantobure.m APCIantobure.m APCIantobure.m APCIantobure.m APCIantobure.m	3	

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.

Ready 🛅

- You have to clear the results first.
- a Click **Clear Results** in the Add-Ins tab in the Ribbon.

**III II** 100% (-)

- **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

# 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.

ite	ep	D	etailed Ins	structions		Com	ments	
	Open the Quantitative Analysis template \MassHunter\Report Templates\Quant\Letter\ISTD\ <i>iii_</i> 3_Custom_ISTD_Summary.xl		Open a Q template template, iii_3_Cus	e instructions uantitative Ar " on page 42 t , tom_ISTD_Su i" are your ini	nalysis to open the ummary.xltx,	<ul> <li>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.</li> </ul>		
	<ul> <li>Move the Volume column to the end of the table.</li> <li>Move the cursor to the edge o the cell until it changes to the Move cursor.</li> </ul>	b f	Click on t Volume. column i Move the until the	the cell conta This column i n the table. e cursor to the cursor change	Sequence Table. ining the word s the fourth e edge of the cell es to a four sided	de	he shape of the cursor changes epending upon where the cursor i binting.	
	Home Insert Page Layout Formulas Data Process Report ☐ Clear Results ♣Add Data ♣Add Graphics	Review	arrow, arrow, ary.xltx - Microsof View Develop Mitting 🎘 Advanced	t Excel per Add-Ins Acrob		- 8 X		
	Home Insert PageLayout Formulas Data Grocess Report 🕤 Clear Results 췍플Add Data 췍글Add Graphics Custo	Review	ary.xltx - Microsof View Develop	t Excel per Add-Ins Acrob	at Design 🕼	) _ = X		
	Home Insert PageLayout Formulas Data	Review	ary.xltx - Microsof View Develoj titting 🎘 Advanced	t Excel per Add-Ins Acrob Properties 🏈 Validate Desi	at Design (6)			
	Home Insert Page Layout Formulas Data Process Report S Clear Results Add Data Add Graphics Cunto D8 S S S S S S S S S S S S S S S S S S S	Review	ary.xltx - Microsof View Develop	t Excel per Add-Ins Acrob	at Design 🕼	) _ = X	Sequence Table.	
	Home     Insert     Page Layout     Formulas     Data       Process Report     Clear Results     Add Data     Add Graphics       Data     Custo     Custo     Custo       Data     Setch Info     B     C       Batch Info     B     C     Custo       Batch Data Path     Anahysis Time     Anahysis Time     Reporter Hame       Last Calib Update     Batch State     Sequence Table     SampleID	Review	ary.xltx - Microsof View Develop Advanced E	t Excel per Add-Ins Acrob Properties 2 Validate Desi F G	at Design (6)	z J	Sequence Table. When you move the column, the Volume cell and the cell directly under it are moved	
1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6	Home     Inset     Page Layout     Formulas     Data       Process Report     Clear Results     Add Data     Add Graphics       Custo     Custo     Custo       D8     C     Custo       Batch Info     Batch Data Path     Analysis Time       Analysis Time     Report Filame     Reporter Hame       Last Calib Update     Batch State     SampleID       Sequence Table     CompoundID     Sample Name       Custo     CompoundID     CompoundID       SampleID     CompoundID     CompoundID	Review Add Formu n Toolbars	E Level v Sam	Excel  t Excel  Properties Validate Desi  F G  ple Ty( Acq Method F(  ntonTim	at Design (6)	z J	Sequence Table. When you move the column, the Volume cell and the cell	
	Home     Insert     Page Layout     Formulas     Data       Process Report     Clear Results     Add Data     Add Graphics       D8 <ul> <li>Image: Clear Results</li> <li>Ima</li></ul>	Review Add Formu n Toolbars	E Level v Sam	Excel  t Excel  Properties Validate Desi  F G  ple Ty( Acq Method F(  ntonTim	at Design (6)	) _ 5 X	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	

Figure 35 Selecting the Volume column in the Sequence Table

Task 4. Move a column in a table

Step	Detailed Instructions	Comments
	<ul> <li>d Click and drag the cursor to the end o 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.</li> <li>e Release the cursor at the end of the table.</li> </ul>	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
Home Insert Page Layout Formulas Dz		- E X - E X - C X -
Home Inset Page Layout Formulas DI Parte B I I I I I I I I I I I I I I I I I I	ata Review View Developer Add-Ins Acrobat Design           Image: Seven per state         Image: Sevenp	e
Home     Insert     Page Layout     Formulas     DI       Pote     A     Image: A market and the second s	ata Review View Developer Add-Ins Acrobat Design Sector 2 Sector	C = X Fina & Select
Home Inset Page Layout Formulas DD Pate A Pate A Pa	ata Review View Developer Add-Ins Acrobat Design Second Constraints Constrai	The Volume column has been moved to the end of the table.
Home Inset Page Layout Formulas Dr Patt Tahoma 8 A A A E E E E Patt B Z U P P A A E C A B A A B C 1 Batch Info 2 Batch Data Path 3 Analysis Time A B C 1 Batch Update B Analyst Hame 6 Last Calib Update B Batch State 6 Sequence Table 8 SampelD A Acquisition Filey Sample Hame	ata Review View Developer Add-Ins Acrobat Design Sector Constraints Conditional Formatting - Sector Add-Ins Acrobat Design Sector Constraints - Sector -	The Volume column has bee moved to the end of the table. This table has some hidden
Home Inset Page Layout Formulas DL Paste J L J	ata Review View Developer Add-In: Acrobat Design Ceneral  Ceneral   The Volume column has been moved to the end of the table. This table has some hidden columns. You do not need to move this column after the	
Home Inset Page Layout Formulas DU Pate Discrete Compound D B EX Discrete Compound D 1 Guantization Results 1 Guantization	ata Review View Developer Add-In: Acrobat Design Ceneral  Ceneral   The Volume column has been moved to the end of the table. This table has some hidden columns. You do not need to move this column after the	

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

Batch Info Batch Data Path

Analysis Time

Report Time

7 Sequence Table 8 Acquisition File 9 CMAMBIk\_01.d 10 CMAMCal\_L1.d

11 CMAMCal\_L1.d 11 CMAMCal\_L2.d 12 CMAMCal\_L3.d 13 CMAMCal\_L4.d

14 CMAMCal\_L5.d 15 CMAMQC\_L2.d

16 CMAMQC\_L4.d 17 CMAMSam\_01.d

18 CMAMSam\_02.d

19 CMAMSam 03.d H ← → H Summary ? Ready

Last Calib Update

Task 4. Move a column in a table

#### Task 4. Move a column in a Quantitative Analysis table

Step	Detailed Instructions	Comments
B Test the changes to the template.	<ul> <li>a Click Process Report.</li> <li>b Click the Browse button.</li> <li>c Navigate to the DrugsOfAbuse \ QuantReports \DrugsOfAbuseDemo folder.</li> <li>d Select report.results.xml.</li> <li>e Click Open.</li> <li>f Click OK.</li> <li>g Find the Sequence Table. The last column is now Volume.</li> </ul>	<ul> <li>The Process Report command is part of the MassHunter toolbar in the Add-Ins tab in the Ribbon.</li> </ul>
	tom_JSTD_Summary.xitx - Microsoft Excel teriew View Developer Add-Ins Acrobat dd Formatting & Advanced Properties & Validate Design ① @	- = ×
Custom Too		

Acq Method File

APCIautotune.m

Volume

5.00 5.00

5.00

5.00 5.00 5.00 5.00

5.00

5.00

5.00

5.00

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

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z AAABACADAEAFAGAHAI AJAKALAMANAO

Processed

Sample Type

Blank Calibration

Calibration

Calibration

Calibration

Calibration

QC

QC

Sample

Sample

Sample

C:\MassHunter\Data\DrugsOfAbuse\QuantResults\DrugsOfAbuseDemo.batch.bin

Analyst Name

**Batch State** 

Reporter Name

Level

L1

L2 L3 L4 L5 L2 L4

1/18/2010 11:13 AM

1/18/2010 11:18 AM

1/18/2010 11:13 AM

Sample Name CMAM\_01 CMAM\_06

CMAM\_10

CMAM\_10 CMAM\_11 CMAM\_14 CMAM\_17 CMAM\_09

CMAM\_15

CMAM\_22

CMAM\_08

CMAM 12

The Volume column is now

at the end of the table.

Task 4. Move a column in a table

Task 4. Move a column in a Quantitative Analysis table	Task 4.	Move a	column in	a Quantitative	Analysis table
--	---------	--------	-----------	----------------	----------------

Step	Detailed Instructions	Comments
<ul> <li>4 Save the changes to the template <i>iii</i>_4_Custom_ISTD_Summary.xltx.</li> <li>You have to clear the results first.</li> </ul>	<ul> <li>a Click Clear Results in the Add-Ins tab in the Ribbon.</li> <li>b Click the Microsoft Office Button and then click Save As and click Other Formats.</li> <li>c In the Save As dialog box, type <i>iii</i>_4_Custom_ISTD_Summary.xltx.</li> <li>d Verify the folder selected in Save in is correct.</li> <li>e Click Save.</li> </ul>	<ul> <li>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).</li> <li>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.</li> </ul>

Change the formatting of this

header to match the other headers in this table.

•

# 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 d	column to	al	Quantitative	Anal	ysis table
--	---------	---------	-----------	----	--------------	------	------------

Step		D	Detailed Instructions		Comments	
1	Open the Quantitative Analysis template \MassHunter\Report Templates\Quant\Letter\ISTD\ iii_4_Custom_ISTD_Summary.xltx.	а	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 " <i>iii</i> " 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 <b>Familiarization Templates</b> folder.	
2	<ul> <li>Add a column to the Sequence</li> <li>Table to the left of the Acquisition</li> <li>File column in the Sequence Table.</li> <li>Change the name of this column to Location.</li> </ul>		Find the table labeled <b>Sequence Table</b> . Click on the cell containing the words <b>Acquisition File</b> . This column is the second column in the table.	•	The <b>Data File</b> column was renamed to <b>Acquisition File</b> in "Task 1. Rename a column header in a table" on page 53.	

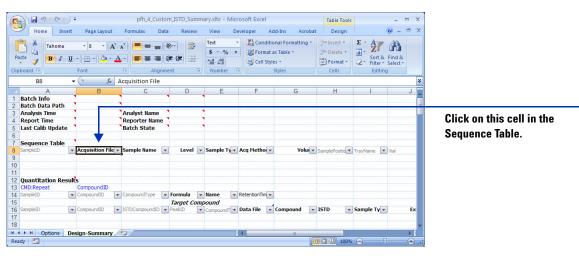


Figure 38 Selecting the Acquisition File cell in Excel

Task 5. Add a column to a table

Step	Detailed Instruct	ions	Commen	ıts
	c Right-click this Table columns	s cell and click <b>Insert &gt;</b> <b>to the left</b> .		ick the column to the right of cation where you want to add mn.
	_4_Custom_ISTD_Summary.xltx - Microsoft Excel	Table Tools	_ = ×	
Paste J BIU Clipboard 5 Font 5	■ ● ● ● ● ● ● ● ● ● ● ● ● ● ● ● ● ● ● ●	Sort &	Find & Select *	
B8 ▼		G H I	*	
Batch Info       Batch Data Path       Analysis Time       Analysis Time       Last Calib Update         Tahoma * 8 *	Name			
/ Sequence Table	ame v tevel v Sample Tv Acq Hetho(v	Volu( v SamplePositid v TrayName (v	Vial	Click this command. The new column is added to the left of the current column.
13 CMD:Repeat Compound Paste Special				
14 SampleID CompoundI Refresh	me ReletionTim			
16 SampleID CompoundI	Table Columns to the L	eft und 👻 ISTD 💽 Sample Ty 💌	Ex	
17 <u>D</u> elete 18 Select	Table Rows Above			
Clear Conten	**		× 1	
Ready S	ns P	III II 100% 🗩 🗸		
Sort				
Filter				
Table				
XML				

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 table

Step	Detailed Instructions Co	mments
	Portulas     Data     Review     View     Developer     Add-Ins     Acrobat     Design     @ - ○       X     Image: State and the sta	X You can also use the icons in the Font group.
A B 1 Batch Info 2 Batch Data Path 3 Analysis Time 4 Report Time 5 Last Calib Update 6 Sequence Table 8 SempleID 10 11 12 Quantitation Results 3 (MD/Repeat Compound	Acquitation of the second state     Level • Sample Ty(• Acq Hethod F(• Volu(• SamplePosit)• TrayName       Copy     Sample Positie       Paste     Special	To change the header to look like the other headers in the table, you click the Bold icon and also change the font color to black.
14         SampleID         ▼ Comp pundID         [s]           15         16         SampleID         ▼ CompoundID           16         SampleID         ▼ CompoundID         17           17         18         ■         ■           18         ■         ■         ■           Ready         ■         ■         ■	Insert Nd	<ul> <li>"Laboratory 1" is added to</li> <li>this cell.</li> </ul>

#### Task 5. Add a column to a Quantitative Analysis table

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 table

Task 5. Add a column to a C	Quantitative Analysis table
-----------------------------	-----------------------------

Step		Detail	ed Instru	ctions		Comme	nts
<b>1 1 1 1 1</b>	•	pfh_4_Custom_ISTD_Summa	ry.xltx - Microsof	t Excel		_ = ×	
	sert Page Layout	Formulas Data Review View	Developer	Add-Ins Acr	obat	🥑 _ 📼 🗙	
Process Report 🧃	Clear Results  🖶 Add Dal	a 📲 Add Graphics 🍋 Add Formatting 🕇	Relation Proper	ties 🌛 Validate D	esign 🚯 🖗 Test Quant		
		Custom Toolbars					
A1	▼ (* <i>f</i> x Ba	atch Info				*	
	EFGHIJ	K L M N O P Q R S T	UVWX	Y Z AA AB A	CAD AE AF AG AH AI	AJ AK AL AM A	
1 Batch Info 2 Batch Data Pat							
2 Batch Data Pat 3 Analysis Time	1/18/2010 11	r\Data\DrugsOfAbuse\QuantResults\Drug 1:13 AM Analyst Name	ISOTADUSEDemo.Da	atch.bin			
4 Report Time	1/18/2010 11					=	The first column is now
5 Last Calib Upda			Processed				
6							Location.
7 Sequence Tabl						100	
	cquisition File	Sample Name	Level	Sample Type	Acq Method File	Volum	
	MAMBk_01.d MAMCal L1.d	CMAM_01 CMAM_06	L1	Blank Calibration	APCIautotune.m APCIautotune.m	.5.0 5.0	
	MAMCal_L1.d MAMCal_L2.d	CMAM_06 CMAM_10	L1 L2	Calibration	APCIautotune.m	5.0	When you Clear Results, th
	MAMCal_L3.d	CMAM_11	L3	Calibration	APCIautotune.m	5.0	
	MAMCal L4.d	CMAM_14	14	Calibration	APCIautotune.m	5.0	formula ="Laboratory 1" is
	MAMCal L5.d	CMAM 17	L5	Calibration	APCIautotune.m	5.0	•
15 Laboratory 1 (	MAMQC_L2.d	CMAM_09	L2	QC	APCIautotune.m	5.0	not visible. However, it is
16 Laboratory 1 0	MAMQC_L4.d	CMAM_15	L4	QC	APCIautotune.m	15.C	atill wood whonever you
	MAMSam_01.d	CMAM_22		Sample	APCIautotune.m	.5.C	still used whenever you
	MAMSam_02.d	CMAM_08		Sample	APCIautotune.m	.5.C	process the report.
	MAMSam_03.d	CMAM_12		Sample	APCIautotune.m	.5 <b>.</b> 0	process me report.
20							
21 Quantitation R	esults					<b>*</b>	

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

# 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 A	nalysis table

Step	Detailed Instructions	Comments
1 Open the Quantitative Analysis template \MassHunter\Report Templates\Quant\Letter\ISTD\ <i>iii_5_</i> Custom_ISTD_Summary.xltx.	f Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, <i>iii_5_Custom_ISTD_Summary.xltx.</i> , where " <i>iii</i> " are your initials.	<ul> <li>If you did not do the previous task, example templates are available of the Agilent Technologies MassHunter Reporting User Information DVD in the Familiarization Templates folder.</li> </ul>
<ul> <li>Display the XML source.</li> <li>Hint: right-click a cell that is already mapped to display the shortcut menu.</li> </ul>	<ul> <li>a Find the cell containing the words Batch Data Path.</li> <li>b Right-click the cell next to this cell.</li> <li>c Click XML &gt; XML Source.</li> </ul>	<ul> <li>If the Developer tab isn't showing:</li> <li>a Click the Microsoft Office Button and then click Excel Options.</li> <li>b In the Excel Options dialog box, mark the Show Developer tab in the Ribbon check box.</li> <li>c Click OK.</li> </ul>

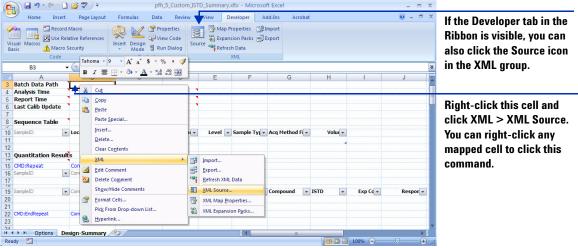


Figure 42 Displaying the XML Source task pane in Excel

Task 6. Add a mapped column to a table

Task 6. Add a mapped column to a Quantitative Analysis table
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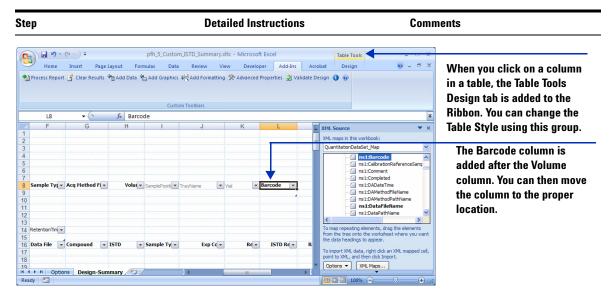
Step					Detailed Instructions					Comments		
<ul> <li>3 Add the column Barcode to the end of the Sequence Table.</li> <li>• Hint: click on two items in the Sequence Table to identify the correct section of the XML Source.</li> <li>a Find the table labeled b Click the Acquisition c Click the Level column content of the XML source.</li> </ul>								<ul> <li>File column.</li> <li>the table, the list of ele XML Source window al</li> <li>If the element in the lis Bold letters, that item i mapped or used in the</li> </ul>		you click the mapped columns in a table, the list of elements in the AL Source window also changes. he element in the list is shown in Id letters, that item is already upped or used in the worksheet. Iments in the same map cannot used more than once.		
н	Iome Insert	Page Layou	dd Data 🍓 Add Graphics 🗄	Review	View D	eveloper Add-In			<u> </u>		When you click on the Leve column, the element ns1:LevelName in the XML	
E	E8 -	• (• f;	Level							×	Source window is	
1	A	В	С	D		F	G	XML Source		▼ ×	highlighted.	
1 Batch J								XML maps in this workbook:			ingingitou	
	Data Path							QuantitationDataSet Map		~		
Analysi		1	Analyst Name					· · · · ·		~		
4 Report		1	Reporter Name					- 🗐 ns1:InjectionsPer		^		
	alib Update		Batch State					ns1:InjectorVo				
6								- 🗐 ns1:Ins rumentNa				
	ence Table	Location	▼ Acquisition File ▼ 9			Sample Tyr - Acq			pe			
8 SampleID 9		Location	Acquisition File	ample Nal 🔻	Level		rietno	ns1:LevelName	1			
9								ns1:Locked			"ns1:" is part of the syntax	
10								ns1:MatrixSpikeG	oup			
	itation Resul	P.c.						ns1:OutlierCCTim		v	of the element in the XML	
3 CMD:Rep		CompoundID						<		>	•••••••••••••••••	
4 SampleID		CompoundID	CompoundType	ormula 🔽	Name 🔻	RetentionTim -		To map repeating elements, drag t	he element	s	source window. Every item	
14 Sampleto	-	- compoundib		Target Comp				from the tree onto the worksheet			•	
16 SampleID	D	CompoundID	▼ ISTDCompoundID ▼ F		CompoundT 🔻	Data File 🔽 Con	npound	the data headings to appear.			in the XML Source window	
17	L							To import XML data, right dick an X	ML mapped	d cell,		
18								point to XML, and then dick Import			starts with "ns1:".	
19								Options  XML Maps				
	Options De	esign-Summar	y 😰 📃	4			▶					
								100% 🕞 🗌		÷. (†)		

Figure 43 Selecting the Level column in Excel

- d Scroll until the column after the end of the Sequence Table is visible.
   A blue triangle appears in the lower right corner of the last column in a
- 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 table

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



In most cases, you can only add a mapped column to a table if the mapped column is from the same section in the XML source as the other columns in the table. First, you identify the section in the XML source by clicking 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 table

Step		Detailed Ins	truction	S	Comments				
	pfh_5_Custon	n_ISTD_Summary.xltx -	Microsoft Exce	ł	_ = ×				
Home Insert Page Li	ayout Formulas Data Revie	w View Develop	er Add-Ins	Acrobat	🕑 – 🖷 X				
🐴 Process Report 🧭 Clear Results 🕈	🖥 Add Data 🐁 Add Graphics 👫 Add F	ormatting 🎇 Advanced I	Properties 🎅 V	alidate Design 🚯 🛞					
						The last column in the			
	Custom Toolbar	s							
A1 • (*	∫ <sub>∞</sub> Batch Info				×	Sequence Table is now the			
	K L M N O P Q R S	TUVWXY	Z AA AB A	AD AE AF AG AH AI A	J AK AL AM AN AO AP AQ 🕎	Barcode column.			
Info         Image: Comparison of the system           2         Jata Path         C:\MassHunt           3         s Time         1/18/2010 1           4         Time         1/18/2010 1           5         IIb Update         1/18/2010 1           6          1/18/2010 1	1:18 AM Reporter Name	Processed	h.bin		=				
7 nce Table									
8 Acquisition File 9 y 1 CMAMBk_01.d	Sample Name CMAM 01		Sample Type Blank	Acq Method File	5.00 BarCode1				
10 y 1 CMAMCal L1.d	CMAM_06	L1	Calibration	APCIautotune.m	5.00 BarCode123				
11 y 1 CMAMCal_L2.d	CMAM_10	L2	Calibration	APCIautotune.m	5.00 BarCode123				
12 'y 1 CMAMCal_L3.d	CMAM_11		Calibration	APCIautotune.m	5.00 BarCode123				
13 y 1 CMAMCal_L4.d	CMAM_14		Calibration	APCIautotune.m	5.00 BarCode123				
14 y 1 CMAMCal_L5.d	CMAM_17		Calibration	APCIautotune.m	5.00 BarCode123				
15 y 1 CMAMQC_L2.d 16 y 1 CMAMQC_L4.d	CMAM_09 CMAM_15		QC	APCIautotune.m APCIautotune.m	5.00 BarCode123				
16 Y 1 CMAMQC_L4.d 17 y 1 CMAMSam 01.d	CMAM_15 CMAM_22		QC Sample	APCIautotune.m	5.00 BarCode123 5.00 BarCode123				
18 y 1 CMAMSam_02.d	CMAM 08		Sample	APCIautotune.m	5.00 BarCode123				
19 v 1 CMAMSam 03.d	CMAM 12		Sample	APCIautotune.m	5.00 BarCode123				
Summary 2									

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

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

# 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\ <i>iii_6_</i> Custom_ISTD_Summary.xltx.	<ul> <li>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.</li> </ul>	<ul> <li>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.</li> </ul>
<ul> <li>Add a filter to the Quantitation Results table using the Advanced Properties dialog box.</li> <li>Only include data files that have an expected concentration.</li> </ul>	<ul> <li>a Find the second table in the section Quantitation Results.</li> <li>b Click the column labeled Exp Conc This column is the tenth (10th) column in the table.</li> <li>c Click Advanced Properties.</li> <li>d Select NonBlanks in the Filter value box when the Exp Conc column is selected.</li> </ul>	<ul> <li>The Advanced Properties icon is part of the MassHunter toolbar in the Add-Ins tab in the Ribbon.</li> </ul>
	e Click Set Filter. f Click Close.	
Advanced Properties Templet [Design Worksheet ] Cell Table ] Table groups and the second seco	e Click Set Filter. f Click Close.	Select NonBlanks as the Filter Value and then click Set Filter.
Template         Design Worksheet         Cell         Table           Table properties         Column         Column           Table core         Passes         Column           The core of the properties         Column         Image: Column           The core of the properties         Passes         Passes	e Click Set Filter. f Click Close.	
Template         Design Worksheet         Cell         Table           Table properties         Column         Column           Table core         Pastor         Column           The core of the properties         Pastor         Pastor	e Click Set Filter. f Click Close. Aum propertes Width Propertes Filter mpoundID Hoden Hoden Let 7 ppe 12.5 ind 12.5 ISTD	
Template         Design Worksheet         Cell         Table           Table properties         Column         Column           Associate with the following table or graphics         Fill         Fill           Hide header row         Column         ISTOC           Table contents transposed to         Columns         Cate Fill           Hide empty cells         Sandid         Sandid	e Click Set Filter. f Click Close. Aum properties Width Properties Filter mpoundID Hidden Cocessante (UAL astation of the filter) is of 12.5 mpot 12.5 mpot cocessante (UAL astation of the filter) t Text width rest	Value and then click Set Filter.         The filter is shown in the Filter

**Figure 46** Add a filter to the Sequence Table using the Advanced Properties dialog box

Task 7. Add a filter to a table

Step	Detailed Instructions	Comments
<ul> <li>Add a filter to a table using Excel.</li> <li>Add a text filter to the column Acquisition File in the Sequence Table.</li> <li>Only include an Acquisition File if the file name contains "Blk" or "Cal".</li> </ul>	<ul> <li>a Find the table labeled Sequence Table.</li> <li>b Click on the arrow in the cell labeled Acquisition File. This column is the third column in the table.</li> <li>c Click Text Filters &gt; Contains. The Custom Auto Filter dialog box is opened.</li> </ul>	<ul> <li>A filter allows you to only include a row in the table if it passes the filter.</li> </ul>
	iummary.xltx - Microsoft Excel Table Tools	

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

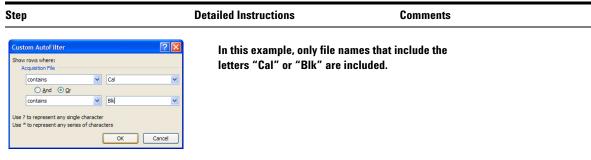
				Cus	tom To	olbars									
	C8	•	( fx /	Acquisition File											
	A		В	С		D	E		F	G		н	L I	J	
5															
1	Sequence Table				_			_							_
	SampleID	-	Location	Acquisition File	San	nple Na 💌	Level	<ul> <li>Sam</li> </ul>	ple Tyj 🔻	Acq Method Fi	-	Volui 👻	SamplePosit	TrayName	-
		₹↓	Sort A to Z		ĺ										
		Z↓	Sort Z to A												
	Quantitation Res		Sort by Color		_										
	CMD:Repeat	K	Clear Filter From	"Acquisition File"				_							
	SampleID		Filter by Color	+			Name	Reter	ntionTim 👻	•					
5			Text Filters		Tan	net Comn	ound	_		4					-
	SampleID		Text Linters		_	Equals		Data	File 💌	Compound	<ul> <li>ISTD</li> </ul>		Sample Ty 💌	Exp C	•
7			(Select All)	)		Does <u>N</u> ot	Equal								
3			(Blanks)			Begins W	ith								
9	CMD:EndRepeat					Ends With									
1	CMD:Enukepear					-		_							
2						Contains.									
						Does Not	Contain								
3						Custom Ei		-							

**Figure 47** Add a filter to the Sequence Table using Excel features

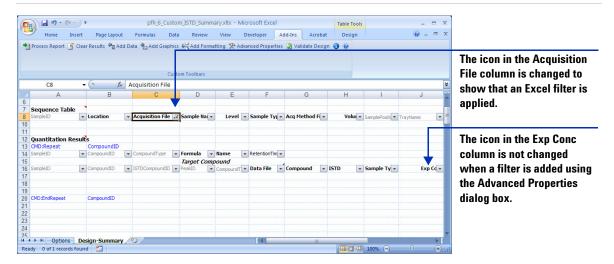
- **d** Type Cal in the first text field.
- e Click Or.
- f Select contains in the second box.
- **g** Type Blk in the second text field.
- h Click OK.

Task 7. Add a filter to a table

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







#### Figure 49 A filter is added to the Acquisition File column

Task 7. Add a filter to a table

Step	Detailed Instructions	Comments				
<b>4</b> Test the changes to the template.	<ul> <li>a Click Process Report.</li> <li>b Click the Browse button.</li> <li>c Navigate to the DrugsOfAbuse\ QuantReports\DrugsOfAbuseDemo folder.</li> <li>d Select report.results.xml.</li> <li>e Click Open.</li> <li>f Click OK.</li> <li>g Find the Sequence Table. The only acquisition files that are included contain either Cal or Blk.</li> <li>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.</li> </ul>	<ul> <li>The Process Report command is part of the MassHunter toolbar in the Add-Ins tab in the Ribbon.</li> </ul>				

Task 7. Add a filter to a table in a Quantitative Analysis template
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9	1 3 -	(" - ) =			ofh 6	Custom IST	D_Summary	vity - Mice	osoft Evcel				= Y	
C	Home	Insert	Page Layout	Formulas	Data	Review	View [	Developer	Add-Ins A	robat		(	0 _ = ×	The Sequence Table now
*	Process Repor	rt 🕑 Clea F	Results 👫 Add	I Data Add	Graphics 🌵	•	ting 🎌 Adv	anced Prop	erties 🎅 Validate	Design 🚯 🧔				only contains six rows. Before the filter was added,
	A1	-	• fx	Batch Info									×	the Sequence Table
7		D E F	GHI		N O F	QR:	3 T U '	X W X	Y Z AA AB	AC AD AE AF	AG AH AI	AJ AK AL A	M AN AO	contained eleven rows. Each
	Location	Acquisit	tion File		Sample Na	ame		Level	Sample Type	Acq Method	File	V	olume Barc	Acquisition File contains
	Laboratory 1	CMAMBIK			CMAM_01				Blank	APCIautotune.			5.00 Bar	•
	Laboratory 1	CMAMCa			CMAM_06			L1	Calibration	APCIautotune.			5.00 Bart	either "Cal" or "Blk" in the
	Laboratory 1	CMAMCa			CMAM_10			L2	Calibration	APCIautotune.			5.00 Bart	
	Laboratory 1	CMAMCa			CMAM_11			L3	Calibration	APCIautotune.			5.00 Bar(	name.
10	Laboratory 1	CMAMCa			CMAM_14			L4	Calibration	APCIautotune.			5.00 Bar(	
	Laboratory 1	CMAMCa	l_L5.d		CMAM_17			L5	Calibration	APCIautotune.	.m		5.00 Bar(	
15	Quantitatio	n Results											_	Every row in this table has
	Target Com		Amp			- <b>V</b>							_	Every row in this table has
	Data File		npound	ISTD	S	ample Type	Exp Cor	nc Resp	ISTD Resp	Resp Ratio	Final Conc	Accuracy	_	an expected concentration.
19	CMAMCal_L1.d	Amp	)	Amp-d5		Calibratio	on 2.50	00 658		0.4725	3.3303	133.2	_	
20	CMAMCal_L2.d	Amp	, ,	Amp-d5		Calibratio	on 5.00	1052		0.8154	5.7475	114.9	_	
21	CMAMCal_L3.d	Amp	, ,	Amp-d5		Calibratio	n 12.50	2673		1.9409	13.6808	109.4	_	
22	CMAMCal_L4.d	Amp	, ,	Amp-d5		Calibratio	on 25.00	00 4952		3.7959	26.7560	107.0	_	
	CMAMCal_L5.d		5	Amp-d5		Calibratio	on 125.00	18605		17.6606	124.4842	99.6	_	
	CMAMQC_L2.d		0	Amp-d5		ç	C 5.00	00 1006		0.7419	5.2293	104.6	_	
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Rea	dy 🛅										100%	<u> </u>	.;	

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

Task 7. Add a filter to a table

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

Step	Detailed Instructions	Comments				
<ul> <li>Save the changes to the template <i>iii</i>_7_Custom_ISTD_Summary.xltx</li> <li>You have to clear the results first.</li> </ul>	<ul> <li>a Click Clear Results in the Add-Ins tab in the Ribbon.</li> <li>b Click the Microsoft Office Button and then click Save As and click Other Formats.</li> <li>c In the Save As dialog box, type <i>iii_7_Custom_ISTD_Summary.xltx.</i></li> <li>d Verify the folder selected in Save in is correct.</li> <li>e Click Save.</li> </ul>	<ul> <li>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).</li> <li>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.</li> </ul>				

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

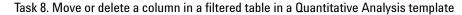
You can add a filter to a column in a table in two different ways. If you use the Advanced Properties dialog box to add a filter, you can still easily move and delete a column. However, if you use Excel features to add a filter to a table, you have to remove the filter before you can move or delete a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

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, <i>iii_</i> 7_Custom_ISTD_Summary.xltx, where " <i>iii</i> " are your initials.	<ul> <li>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.</li> </ul>
<ul> <li>2 Delete the Volume column.</li> <li>Hint: you only click the column header if you want to delete the column.</li> </ul>	<ul> <li>a Find the Sequence Table.</li> <li>b Select the column labeled Volume and the cell beneath it. This column is the eighth (8th) column in the table.</li> <li>c Right-click the Volume column and try to click Delete &gt; Table Columns. You cannot because this command is grayed out.</li> <li>d Click only the cell labeled Volume.</li> <li>e Right-click the Volume column and click Delete &gt; Table Columns. You can delete this column ow.</li> </ul>	• The Sequence Table has an Excel filter added to it.
<ul> <li>Move the Barcode column.</li> <li>You have to remove the filter before you can move a column.</li> </ul>	<ul> <li>a Find the Sequence Table.</li> <li>b Click the column labeled Barcode and on the cell beneath it. This column is the eighth (8th) column in the table.</li> <li>c Move the cursor to the edge of the cell until the cursor changes to a four sided arrow, * * .</li> <li>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.</li> <li>e Click OK in the error message</li> </ul>	<ul> <li>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".</li> </ul>

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

e Click OK in the error message.

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



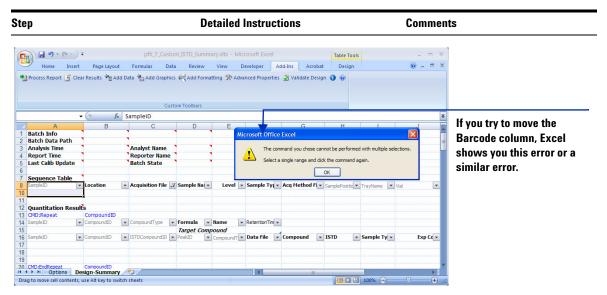


Figure 51 A filter is added to the Acquisition File column

- 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.
- I 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

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Last Calib Update				Batch State									
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eady 0 of 1 records fo											100% 🕞 —	- <b>(</b>	

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

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.
- I 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

#### **Detailed Instructions** Step Comments 🔁 🖌 🖉 - (° - ) = = x pfh 7 Custom ISTD Summary.xltx - Microsoft Excel Table Too Home Insert Developer Desig 0 -Page Layout Add-Ins The Acquisition File column 軩 Process Report 🧃 Clear Results 👫 Add Data 🐁 Add Gra iced Properties 🌍 Validate Design 🚯 has the text filter again. D8 fx Barcode ¥ Batch Info Batch Data Path Analysis Time Analyst Na Report Time Reporter Na Last Calib Undate Ratch State The Barcode column is now Sequence Table after the Acquisition File - Location Acquisition File J Barcode Sample Na 🗸 Level Sample Type -Aca Methor • column 12 **Ouantitation Results** CMD:Repeat 13 14 CompoundID CompoundID ▼ Name ▼ RetentionTim ▼ CompoundType Formula 15 Target Compound CompoundID 16 ▼ ISTDCom Data File ▼ Sample Ty ▼ Exp Cc 👻 dID 💌 Compound ▼ ISTD 18 20 CMD:EndRepeat Components Ready 0 of 1 records found

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

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.
- 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 **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.
- **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.

- The second table in the Quantitation Results section has a filter added to it using the Advanced Properties dialog box.
- 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

Step		Detailed Ins	tructions		Commen	ts
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Home Insert Page L		Review View Develop		Design	<b>⊘</b> _ = ×	
🗎 Process Report 🥤 Clear Results 🕯		🚧 Add Formatting 🏋 Advanced F n Toolbars	roperties 🔮 Validate Design	0 0		
K16 🗸 🕤	∫x Final Conc				*	The Barcode column is
A B C	DE	F G	H I	J	K L	
2					=	after the Acquisition File.
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4 Reporter Nat 5 Batch State	ne					
6						
7						
8 Location  Acquisition Fil 10	e 📝 Barcode 🛛 💌 Sample I	a 💌 Level 💌 Sample Type	Acq Methor SamplePosit	TrayName	Vial	The Final Course selection is
11						The Final Conc column is
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20 CompoundID					×	
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Task 8. Move or delete a column in a filtered table in a Quantitative Analysis template

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

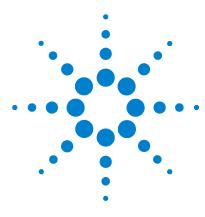
#### Task 8. Move or delete a column in a filtered table in a Quantitative Analysis template

Step		Deta	iled Instructi	ons		Commen	ts
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Process Report	t 🥑 Clear Results 👻 Add Dal	ta 🐁 Add Graphics 👫 Add Formatting	Advanced Properties	🛿 Validate Design 🚯 🧯	)		
V4	• (• fx	Custom Toolbars				×	The Barcode column is
A B C 4 Report Time 5 Last Calib Up 6	1/18/2010 11	1:18 AM Reporter Name	F U V W X Y Z Processed	AA AB AC AD AE A	F AG AH AI AJ A	K AL AM AN AO	moved to after the Acquisition File.
7 Sequence T 8 Location 9 Laboratory 1 10 Laboratory 1	able Acquisition File CMAMBk_01.d CMAMCal L1.d	Barcode BarCode 1 BarCode 123456	Sample Name CMAM_01 CMAM_06	Leve	Sample Type Blank Calibration	Acq Method File APCIautotune.m APCIautotune.m	Acquisition The.
11 Laboratory 1 12 Laboratory 1 13 Laboratory 1 14 Laboratory 1	CMAMCal_L2.d CMAMCal_L3.d CMAMCal_L4.d CMAMCal_L5.d	BarCode 1234567890 BarCode 1234567890 1 BarCode 1234567890 1234 BarCode 1235677890 1234567	CMAM_10 CMAM_11 CMAM_14 CMAM_17	L2 L3 L4	Calibration Calibration Calibration Calibration	APCIautotune.m APCIautotune.m APCIautotune.m APCIautotune.m	The Final Conc column is
15 16 Quantitatio 17 Target Com	n Results bound Amp		↓ -	13	Calbrauur	Arctadiolane.m	moved to after the Exp Conc column.
Data File           19         CMAMCal_L1.d           20         CMAMCal_L2.d           21         CMAMCal_L3.d           22         CMAMCal_L3.d	Amp A Amp A Amp A	Sample Type           Imp-d5         Calibration           Imp-d5         Calibration           Imp-d5         Calibration           Imp-d5         Calibration           Imp-d5         Calibration	Exp Conc         Final Conc           2.5000         3.3303           5.0000         5.7475           12.5000         13.6808           25.0000         26.7560	Resp         ISTD Resp           658         1052           2673         4952	Accuracy 133.2 114.9 109.4 107.0	*	column.
	mary 🕄 Amp A	Calbration	25.0000 26.7560		107.0		

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.



Agilent MassHunter Workstation Software Reporting Familiarization Guide

# Exercise 4 Additional ways to customize a table

Task 1. Add a table to a template86Task 2. Format a table (Transposing and Hiding headers)92Task 3. Add a formula column to a table95Task 4. Add an ISTD column to a Quantitative Analysis template100Task 5. Add a column that is already mapped104

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.

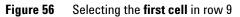
When you add a table to a template using the Add Data commands, a new XML map is added automatically. If you remove this table from the template in the future, make sure to also delete the XML map that was created. Reports print more quickly when you have fewer XML maps. You can delete unused XML maps 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. A	dd a table to	a Qualitative A	Analysis template
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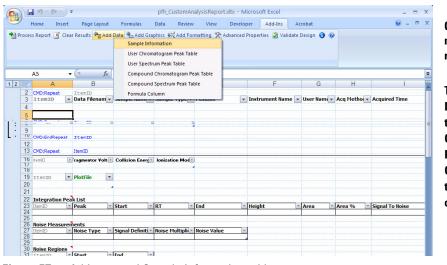
S	tep	D	etailed Instructions	C	Comments
1	Open the Qualitative Analysis template, \ <b>MassHunter\Report</b> Templates\Qual\Letter\ iii_CustomAnalysisReport.xltx.	а	Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 32 to open the template, <i>iii</i> _CustomAnalysisReport.xltx, where " <i>iii</i> " 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 <b>Familiarization Templates</b> folder.
2	<ul><li>Add a second table to show additional Sample Information.</li><li>Add the table inside the Repeat section.</li></ul>		Find the first table in the template. The first two items are <b>ItemID</b> and <b>Data</b> <b>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.

ep				1	Detailed In	structions			Comm	ents
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	Home insert ss Report 👔 Clea	r Results 🆓 Ad		aphics 📲 Add Fo		ed Properties 🔮 Validate	e Design 👔 🥳			Click on this cell in the template.
				Custom Toolbars						
2 4	A5 •	B	С	D	E	E	G	Н		The current position in the
2	CMD:Repert ItemIR	ItemID	▼ Sample Nam( ▼			▪ Instrument Name [			Acquired Time	template is shown here.
: :	217 <u>2-</u> 1		0							=
· 9	- CMUSENDRepear	ItemID								
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16 17 18		ragmentor ¥olt	Collision Energ	lonization Mod						CMD:Repeat row and the
		PlotFile	•							CMD:EndRepeat row are
20			•							
22	Integration Pea	k List								repeated for each ItemID.
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	ItemID 💌		<ul> <li>Signal Definiti</li> </ul>	Noise Multipli	Noise Value	-				data files.
29	Noise Regions		-							

#### Task 1. Add a table to a Qualitative Analysis template



- c Click Add Data > Sample Information Extra rows are automatically added in the Add-Ins tab in the Ribbon.
- 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 template

#### Task 1. Add a table to a Qualitative Analysis template

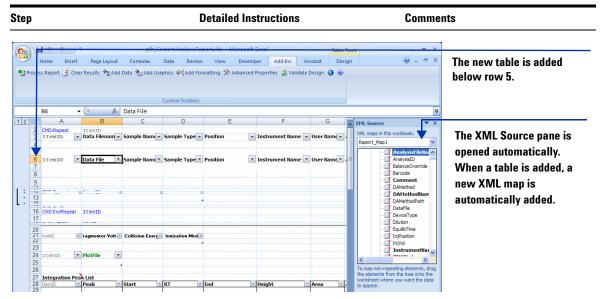


Figure 58 Add a second Sample Information table.

- **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.
- 4 Change the second table to include only the following columns:
  - ItemID
  - Data File
  - Injector Volume
  - Dilution

- 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.
- 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 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.
- 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.

Step **Detailed Instructions** Comments 强 🖉 - (° - ) = pfh CustomAnalysisReport.xltx - Microsoft Excel = x Table Tool Home Insert Page Layout Formulas Data Review View Developer Add-Ins Acrobat Design 📸 Process Report 🧉 Clear Results 🐜 Add Data 🐁 Add Graphics 🖊 Add Formatting 🎇 Advanced Properties 🧕 Validate Design 🚯 👰 C6 - () fx Sample Name ¥ A В XML Source **•** × 2 CMD:Repeat 4L maps in t ▼ Data Filenam ▼ Sam Tahoma ▼ 8 · A A \$ • % , 0 ▼ Instr ent Name 💌 User Name Report\_Map1 ~ Select the columns that you Tilution ^ EquilibTime want to delete. Right-click Data File Instr nt Name 🔻 User Name Cut Ж Сору TniVol and click Delete > Table InstrumentNa Paste IRMStatus Columns. All of the columns l Paste Special. 1 ItemID 13 T LevelName that are selected are MethodType 16 CMD:EndRepeat ItemID Insert • PlateCode removed. PlatePosition Table Colu Delete RackCode 20 21 22 Select Table Rows ragmentor Volt Col TRackPosition Clear Contents SampleID Sampl 24 ItemID Sort . PlotFile -25 Filter 2 26 Ta<u>b</u>le Þ 27 28 Integration Peak List ItemID • Peak ϪML Þ - Star

#### Task 1. Add a table to a Qualitative Analysis template

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 template



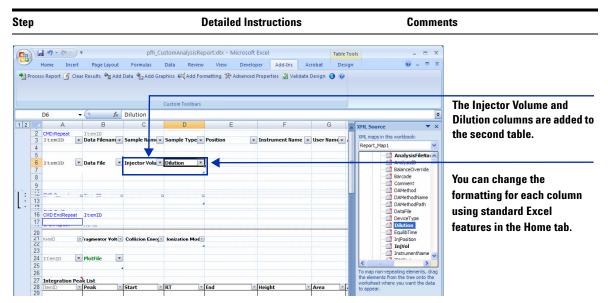


Figure 60 The Injector Volume and Dilution columns are added to the second table

- **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.

Step	Detailed Instructions	Comme	nts
	pfft_GustomAnalysisReportsite Microsoft Exect mulas Data Review View Developer Add-Ins Acrobat 철 Add Graphics 뷰 Add Formatting 갖 Advanced Properties ઝ Validate Design ④ * Custom Toolbars		The first table is transposed and shows the information next to the column header.
2         Data Filename         sulfas_PosMS.d           3         Sample Type         Sample           4         Instrument Name         QTOF PP1           5         Acq Nethod         sulfas_PosMSonly_           6         IRM Calibration Status         Success           7         Comment         Success	L M N O P Q R S T U V W X Y Z AA AB AC AD AE, Sample Name 1ng sulfas Position P1:F1 User Name demo.m Acquired Time 8/16/2008 9:29:01PM DA Nethod Default.m	AF XHL Source V X XML maps in this workbook: Report_Map V Start A Symm Tailin Widt	
8 0 bate File sulfas_PosMs.d Injector Volume 9 Diution 1 12 User Chromatograms 14 Fragmentor Voltage 125 Collision Eaerg × 10 6 +ESI TIC Scan Frag=125.0V sulfas_Po 6 1 0.7 5 0.7 5 0.7 6 0.325 14 0.325 14 0.325	0 Ionization Mode ESI sMS.d 11 1225 1 1	Workscher	The second Sample Information table shows the Injector Volume and the Dilution.

Task 1. Add a table to a Qualitative Analysis template

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.

Step	Detailed Instructions	Comments
1 Open the Qualitative Analysis template, \ <b>MassHunter\Report</b> 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, <i>iii</i> _1_CustomAnalysisReport.xltx, where " <i>iii</i> " are your initials.	<ul> <li>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.</li> </ul>
<ul> <li>2 Format the second table.</li> <li>Do not transpose the second sample information table.</li> <li>Set the width of each column to 15.</li> </ul>	<ul> <li>a Click on a column in the second table.</li> <li>b Click Advanced Properties which is part of the MassHunter toolbar in the Add-Ins tab in the Ribbon.</li> <li>c Clear the Table contents transposed to check box.</li> <li>d Select each Column under Table column properties.</li> <li>e Type 15 in the Text width field.</li> </ul>	<ul> <li>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.</li> <li>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.</li> </ul>

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

#### Task 2. Format a table in a Qualitative Analysis template

Table projecties       Column       Table projecties       Check box         Table projecties       Column       Wdth       Properties       Check box         Table projecties       Column       Hide       15       Hide       Hide	
Table contents transposed to       columns         Hide empty cells       Image: transposed to         Wrap columns across page       2         Combine table rows starting at column       1         Combine table rows starting at column       Image: transposed to         Combine table rows starting at column       Image: transposed to         Combine table rows starting at column       Image: transposed to         Combine table rows starting at column       Image: transposed to         Graphics layout       Image: transposed to         Graphics layout       Image: transposed to         Column sort order       Image: transposed to         Column sort order       Image: transposed to	contents transposed to k is cleared.
	of each column in the et to 15 using the Text width

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.
- **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.

- You do not need to close the Advanced Properties dialog box to switch to a different table.
- The Process Report command is part of the MassHunter toolbar in the Add-Ins tab in the Ribbon.

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

#### Task 2. Format a table in a Qualitative Analysis template

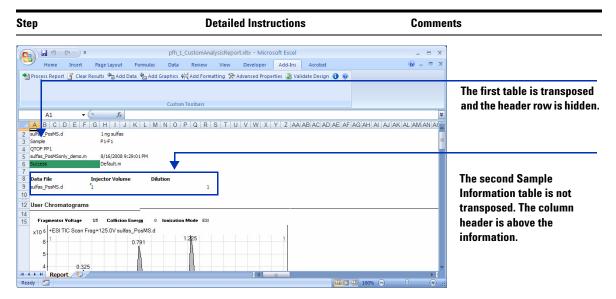


Figure 63 Verifying a new Sample Information table is added to the template

- 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
Templates\Qua	sHunter\Report Il\Letter\ nalysisReport.xltx,	a Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 32 to open the template, <i>iii_2_CustomAnalysisReport.xltx,</i> where " <i>iii</i> " are your initials.	<ul> <li>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.</li> </ul>
End in the Int Table. • Label the colu • Change the for difference of	right of the column egration Peak List umn <b>PWFH</b> . ormula to show the the start of the end of the peak.	<ul> <li>a Find the table labeled Integration Peak List.</li> <li>b Click on the cell containing the words End. This column is the fifth column in the table.</li> <li>c Click Add Data &gt; Formula Column in the Add-Ins tab in the Ribbon.</li> <li>d Follow the instructions in "Task 1. Rename a column header in a table" on page 53 to rename the column to PWFH.</li> <li>e Click the Formulas tab in the Ribbon.</li> <li>f Hide the XML Source pane, if it is visible.</li> </ul>	<ul> <li>The Add Data &gt; Formula Column command adds the column to the right of the column selected.</li> <li><b>PWFH</b> is an abbreviation for Peak Width Full Height.</li> <li>You can manually enter formulas if you know the syntax, without using the Excel Function Arguments dialog box.</li> </ul>

Task 3. Add a formula column to a table

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

Step	Detailed Instructions	Comme	nts
Home Insert Page Layout Formulas Dat	omAnalysisReport.xltx - Microsoft Excel ta Review View Developer Add-Ins Ad	Table Tools _	
Jack         Z AutoSum         IP Logical         Logical         Date & Reference           Inset         Inset	As * Manager III: Create from Selection Defined Names Fig.	pendents 🔶 - Arrows - 🙆 Watch Window ormula Auditing Calculation Calculation	This tab in the Ribbon helps you add a formula to the
F23         C         file         Enter formula her           12         A         B         C           6         IttemD         Data         Injector Volute         Data           7         9         9         9         9         9         10         Injector Volute         Data           13         13         13         11         12         0	D E F	G H I	table. For information about formulas and functions, see the online Help for Microso Excel 2007 or Excel 2010.
20     ************************************		Hormula H	The new column PWFH is to the right of the End column. The Excel comment, "Formula" is added to this column.

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
- 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.
- I 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.
- 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 table

Function Library       Defined Names       Formula Auditing       Calculation         SUM <ul> <li>X</li> <li>A</li> <li>B</li> <li>C</li> <li>T temTD</li> <li>X</li> <li>X<th>tep</th><th></th><th></th><th></th><th></th><th>Deta</th><th>iled Instr</th><th>uction</th><th>S</th><th></th><th>Con</th><th>nme</th></li></ul>	tep					Deta	iled Instr	uction	S		Con	nme
Institute		Home Inser	Page Layou	t Formulas	Data	Review View	w Developer	Add-Ins		Design	- 0	
12       A       B       C         5       ItemID       Data File       Injector Volu       Dilution         6       ItemID       Data File       Injector Volu       Dilution         9       Injector Volu       Dilution       IteI[[#This Row],[End]]       Itei[[#This Row],[Start]]       Itei       0         1       IteI[[#This Row],[Start]]       Itei       0       IteI[[#This Row],[Start]]       Itei       0         1       IteI       IteI       IteI       IteI       0       IteI       0         1       IteI       IteI       IteI       IteI       0       IteI       0         1       IteI       IteI       IteI       IteI       IteI       0       IteI       0         1       IteI		Recently Use	d * 🔒 Text *	🖗 Math me = 🍘 More	& Trig *	Name Manager	Use in Formula •	-Ç∦ Tra	ce Dependent move Arrows	ts 🚸 - 🛱 Wat Wind	ch Calculation	
5       T CEND       Data File       Injector Volu       Dilution         6       T CEND       Data File       Injector Volu       Dilution         7       Number 2       List [[[This Row], [End]]       Es       =       0         1       Number 2       List [[[This Row], [End]]       Es       =       0         1       Immon       Item 10       Item 10       Adds all the numbers in a range of cells.       =       0         10       Item 0       Plagmentor Yot 2       Cotitision Energie       Ionizative       Formula result =       0         20       Item 0       Plagmentor Yot 2       Cotitision Energie       Ionizative       Formula result =       0         23       Item 0       Place N test       Estart       Rt       End       PPWH       I Height       Area %		SUM			1[[#This Ro	Function Argu	iments				[	2 🛛
The second	5 6 7 8 9 : : : :	ItemID			lu 💌 Dilutior	Nur Ni	umber2 -List1[[#Th		ul 📧	= 0		
24         rtem10 <ul></ul>	16 17 20 21 22	CMD:EndRepeat		Collision Er	erc Ionizati		10.000000000 <del>.</del> 000000000	r2: number 1,	number2, ar ed in cells, inclu	e 1 to 255 numb	ers to sum. Logical values ani arguments.	i text
28 ItemID · Peak · Start · RT · End · PFWH · Height · Area · Area %	24 25 26	4 ItemID ( 5 6		•			5				OK Cano	e
29 [This Row], [Start]])	28	B ItemID		- Start	₹ RT	🗾 End		VH Row],[Start]])	- Height	- Area	Area %	

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

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.

f Inse Fund	ert and an and a second y Us	t Page Layout	Formulas Cookup & Math & 1 e + More Fu	Data R & Reference rig *	Name Contact	Developer Add re Hume S n Formula * te from Selection	-Ins Acrobat	Watch Window	Ø − ■	A formula starts with the equal sign. This formula i
	SUM				End]],-List1[[#Thi					a sum of the two items
12	A 6	В	SUMmumpe	1, (number2), (	numpet3],) ) E	F	G	H	1	listed. The blue part of the
	6 ItemID 7 8 9 13 16 CMDEndRepea 17 20	.a	Injector Volu		•					formula refers to the valu in the End column. It is color-coded to match the outline of the cell in the Integration Peak List tabl
	Z1 ItemID Z2	▼ <sup>:</sup> ragmentor ¥olt	Collision Energ	Ionization I	Aode					The green part of the
	25	▼ PlotFile ▼								formula refers to the valu
	26				- <u> </u>					in the Start column. It als
	27 Integration P 28 ItemID		Start	- RT	- End	- PFWH	~ Height	~ Area	~ Area %	- in an law and ad
	29 30	- Curk	Store	NI I	Linu	=5UM(List1[				is color-coded.

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

Task 3. Add a formula column to a table

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

	Detailed Instructions	Comments
Test the changes to the template.	<ul> <li>a Click the Add-Ins tab in the Ribbon.</li> <li>b Click Process Report.</li> <li>c Click the Browse button.</li> <li>d Navigate to the \MassHunter \Reports\Temp folder.</li> <li>e Double-click one of the folders that contains analysis results.</li> <li>f Select Report.xml.</li> <li>g Click Open.</li> <li>h Click OK.</li> <li>i Find the Integration Peak List table. The PWFH column contains the difference between the End and the Start of the peak.</li> </ul>	<ul> <li>The Process Report command is part of the MassHunter toolbar in the Add-Ins tab in the Ribbon.</li> </ul>

Figure 67 Verifying the formula column in the Integration Peak List table.

Task 3. Add a formula column to a table

S	tep	Detailed Instructions	Comments	
4	Save the changes to the template, <i>iii</i> _3_CustomAnalysisReport.xltx, where <i>iii</i> are your initials.	<ul> <li>a Click Clear Results in the Add-Ins tab in the Ribbon.</li> <li>b Click the Microsoft Office Button and then click Save As and click Other Formats.</li> <li>c In the Save As dialog box, type <i>iii_3_</i>CustomAnalysisReport.xltx, where <i>iii</i> are your initials.</li> <li>d Verify the folder selected in Save in is correct.</li> <li>e Click Save.</li> </ul>	<ul> <li>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).</li> <li>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.</li> </ul>	

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

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

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

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

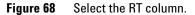
Task 4. Add an ISTD mapped column to a Quantitative Analysis table
--

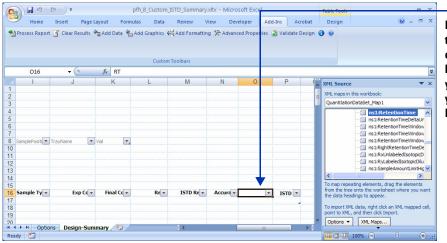
Step	Detailed Instructions	Comments
1 Open the Quantitative Analysis template, \MassHunter\Report Templates\Quant\Letter\ISTD\ Parts\ <i>iii_</i> 8_Custom_ ISTD_Summary.xltx template.	a Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, <i>iii_8_</i> Custom_ISTD_Summary.xltx., where " <i>iii</i> " are your initials.	<ul> <li>If you do not have this template, example templates are available or the Agilent Technologies MassHunter Reporting User Information DVD in the Familiarization Templates folder.</li> </ul>
<ul> <li>2 Add two columns to the Target Compound table.</li> <li>Add the Retention Time column and change the name to RT.</li> <li>Add the ISTD Retention Time column and change the name to ISTD RT.</li> </ul>	<ul> <li>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.</li> <li>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.</li> <li>c Right-click the RT column header and click the B button to make the header match the font in the other headers.</li> <li>d Right-click the RT column header and click the Format Cells command.</li> <li>e Click the Alignment tab.</li> <li>f Select Right (Indent) in the Horizontal list. Click OK.</li> <li>g Click the RT column header.</li> <li>h Click the Add Data &gt; ISTD Column command.</li> <li>i Select RT from the Select Column Dialog box.</li> <li>j Click OK.</li> <li>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.</li> </ul>	<ul> <li>An ISTD column is added to the right of the selected column.</li> <li>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.</li> <li>(optional) You right-click the value for the RT and the ISTD RT and clic the Format Cells command to select the number of decimal places.</li> <li>(optional) You can set the width of the RT and ISTD RT column to</li> </ul>

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

Task 4. Add an ISTD mapped column to a	Quantitative Analysis table
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Step	Detailed Instructions	Comments
Select Column Pick a column SampleID CompoundID ISTDCompoundID PeakID CompoundType		t with the word ISTD. These columns are umns. Do not select any of these
Composite type Data File Compound Exp Conc File Accuracy Response ISTD Resp Accuracy RI	add an ISTD column. This col	D has to be part of the table in order to umn is automatically added when you t already included. the ISTDCompoundID
OK Cancel		





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 column to a Quantitative Analysis template

Task 4. Add an ISTD mapped column to a Qu	Quantitative Analysis table
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Step	Detailed Instructions	Comments	
<b>3</b> Test the changes to the template.	<ul> <li>a Click Process Report.</li> <li>b Click the Browse button.</li> <li>c Navigate to the DrugsOfAbuse\ QuantReports\DrugsOfAbuseDemo folder.</li> <li>d Select report.results.xml.</li> <li>e Click Open.</li> <li>f Click OK.</li> <li>g Find the Target Compound Table.</li> <li>h Scroll to the end of the Sequence Table. The Barcode column is now the</li> </ul>	<ul> <li>The Process Report command is part of the MassHunter toolbar in the Add-Ins tab in the Ribbon.</li> </ul>	

last column in the Sequence Table.

•	1	(21 - ) ≠			pfh_8_Custom_ISTE	_Summary.	dtx - Micros	oft Exce	1			_ = X	
8	Home	Insert	Page Layou	t Formulas	Data Review V	/iew Dev	eloper A	dd-Ins	Acrobat			0 _ = ×	
1	Process Report	📑 Clear Re	sults 🖣 Ad	dd Data 🐐 Add Gr	aphics 👫 Add Formattir	ig 🔆 Advan	ed Properties	s 🍠 Vali	date Design 🚯 (	9			
													The last two columns in
					Custom Toolbars								
	A1	- 6	fa	Batch Info								*	the Target Compound tabl
						-							<b>J</b> 1
			GHI	JKLM	N O P Q R S	IUV	WXY	ZAA	AB AC AD AE A	AF AG AH A	I AJ AK AL	AM AN AO AP	are the RT and ISTD RT
	Quantitatior Target Comp		Amp										
	<i>Target Comp</i> Data File		ound	ISTD	Sample Type	Exp Conc	Final Conc	Resp	ISTD Resp	Accuracy	RT	ISTD RT	
	CMAMCal L1.d	Amp	, ound	Amp-d5	Calibration	2,5000	3,3303	658	1510 Hesp	133.2	2,10050434	2.076037963	The RT column is the
	CMAMCal_L2.d	Amp		Amp-d5	Calibration	5.0000	5.7475	1052		114.9	2.10050434	2.076037963	
21 0	CMAMCal_L3.d	Amp		Amp-d5	Calibration	12.5000	13.6808	2673		109.4	2.10050434	2.076037963	retention time of that
22 0	CMAMCal_L4.d	Amp		Amp-d5	Calibration	25.0000	26.7560	4952		107.0	2.10050434	2.076037963	
23	CMAMCal_L5.d	Amp		Amp-d5	Calibration	125.0000	124.4842	18605		99.6	2.10050434	2.076037963 😑	compound. The ISTD RT
	CMAMQC_L2.d	Amp		Amp-d5	QC	5.0000	5.2293	1006		104.6	2.10050434	2.076037963	compound. The ISTD III
	CMAMQC_L4.d	Amp		Amp-d5	QC	25.0000	27.8011	4715		111.2	2.10050434	2.076037963	column is the retention
26			1										column is the retention
	Target Comp		Cocaine	ISTD							2019-0		time for the internal
	Data File CMAMCal L1.d	Cocair	ound	Cocaine-d3	Sample Type Calibration	2,5000	Final Conc 2.3077	Resp 5189	ISTD Resp	Accuracy 92.3	RT 2.448179215	1STD RT 2.447916667	
	CMAMCal_L1.d	Cocair		Cocaine-d3	Calibration	5.0000	4.2681	9716		92.5	2.448179215	2.447916667	standard for that
	CMAMCal_L2.d	Cocair		Cocaine-d3	Calibration	12,5000	11.5536	25187		92.4	2.448179215	2.447916667	Standard for that
	CMAMCal L4.d	Cocair		Cocaine-d3	Calibration	25,0000	25.2713	50703		101.1	2,448179215	2,447916667	
	CMAMCal_L5.d	Cocair	e	Cocaine-d3	Calibration	125.0000	125.0735	199967		100.1	2.448179215	2.447916667	
34 0	CMAMOC L2.d	Cocair	e	Cocaine-d3	oc	5.0000	4.2837	9246		85.7	2.448179215	2.447916667 🗵	
		nary / 🕲 /											
Read	iy 🛅										100% 😑 🗕	- 🛡:j	

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

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

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

Step	Detailed Instructions	Comments	
<ul> <li>4 Save the changes to the template, <i>iii</i>_9_Custom_ISTD_Summary.xltx.</li> <li>You have to clear the results first.</li> </ul>	<ul> <li>a Click Clear Results in the Add-Ins tab in the Ribbon.</li> <li>b Click the Microsoft Office Button and then click Save As and click Other Formats.</li> <li>c In the Save As dialog box, type <i>iii</i>_9_Custom_ISTD_Summary.xltx.</li> <li>d Verify the folder selected in Save in is correct.</li> <li>e Click Save.</li> </ul>	<ul> <li>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).</li> <li>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.</li> </ul>	

Task 5. Add a column that is already mapped

# 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.

Step		De	Detailed Instructions		Comments	
1	Open the Qualitative Analysis template \ <b>MassHunter\Report</b> <b>Templates\Qual\Letter\</b> <b>iii_3_CustomAnalysisReport.xltx</b> , where <i>iii</i> are your initials.	a	Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 32 to open the template, <i>iii_3_</i> CustomAnalysisReport.xltx, where " <i>iii</i> " 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 <b>Familiarization Templates</b> folder.	
2	Add the item AnalysisFileName to the first column in row 10.	a b c d e	Find the second table in the template. The items in this table are <b>ItemID</b> , <b>Data File, Injector Volume</b> and <b>Dilution</b> . In the table, click <b>Data File</b> . Right-click and click <b>XML &gt; XML</b> <b>Source</b> . Click the <b>Dilution</b> column. Try to add the AnalysisFileName item to the end of the table. An error message is displayed.		<ul> <li>In the XML Source window, both of these items are shown in bold which means that this item is already being used.</li> <li>See "Task 6. Add a mapped column to a table" on page 70 for instructions on adding a mapped column to a table.</li> </ul>	
N	Nicrosoft Office Excel This element has already been mapped. An element	cannot	De mapped more than once.			

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

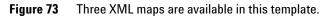
Task 5. Add a column that is already mapped

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

Step		Detailed Instructions	Comments
		<ul> <li>f Click XML Maps in the XML Source pane. The XML Maps dialog box is opened.</li> <li>g Click Add in the XML Maps dialog box.</li> <li>h Navigate to the Report Templates/Qual/Letter folder.</li> <li>i Select AnalysisReport.xsd for this template.</li> <li>j Click Open.</li> <li>k Click OK.</li> </ul>	<ul> <li>Two maps are already available in the XML Maps dialog box.</li> <li>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.</li> </ul>
Select XML Source	:e	⑦⊠ Analys	isReport.xsd - Analysis report
Look in:	Letter	Compo	undReport.xsd - Compound report
My Recent Documents	CompoundReport.xsd Graphic.xsd QualitativeMethodReport.xsd	Graphi	c.xsd - Graphic report
My Documents My Computer My Network Places		Qualita	ativeMethodReport.xsd - Qualitative is Method Report
	File name: Files of type: All XML Data Sources (*.xml; *.xe	New Source	uantitative Analysis template, the XML

**Figure 72** Add another map file.

KML Maps XML maps in th	is workboo	k:	2	
Name	Root	Namespace		Report Map - original map file
Report_Map	Report	<no namespace=""></no>		• .
Report_Map1	Report	<no namespace=""></no>		Panart Man1 automatically added in Taak 1 when th
Report_Map2	Report	<no namespace=""></no>		Report_Map1 - automatically added in Task 1 when th table was added
<		Ш	>	Report_Map2 - added manually in this task
<u>R</u> ename		dd <u>D</u> elete	OK Cancel	



Task 5. Add a column that is already mapped

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

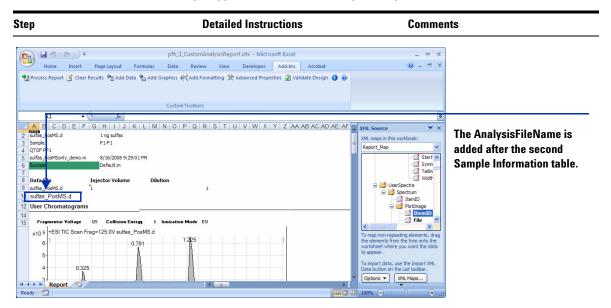
Step	<b>Detailed Instructions</b>	Comments
	<ul> <li>I Select Report_Map Source pane.</li> <li>m Add the mapped col AnalysisFileName of row 10.</li> </ul>	lumn,
pfh_3_CustomA	nalysisReport.xltx - Microsoft Ex Review View Add-Ins Acrobat	$\frac{1}{2} = \frac{1}{2} \times $ The Analysis FileName is
A         A         A         A         A         A         A         A         A         B         A         A         A         B         B         A         A         A         B         B         A         A         A         A         B         B         C		tting · * Delete - Format · Cells * Cells * Cell
A10 • 🤄 🌆		📧 column header is not
A B C Formula Bar 2 (DPDReport Trem1) 3 Trem1 V Data Filenam V Sample Nam(v Sample Type V 4 6 Trem10 V Data File V Injector Volu V Dilution V 7 8	E F =	XML Source        NML maps in this workbook:        NML maps in this workbook:        Report Her        SempleInformationTable        AcqNethodIame        AcqNethodIame
10 10 11 CHU EndRepeat IT CHTD 11 CHU EndRepeat IT CHTD 15 10 10 10 10 10 10 10 10 10 10 10 10 10		AcquiredTime AnalysisTektame AnalysisTektame To nap on-repeating elements, drag the elements from the tree onto the worksheet where you want the data to appear.
22 11 Integration Peak List 12 Integration Peak List 14 Ready 14 Ready		To import data, use the Import XML Data button on the List toobar. ( Coptions • ) XML Maps The Import and the Import XML Data button on the Coptions • ) XML Maps • • • • • • • • • • • • • • • • • • •

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



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

Verifying that the AnalysisFileName is repeated Figure 75

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 **c** In the Save As dialog box, type 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.
  - 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.

Task 5. Add a column that is already mapped



Agilent MassHunter Workstation Software Reporting Familiarization Guide

# Exercise 5 Graphics

Task 1. Adding graphics to a template110Task 2. Display multiple graphics per row113

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.



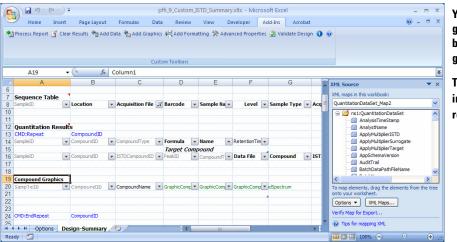
Task 1. Adding graphics to a template

# 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. Ad	d graphics to	a Quantitative	Analysis template

Step	Detailed Instructions	Comments
1 Open the Quantitative Analysis template, \MassHunter\Report Templates\Quant\Letter\ISTD\ Parts\ <i>iii_9_</i> Custom_ ISTD_Summary.xltx template.	a Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, <i>iii_9_Custom_ISTD_Summary.xltx.,</i> where " <i>iii</i> " are your initials.	<ul> <li>If you do not have this template, example templates are available or the Agilent Technologies MassHunter Reporting User Information DVD in the Familiarization Templates folder.</li> </ul>
<ul> <li>Add target compound graphics.</li> <li>Add them in the Quantitation Results repeating section.</li> </ul>	<ul> <li>a Click in the first column in the last rows before the CMD:EndRepeat CompoundID row.</li> <li>b Click Add Graphics &gt; Compound Graphics.</li> </ul>	<ul> <li>Refer to "Task 3. Add a single repeating section" on page 127 for an explanation of repeating sections.</li> <li>Three different graphics are added in the Compound Graphics table.</li> </ul>



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.



#### Graphics Task 1. Adding graphics to a template

5

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

#### Task 1. Add graphics to a Quantitative Analysis template

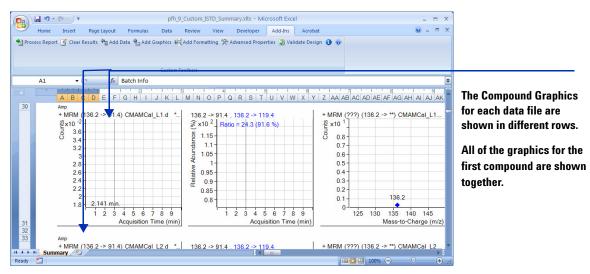


Figure 77 The compound graphics are added after the Target Compound table

Task 1. Adding graphics to a template

### Task 1. Add graphics to a Quantitative Analysis template

Step	Detailed Instructions	Comments
<ul> <li>4 Save the changes to the template, <i>iii</i>_10_Custom_ISTD_ Summary.xltx.</li> <li>You have to clear the results first.</li> </ul>	<ul> <li>a Click Clear Results in the Add-Ins tab in the Ribbon.</li> <li>b Click the Microsoft Office Button and then click Save As and click Other Formats.</li> <li>c In the Save As dialog box, type <i>iii</i>_10_Custom_ISTD_Summary.xltx.</li> <li>d Verify the folder selected in Save in is correct.</li> <li>e Click Save.</li> </ul>	<ul> <li>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).</li> <li>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.</li> </ul>

5

# Task 2. Display multiple graphics per row

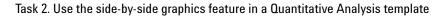
If you have graphics in a template, you can specify the relative width and height for those graphics.

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		D	Detailed Instructions		Comments	
1	Open the Quantitative Analysis template, \MassHunter\Report Templates\Quant\Letter\ISTD\ Parts\ <i>iii</i> _10_Custom_ ISTD_Summary.xltx template.	а	Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, <i>iii10Custom_ISTD_Summary.xltx.,</i> where " <i>iii</i> " 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 <b>Familiarization Templates</b> folder.	
2	<ul> <li>Change the size of the graphics in the Compound Graphics table.</li> <li>Make the width of each graphic 1/6th of the width of the page.</li> <li>Make the height of each graphics 1/6th of the height of the page.</li> </ul>	b	Click one of the graphics in the Compound Graphics table. Click Advanced Properties in the Add-Ins tab in the Ribbon. Select 1/6 for the Graphic size relative to page width and Height boxes for each graphic. Mark the Continue graphics across the page check box. Click Close.	•	Make sure to change the width and height for each graphic.	

Task 2. Display multiple graphics per row



		X
Advanced Properties       Template   Design Worksheet   Cell   Table         Table corporties       Associate with the following table or graphics       Hide header row       Table contents transposed to       Indice more contents transposed to       Combine table rows sarving at column       Combine table rows starting at column       Combine table rows starting at column       Lise super-header       If continue graphics across the page       Stack graphics vertically	Table colum properties     Filter       Colum     Width     Piperties       Semple:Dig     Edited       Semple:Compound's management     Edited       Oraphic Compound's Graphic(6,6)     Graphic(6,6)       Graphic Compound's Graphic(6,6)     Graphic(6,6)       Graphic Compound's Graphic(6,6)     Graphic(6,6)       Graphic Compound's Graphic(6,6)     Graphic(6,6)       Graphic Compound's Graphic Size relative to page width     116       © Frondia     Preset graphics row height     Meight       Column sort order     Uncorted     © Ascending       Filter value	Set the relative graphic width and height for each of the graphics.
XML mapped list Graphic(6,6)	Close	The Stack graphics vertically

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.

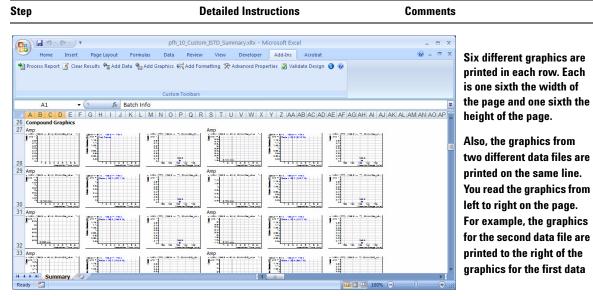
check box changes how the graphics are organized on the page. If this check box is cleared, then the related graphics are printed side-by-side. If this check box is marked, then related graphics are printed on consecutive rows.

#### 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. Display multiple graphics per row



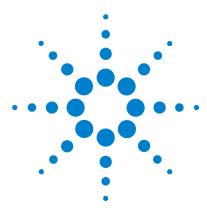
#### Task 2. Use the side-by-side graphics feature in a Quantitative Analysis template

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.

Task 2. Display multiple graphics per row



Agilent MassHunter Workstation Software Reporting Familiarization Guide

# Exercise 6 Advanced topics

Task 1. Add a page break and a sheet break118Task 2. Use Test Mode122Task 3. Add a single repeating section127Task 4. Add a nested repeating section131Task 5. Change values on the Options worksheet135Task 6. Add a formula using the IF function138Task 7. Use the VLOOKUP function142

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.



Agilent Technologies

Task 1. Add a page break and a sheet break

## 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 Qualitative Analysis template" on page 44 for more information.

Task 1. Add a page break and a sheet break

S	tep	D	etailed Instructions	C	Comments
1	Open the Quantitative Analysis template, \MassHunter\Report Templates\Quant\Letter\ISTD\ Parts\ <i>iii_</i> 11_Custom_ ISTD_Summary.xltx template.	а	Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, <i>iii</i>	•	If you do not have this template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the <b>Familiarization Templates</b> folder.
2	<ul> <li>Add a sheet break to the Quantitation Results section.</li> <li>Select Compound to label the worksheet.</li> </ul>	b c d	Select the row containing the SampleID column in the Quantitation Results section. Right-click the row and click Insert. A row is added above the table. Click the first column in this new row. Click Add Formatting > Sheet Break in the Add-Ins tab in the Ribbon. Select Compound. Click OK.	•	template, you can add it to the template and hide that column or cell.
3	Add a page break before the graphics in the Quantitation Results section.	-	Click the first column in the row that is above the Compound Graphics label. Click <b>Add Formatting &gt; Page Break</b> 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

tep	Detailed Instru	ctions	Comments
• • • •	pfh_11_Custom_ISTD_Summary.xltx - N	Aicrosoft Excel	_ 🗆 X
Home Insert Page Layo	Add Data 🐮 Add Graphics 👫 Add Formatting 🔆 Advanced F	Acrobat Properties 🔮 Validate Design 🚯 🛞	When you add a Sheet Bre you select an item to use to label the new worksheet.
A16 • 6	Custom Toolbars CMD:SheetBreak		you do not select an item, t
Alb C A B	C D E F	G H	the name of the design
Quantitation Results     CompoundID     CMD SheetBreak     CompoundID     SampleID     CompoundID	▼ CompoundType ▼ Formula ▼ Name ▼ Target Compound ,		worksheet is used to label each of the new workshee
1 SampleID CompoundID 2 3 4 CMD:PageBreak	VISTDCompoundID V PeakID V CompoundTV Data File	▼ Compound ▼ ISTD ▼	Exp Ce v Final
28 29 30	CompoundName     GraphicComp     GraphicComp     GraphicComp     GraphicComp	p[▼]dSpectrum	You do not select a column when you add a page brea
31 CMD:EndRepeat CompoundID			
Ready Ready	Insert Worksheet (Shift+F11)	<b>III II</b> 100% —	

#### Task 1. Add a page break and a sheet break

Figure 80 Adding a sheet break and a page break.

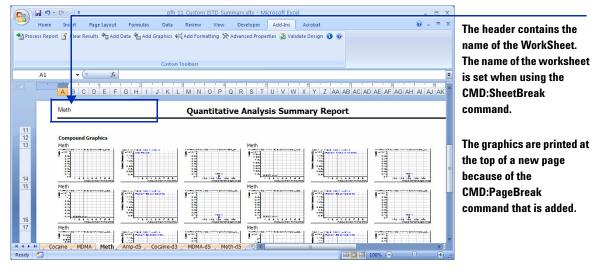
- **4** Add the sheet name to the Header of the worksheet.
- a Click the View tab.
- **b** Click the **Page Layout** button.
- c Click the left hand portion of the Header.
- d Click the Header & Footer Tools tab.
- e Click the Sheet Name button under Header & Footer Elements in the Header & Footer Tools 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

S	tep	D	etailed Instructions		Comments	
5	Test the changes to the template.	a b c d e f g h i j	Click <b>Process Report</b> . Click the <b>Browse</b> button. Navigate to the <i>DrugsOfAbuse\</i> <i>QuantReports\DrugsOfAbuseDemo</i> folder. Select <i>report.results.xml</i> . Click <b>Open</b> . Click <b>OK</b> .	•	The Process Report command is part of the MassHunter toolbar in the Add-Ins tab in the Ribbon.	
		k	The compound graphics are printed starting at the top of the next page.			

Task	1 A	dd a	nage	break	and a	sheet	break
nuon		սսս	pugo	DIGUN	und u	011001	DIGUN



**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	
<ul> <li>6 Save the changes to the template, <i>iii</i>_12_Custom_ISTD_ Summary.xltx.</li> <li>You have to clear the results first.</li> </ul>	<ul> <li>a Click Clear Results in the Add-Ins tab in the Ribbon.</li> <li>b Click the Microsoft Office Button and then click Save As and click Other Formats.</li> <li>c In the Save As dialog box, type <i>iii</i>_12_Custom_ISTD_Summary.xltx.</li> <li>d Verify the folder selected in Save in is correct.</li> <li>e Click Save.</li> </ul>	<ul> <li>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).</li> <li>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.</li> </ul>	

### Task 1. Add a page break and a sheet break

Task 2. Use Test Mode

# 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.

S	tep	Detailed Instructions Comments
1	Make a backup copy of the file "MassHunter Reporting Quant.config".	<ul> <li>a Open the Windows Explorer program.</li> <li>b Navigate to the C:\Program Files\ Microsoft Office\Office12\Library folder.</li> <li>c Right-click the MassHunter Reporting Quant.config file and click Copy.</li> <li>d Click Edit &gt; Paste to add a copy of the config file to the current folder.</li> <li>e Right-click the new file, Copy of MassHunter Reporting Quant.config and click Rename.</li> <li>f Type backup_MassHunter Reporting</li> </ul>
2	Remove the <b>Read-only</b> attribute from the original config file.	<ul> <li>Quant.config.</li> <li>a Right-click the MassHunter Reporting Quant.config file and click Properties.</li> <li>b Clear the Read-only check box in the Attributes section, if necessary.</li> <li>c Click OK.</li> </ul>

Task 2. Use Test mode

### Task 2. Use Test mode

S	tep	D	etailed Instructions	C	Comments		
3	Change the TestMode enabled line from <b>False</b> to <b>True</b> .	b	Notepad, click <b>File &gt; Save</b> .				
4	Open the Quantitative Analysis template, \MassHunter\Report Templates\Quant\Letter\ISTD\ Parts\ <i>iii_</i> 12_Custom_ ISTD_Summary.xltx template.	а	Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, <i>iii12_Custom_ISTD_Summary.xltx.</i> , where " <i>iii</i> " are your initials.	•	If you do not have the <i>iii_</i> 12_Custom_ISTD_Summary.xltx template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the <b>Familiarization Templates</b> folder.		

6	Home In	sert	Page Layout	Formulas	Dat	ta Revie	w Vie	w De	veloper	Add-Ins	Acroba				U	_ = >	t
1	Process Report 🧃	Clear	Results 🏪 Ad			s 📲 Add F	ormatting	🔆 Advar	nced Propertie	s 🍠 Valid	ate Desig	n 🚯 🔞	Test	Quant -			When you enable T
						Custom 1	oolbars						6 	Import XML Dat Copy Data to R Format Report			Mode, a new menu
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4	А		В	(	2	D		E	F		3	Н	-	1	J	-	Reporting toolbar.
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	Sequence Table																the report which ca
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	CMD:PageBreak																
2																	*
- 4	Design-	Sum	mary 🦯 🖓 🦯								_		_	100% 🔾		→ I +	

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**Figure 82** The Test Mode menu.

Task 2. Use Test Mode

5 Test the steps in the Test Mode

#### Task 2. Use Test mode

#### Step

menu.

#### **Detailed Instructions**

- 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.

#### Comments

- 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.

-	Home Insert		Page Layout		Formulas Data	Review		View De	reloper A	dd-Ins	Acrobat			0	-	•
1	Process Report 🥑 Clea	ar F	Results 🖣 Add [	Da	ta 🐁 Add Graphics	4분 Add For	ma	tting 🛠 Advan	ced Properties	🏹 Val	iidate Desig	n 🚯 🖗 Test C	Quant *			
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	Batch Info	1	-	٦				_			-			-		
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	Analysis Time	2	010-01-18 11:1	3	Analyst Name											
	Report Time	2	010-01-18 11:1	8	Reporter Name		•	(								
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6																
7	Sequence Table	1														
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0		L	aboratory 1		CMAMCal_L1.d	BarCode 1234	156	CMAM_06	L1	Calbra		APCIautotune.m	P1-C6			
1	2	2 Li	aboratory 1		CMAMCal_L2.d	BarCode 1234	156	CMAM_10	L2	Calibra		APCIautotune.m	P1-C10			
2	3	Li	aboratory 1		CMAMCal_L3.d	BarCode 1234	156	CMAM_11	L3	Calibra	tion	APCIautotune.m				
3	4	ł Li	aboratory 1		CMAMCal_L4.d	BarCode 1234	156	CMAM_14	L4	Calibra	tion	APCIautotune.m	P1-C14			
4			aboratory 1		CMAMCal_L5.d	BarCode 1239			L5	Calibra	tion	APCIautotune.m				
5			aboratory 1		CMAMQC_L2.d	BarCode 1234			L2	QC		APCIautotune.m				
6			aboratory 1		CMAMQC_L4.d	BarCode 1234			L4	QC		APCIautotune.m				
7			aboratory 1		CMAMSam_01.d	BarCode 1234				Sample		APCIautotune.m				
8			aboratory 1		CMAMSam_02.d	BarCode 1234				Sample		APCIautotune.m				
9	10	Li	aboratory 1		CMAMSam_03.d	BarCode 1234	156	CMAM_12		Sample		APCIautotune.m	P1-C12			
0																
1																

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

Ste	p				D	etailed	Instruc	tions				Comme	ents	
					g	Click 1 Repor	ēst Qu t.	ant > (	Copy I	Data t	)			
Ģ		(°I • ) <del>•</del>			pfh_12_Custom_	ISTD_Summai	y.xltx - Micr	osoft Excel					×	
	Home	Insert	Page Layout	Formulas	Data Review	View D	eveloper	Add-Ins	Acrobat			🕜 🗕 =	a x	After the second step, th
	41		( fx	Batch Info	Custom Toolb	ars							×	data is placed onto the appropriate worksheet
_	A1	•				-	-						*	and it is filtered, but it is
216	A		В	С	D	E	F	G		Н		J	-	wetter were the different to be
	CMD:PageE	Irook												not formatted. Also, the
218	CIVID.FageL	liean												and the second sector of the stands
	Compound G	raphics												graphics are not include
	SampleID		CompoundID	CompoundName	GraphicComp -	GraphicCom	GraphicComp	▼ dSpectrum						In the new set of the
221		0		0 Amp	PeakChromatog				1.0.0.0.emf					in the report yet.
222		0		1 Amp-d5		r PeakQualifiers								
223		0		2 Cocaine	PeakChromatog	PeakQualifiers	PeakSpectrum	PeakSpectrun	n.0.0.2.emf					
224		0		3 Cocaine-d3	PeakChromatog	r PeakQualifiers)	PeakSpectrum	PeakSpectrun	n.0.0.3.emf					
225		0		4 MDMA		r PeakQualifiers								
226		0		5 MDMA-d5		r PeakQualifiers								
227		0		6 Meth		r PeakQualifiers)								
228		0		7 Meth-d5		r PeakQualifiers								
229		1		0 Amp	PeakChromatog									
230		1		1 Amp-d5		r PeakQualifiers								
231 232		1		2 Cocaine		r PeakQualifiers								
232		1		3 Cocaine-d3		r PeakQualifiers								
233		1		4 MDMA 5 MDMA-d5		r PeakQualifiers) r PeakQualifiers)								
234		1		5 MDMA-d5 6 Meth	PeakChromatog									
235				7 Meth-d5	PeakChromatog									
11	н н 📈 Ме					ign-Summar		e caxouectrun					> 1	
													÷	

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

Task 2. Use Test Mode

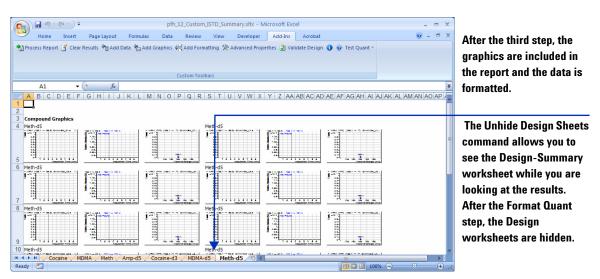
#### Task 2. Use Test mode

#### Step

#### **Detailed Instructions**

Comments

h Click Test Quant > Format Report.



#### 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	sinale	repeating	section
		0		

S	tep	D	etailed Instructions	C	Comments		
1	Open the Quantitative Analysis template, \ <i>MassHunter\Report</i> <i>Templates\Quant\Letter\ESTD\</i> <i>Parts\iii_Custom_QuantReport_</i> <i>ESTD_Summary.xltx</i> .	a	Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, <i>iii_</i> Custom_QuantReport_ ESTD_Summary.xltx, where " <i>iii</i> " are your initials.	•	Make a copy of the QuantReport_ESTD_Summary_B_0 4_00.xltx template and rename it to <i>iii</i> _Custom_QuantReport_ ESTD_Summary.xltx, where "iii" are your initials.		
2	<ul> <li>Add a repeating section at the end of the template.</li> <li>Add the Target Compound table.</li> <li>Repeat this table using the CompoundID.</li> </ul>		Select the first column in row 25. 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. 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>B</b> button in the shortcut menu to change the font.		

Task 3. Add a single repeating section

#### Task 3. Add a single repeating section

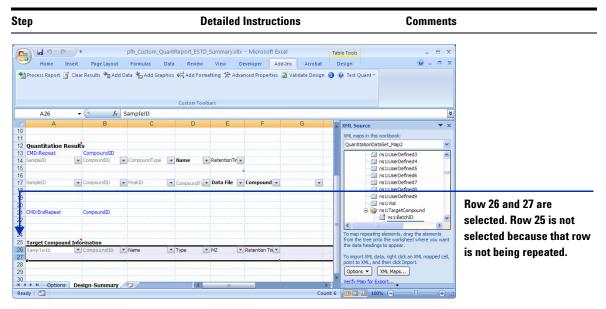


Figure 86 Adding a single repeating section.

- 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

**B** 

Process Re

12 11

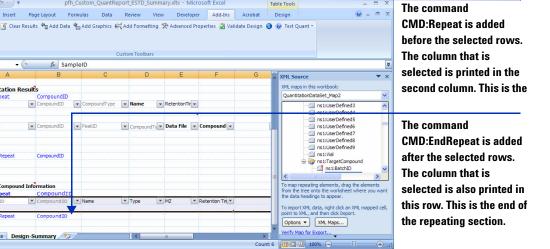
A27

second column. Th	XML maps in this workbook:						tesults	Quantitation I	12
	QuantitationDataSet_Map2						CompoundID	CMD:Repeat	
	ns1:UserDefined3		]	RetentionTir	Name 💌	CompoundType	CompoundID	SampleID	
The command	ns1:UserDefined5	r	Compound V	Data fila		PeakID 💌	CompoundID		15 16
The command	ns 1:UserDefined6		Compound	Data File	CompoundTy	PeakID		SampleID	17 18
CMD:EndRepeat is									19
after the selected							CompoundID	CMD:EndRepeat	20 21
	🖻 🤯 ns1:TargetCompound								22
The column that is	<pre>ns1:BatchID v </pre>								23 24
selected is also pr	To map repeating elements, drag the elements from the tree onto the worksheet where you want						nd Information	Target Compou	
selected is also pi	the data headings to appear.						CompoundID	CMD:Repeat	26
this row. This is th	To import XML data, right click an XML mapped cell,		Retention Tin	MZ	Туре 💌	Name	CompoundID	SampleID	27 28
the repeating sect	Options  XML, and then click Import. XML Maps						CompoundID	CMD:EndRepeat	29 30
and repouting cool	Verify Map for Export	×					sign-Summary 🖉 🖊		31
	· · · · · · · · · · · · · · · · · · ·	Count: 6							2

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

**Detailed Instructions** 

- 3 Test the changes to the template.
- a Click Process Report.
- h Click the Browse button.
- c Navigate to the *DrugsOfAbuse*\ QuantReports\DrugsOfAbuseDemo folder.
- **d** Select *report.results.xml*.
- Click Open. е
- Click OK. f
- Scroll the report until you find the a 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

Comments

Task 3. Add a single repeating section



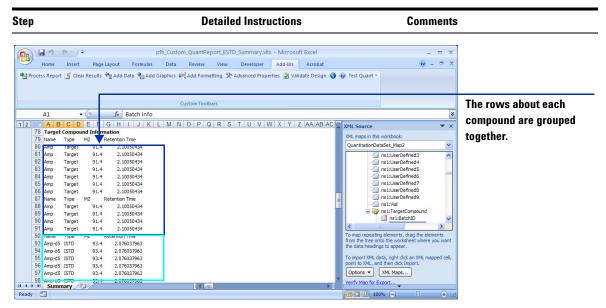


Figure 88 The results after adding a repeating section using the CompoundID

- 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.

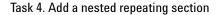
In this task, you group different tables together using a nested repeating section. A nested repeating section is simply a repeating section that is within another repeating section. When repeating sections are nested, the inner repeating section needs to end before the outer repeating section ends.

- 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, <i>iii_</i> 1_Custom_QuantReport_ ESTD_Summary.xltx., where " <i>iii</i> " are your initials.	<ul> <li>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.</li> </ul>
<ul> <li>the end of the template.</li> <li>Add the Compound Graphics inside of the repeating section at the end of the report.</li> <li>Add an inner repeating section repeating on the SampleID.</li> </ul>	<ul> <li>a Select row 29.</li> <li>b Right-click and click Insert to add a new row to the template.</li> <li>c Click the first column in row 30.</li> <li>d Click Add Graphics &gt; Compound Graphics in the Add-Ins tab in the Ribbon.</li> <li>e Select rows 27 to 32. Click the row number 27 and drag to include row 32.</li> </ul>	<ul> <li>Do not include the rows containing the commands CMD:Repeat nor CMD:EndRepeat.</li> </ul>

Task 4. Add a nested repeating section



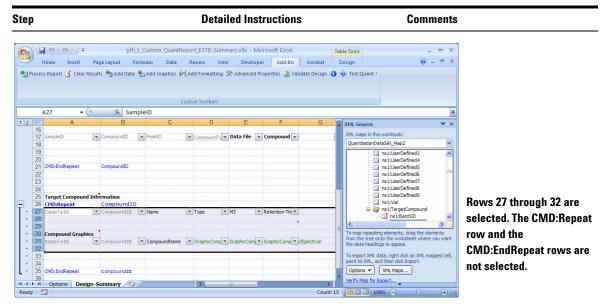


Figure 89 Selecting both tables inside of the Repeating Section

- 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

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

3 Test the changes to the template.

### a Click Process Report.

**Detailed Instructions** 

- **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.

Step

Ready 🛅

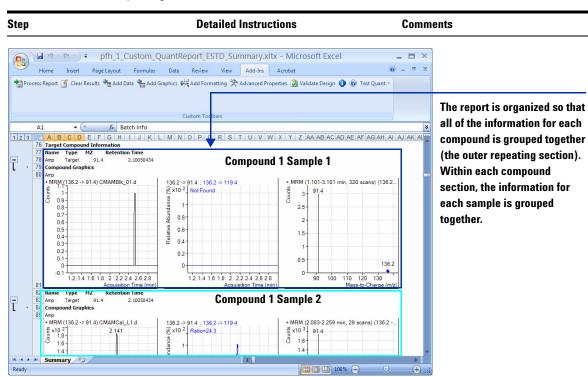
	J. M.	(~ (~ ~ ) <del>+</del>	pfh_1_Cus	stom_QuantRe	port_EST	D_Summar	y.xltx - Micro	osoft Excel		Table Tools		
-	Hor	e Insert Page	Layout Formula	as Data	Review	View	Developer	Add-Ins	Acrobat	Design	(	0 - 🗖
2	rocess R	port 🗹 Clear Results '	Add Data 🐏 A		Add Forn		Advanced Prop	oerties 💆 Vali	date Design 🕻	🌒 👰 Test Quant 👻		
	A28	- (>	<i>f</i> ∗ SampleID	)								
2	3 🔺	A	В	С		D	E	F	G	XMI Source		•
-	· 28 · 29 · 30 · 31	DPD:EndRepeat CompoundIn arget Compound Information (10)Repeat Compound CHD/Repeat SampleID SampleID ♥ Compound; Compound Graphics		on poundID oleID oundID ▼Name ▼Ty			Type 💌 MZ 💌 Retent			To map repeating	aSet_Map2 ns1:UserDefined3 ns1:UserDefined4 ns1:UserDefined6 ns1:UserDefined6 ns1:UserDefined9 ns1:UserDefined9 ns1:TargetCompou is1:Yal ns1:Yal n	e elements
	35 36	CMD:EndRepeat	SampleID CompoundID							To import XML da point to XML, and	ata, right dick an XM d then dick Import. XML Maps	

Task 4. Add a nested repeating section

Comments

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Task 4. Add a nested repeating section



#### Task 4. Add a nested repeating section

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.
- In the Save As dialog box, type *iii*\_2\_Custom\_QuantReport\_ESTD\_Su mmary.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.

template.

6

# 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**.

Step	Detailed Instructions	Comments
1 Open the Qualitative Analysis template \MassHunter\Report Templates\Qual\Letter\ iii_4_CustomAnalysisReport.xltx, where <i>iii</i> are your initials.	a Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 32 to open the template, <i>iii4</i> CustomAnalysisReport.xltx, where " <i>iii</i> " are your initials.	<ul> <li>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.</li> </ul>
<ul> <li>2 Switch to the Options worksheet.</li> <li>Set Use Options to True</li> <li>Set Include Header to False</li> <li>Set Include Footer to False</li> </ul>	<ul> <li>a Click the Options worksheet at the bottom of the program.</li> <li>b Find the Use Options row.</li> <li>c Select True in the Value column.</li> <li>d Find the Include Header row.</li> <li>e Select False in the Value column.</li> <li>f Find the Include Footer row.</li> <li>g Select False in the Value column.</li> </ul>	<ul> <li>Only change the values in the Value column.</li> <li>The Options in the first section only change the report if the Use Options value is True.</li> <li>The options in the second section are not affected by the Use Options value.</li> <li>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</li> </ul>

Task 5. Change values on the Options worksheet

Task 5. Change values on the Options worksheet

Step			Detailed Instructions		Comme	nts
		Formulus Duta Re	omAnalysisReport.xltx - Microsoft Excel <del>rice Vice Beeckper   Add Sin  </del> Formatting 🎘 Advanced Properties 🗿 Validat ars	Aasbat e Design 🗿 🎯	- = x @ - *	Each cell in the Value column is explicitly named. You can see the name of the cell here.
IncluieFooter -	Type Boolean k Boolean	Value TRUE TRUE	Comment		XML Source X XML maps in this workbook: Report_Map1	
Include Header Include Footer Landscape Fit to	Boolean Boolean Integer Integer	FALSE FALSE FALSE 1 0	Page(s) wide Page(s) tall		DAMethodName  DAMethodPath DataFile DeviceType Dilution	Only change the Value
Hide Empty Colu Note: The follov Hide ID Columns	•	TRUE be observed regardle	s of the Use Options value.	=	EquilbTime     ThyPosition     ThyPosition     ThyPosition     ThyPosition     ThyPosition     ThyPosition     ThyPosition     ThyPosition     ThyPosition	column. In this example, the Include Header and Include Footer values are set to
Add Smart Page Breaks and Table Headers Adjust columns to fit data	Boolean	TRUE	Use inserting and merging cells to allow adjusting table column widths		To map non-repeating elements, drag the elements from the tree onto the worksheet where you want the data to appear.	False. The header and footer will not be printed in the
Protect Results	Boolean	FALSE	not an imported option		To import data, use the Import XML Data button on the List toolbar. Options V XML Maps 100% - U + .::	

#### Task 5. Change values on the Options worksheet

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	Comme	nts
Print Preview		mAnalysisReport.xltx - Microsoft Excel	- = ×	
Print Page Zoo Print Zoo	Show Margins Preview		1	The header and the footer are not included in the
		•		The Qualitative Analysis program lets you set several of these options in the user
	sulfas_PozMS.d 1 ng sulfas Sample P1.F1 gr)GP PP1 sulfas_PozMSonly_demo.m 8/16/2008 9:29:01 PM Success Default.m			interface. The values that you set here in the template
	Data File Injector Volume sulfas_PosMS.d 1 sulfas_PosMS.d User Chromatograms	Dilution 1		are overridden by the values in the Qualitative Analysis user interface when you
A Demainer Demail of 2	Fragmentor Voltage 125 Collision Energy	0 Ionization Mode ESI		print from the Qualitative Analysis programs.
Preview: Page 1 of 3			Zoom Out 100% 🕤 🤃 🔃	Analysis programs.

#### Task 5. Change values on the Options worksheet

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

# 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	c hhΔ	formula	usina	the	IF	function
TUSK U.	nuu u	Torniula	using	uic		Tuniction

Step	Detailed Instructions	Comments	
1 Open the Qualitative Analysis template \MassHunter\Report Templates\Qual\Letter\ iii_5_CustomAnalysisReport.xltx, where <i>iii</i> are your initials.	a Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 32 to open the template, <i>iii_5_CustomAnalysisReport.xltx,</i> where " <i>iii</i> " are your initials.	<ul> <li>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.</li> </ul>	
<ul> <li>2 Add a formula column to the second Peak List table.</li> <li>If the formula is not defined, print "Not Found".</li> <li>If the formula is defined, print the formula.</li> </ul>	<ul> <li>a Find the Formula column in the Peak List table that is at the end of the report.</li> <li>b Click the Formula column.</li> <li>c Click Add Data &gt; Formula Column in the Add-Ins tab in the Ribbon.</li> <li>d Click the Formulas tab.</li> <li>e Click Insert Function.</li> <li>f In the Insert Function dialog box, select IF.</li> <li>g Click OK.</li> </ul>	<ul> <li>See the online Help for Excel for a complete description of the IF formula and other possible formulas.</li> </ul>	

Task 6. Add a formula using the IF function

Select the IF function and click OK.	<ul> <li>See the online Help for Excel for a</li> </ul>
Click the Lewisel Acet have	See the online Help for Eycel for a
Click the Lewisel Acet have	See the online Help for Eycel for a
Click the Lewisel Acet have	See the online Help for Eycel for a
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	See the online Help for Eycel for a
Click the Lewisel Acat have	See the online Help for Excel for a
Click the Logical_test box. Click the cell in the Formula column. Type = " " in the Logical_test box. Type "Not Found" in the Value_if_true box. Click the Value_if_false box. Click the cell in the Formula column. Click OK.	complete description of the IF formula and other possible formulas.
	Type = " " in the Logical_test box. Type <b>"Not Found"</b> in the <b>Value_if_true</b> box. Click the <b>Value_if_false</b> box. Click the cell in the Formula column.

Task 6. Add a formula using the IF function

Task 6. Add a formula using the IF function

Step		Detailed Instruc	ctions	Comme	nts
Home Insert Page Layout		M	Add-Ins Acrobat Design	@_ = ×	
Jx Insert Function D Financial ~ Date & Time Function Library	<ul> <li>Math &amp; Trig *</li> <li>More Functions *</li> </ul>	Name Manager III: Create from Selection Defined Names	حَجَّ Trace Dependents مَنْ مَنْ مَنْ مَنْ مَنْ مَنْ مَنْ مَنْ	Watch Vindow Calculation Calculation	You click the cell in the Formula column in the table
1     2     A     B       53     S     Item10     Library Spect ×       54     Function Arguments       IF     Logical_test     This Rowl, [Formula]] = "       Value_jf_true     "Not Found"	C D	ormula]]="","Not Found",List1	F G	XHL Source  XUL maps in this workbook: Report_Map Refer Refer Refer Redet Rede	to get [Formula] added to the Logical_test and the Value_if_false boxes.
Value_if_failse Lst13[[#This Row],[Porm Checks whether a condition is met, and returns on Value_if_failse is the v FALSE	= "Not Found			To map non-repeating elements, drag the elements from the tree onto the worksheet where you want the data to appear.	
Help on this function Help on this function H ↔ Help on this function Edit C		OK Cance		To import data, use the Import XML Data button on the List toolbar. Options  XML Maps	

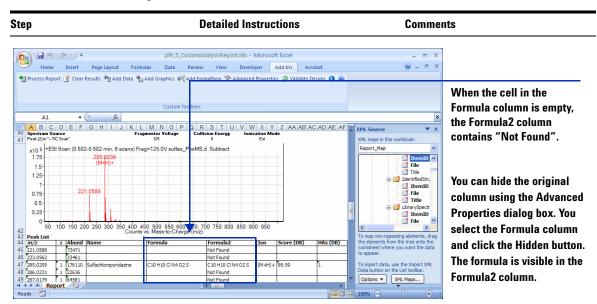
#### Task 6. Add a formula using the IF function

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



Task 6. Add a formula using the IF function

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.

Agilent MassHunter Workstation Software Reporting Familiarization Guide

- 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

# Task 7. Use the VLOOKUP function

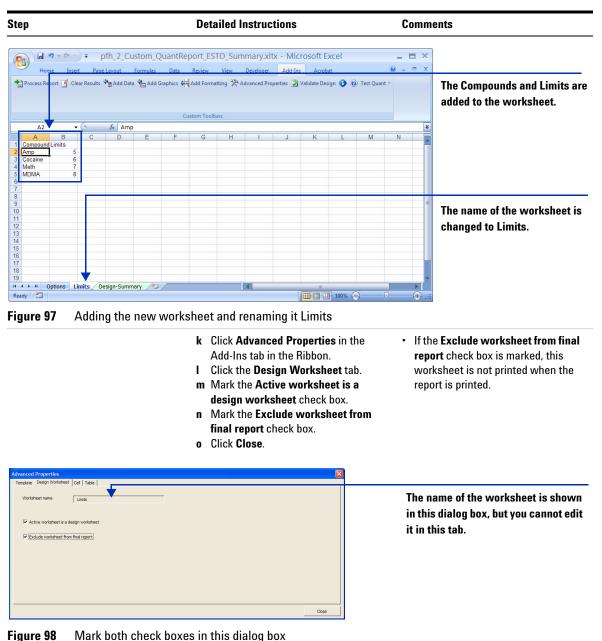
In this task, you use the function VLOOKUP in a template to look up limits for different compounds. The VLOOKUP function allows you to look in a table to find a specific value, and then it returns another value in that row. The main steps that you need to do are:

- **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.

Step	Detailed Instructions	Comments	
1 Open the Quantitative Analysis template, \MassHunter\Report Templates\Quant\Letter\ESTD\ Parts\ <i>iii_2_</i> Custom_QuantReport_ESTD _Summary.xltx.	a Follow the instructions in "Task 4. Open a Quantitative Analysis template" on page 42 to open the template, <i>iii_2_Custom_QuantReport_ ESTD_Summary.xltx.</i> , where " <i>iii</i> " are your initials.	<ul> <li>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.</li> </ul>	
<ul> <li>Add a new worksheet to the template that contains the VLOOKUP range. For this example, we will use the following arbitrary values</li> <li>Amp 5</li> <li>Cocaine 6</li> <li>Meth 7</li> <li>MDMA 8</li> </ul>	<ul> <li>a Press Shift and F11. A new worksheet is added.</li> <li>b Click the first column in row 1.</li> <li>c Type Compounds.</li> <li>d Click the second column in row 1.</li> <li>e Type Limits.</li> <li>f Enter the four compound names in the Compounds column.</li> <li>g Enter the four limits in the Limits column.</li> <li>h Right-click the tab at the bottom of the worksheet.</li> <li>i Click Rename.</li> <li>j Type Limits and press Enter.</li> </ul>	<ul> <li>You can also click the Insert Worksheet tab that is next to the other tabs at the bottom of the program.</li> <li>Instead, you can add the lookup table to the Options tab. The Options tab is not printed when the report is printed.</li> </ul>	

Task 7. Use the VLOOKUP function



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

Task 7. Use the VLOOKUP function

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

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

	pfh_2_Custom_QuantRe	eport_ESTD_Summary.xltx - Microsoft Ex	el Table Tools	_ = ×	The Lookup value is the
Home Insert Page Layour	t Formulas Data	Review View Developer Add	Ins Acrobat Design	0 _ = ×	The Lookup_value is the
fx E AutoSum * D Logical *	🛱 Lookup & Referenc	e * 🔄 🙃 Define Name *	🖙 Trace Precedents 🛛 🔣 Show Formulas		value that you want to look
	间 Math & Trig *	🖉 Use in Formula 👻 🖓			up in the Limits
Insert Function 😰 Financial - 👘 Date & Ti	me 🐐 🎁 More Functions 🐐	Name Manager 🔛 Create from Selection		Vatch Calculation	up in the Linnts
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VLOOKUP - ( X V J	=VLOOKUP([Compou	Function Arguments		2 🖌 🛓	worksheet. 30, you click
123 A A	ВС	VLOOKUP			on the cell in the
1 Batch Info		Lookup_value [Compound]	<b>F</b> = 0	-	
2 Batch Data Path		Table array	🛐 = number		Compound column that
3 Analysis Time	Analyst Nar		= number		•
4 Report Time	Reporter N				contains the results. Do
5 Last Calib Update	Batch State	Range_lookup	🐹 = logical		
6			-		not click on the column
7 Sequence Table		Looks for a value in the leftmost column of a ta	le, and then returns a value in the same row from	a column you specify.	
8 SampleID Data	a File 💽 Sample Nam	By default, the table must be sorted in an asce	ding order.		header.
9		Lookup_value is t	e value to be found in the first column of the table,	and can be a value, a	
10		refe	rence, or a text string.		
12 Quantitation Results					
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14 SampleID Comp		Formula result =			
15		Help on this function	ОК	Cancel	
16					
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Figure 99 Add the Lookup\_value to the Function Arguments dialog box

Step	Detailed Instructions	Comments	
	<ul> <li>I Click the Table_array box in the Function Arguments dialog box.</li> <li>m Click the Limits worksheet tab.</li> <li>n Click and drag to select the area containing the compound names and the limits.</li> </ul>	<ul> <li>When you click the Limits worksheet tab, "Limits!" is added to the Table_array box.</li> </ul>	
Home Insert Page Layout Formulas Data	Report_ESTD_Summary.xltx - Microsoft Excel Table Tools Review View Developer Add-Ins Acrobat Design	<b>- X</b>	
∑         AutoSum         © Logical         Lockup & Refere           Finiset Function         Imarcla         Imarcla	A <sup>2</sup> Use in Formula *     Name     Manager ⊞ <sup>2</sup> Create from Selection     Z, Remove Arrows * ② Evaluate Formula     Wir     Function Arguments	Select the area containing the compound names and limits. You do not include the column headers.	
16 17 18 19 19 19 19 19 19 19 19 19 19 19 19 19			
H + + H Options Limits Design-Summary 2			

Figure 100 Add the Table\_array value to the Function Arguments dialog box

- 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

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

Step	<b>Detailed Instructions</b>	Comments
ascending order) = TR Formula result = Help on this function	Image: ('Amp', 5; 'Cocaine', 6; 'Meth', 7; 'MDMA''       Image: Imag	Select the area containing the compound names and limits. You do not include the column headers. IP function
<ul> <li>4 Add the second formula col check if the Final Concentra below the value in the Limit column.</li> <li>If the value is below the liprint the message "Below</li> </ul>	tion is same table. s <b>b</b> Click <b>Add Data &gt; Formula C</b> <b>c</b> Rename the column "Limit ( <b>mit</b> , <b>d</b> Click the cell containing the	IF function for more information oncolumn.adding a formula column using theCheck".IF function.

- Otherwise, print "Pass".
- 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 <
- I 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.

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

Step	Detailed Instructions	Comments			
Value_if_true below Imit Value_if_false Pass" = Chedis whether a condition is met, and returns one value if TRUE, ar Value_if_true is the value that is return		The quotation marks are automatically added when you leave the field.			
Formula result = #N/A Help on this function	OK Cancel				

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

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

itep		<b>Detailed Instructions</b>					Comments			
						-				
强 🖉 - (* - ) =		uantReport_ESTD_S							The Limite column containe th	
	Page Layout Formulas Data	Review View	Develo	<u> </u>		Acrobat		0 - =		
襘 Process Report 🧭 Clear Re	sults 📲 Add Data 🐁 Add Graphics 🕯	🕂 Add Formatting 🕉	Advanced	1 Proper	ties 🛃 Valida	te Design 🚯 🧕	Test Quant	*	value from the Limits tab that	
									was next to this Compound	
									was next to this compound	
		Custom Toolbars							name.	
A1 🗸 🔄	∫ Batch Info								*	
1 2 3 🔺 A B C D	EFGHIJK M	NOPQR	STI	UV	WXY	ZAAABACA			1	
22 Cocaine							1		The Limit Check column	
23 Data File	Compound	Limits	RT 2.433	Resp	Final Conc 11.8231	Limit Check Pass	Exp Conc	Accuracy		
24 CMAMBk_01.d 25 CMAMCal L1.d	Cocaine	6	2.433	20 5189	2.3077	Pass Below limit	2,5000	92.31	contains the word "Below	
26 CMAMCal L2.d	Cocaine	6	2.454	9716	4.2681	Below limit	5.0000	85.36	Limit" if the Final	
27 CMAMCal L3.d	Cocaine	6	2.459	25187	11.5536	Pass	12,5000	92.43		
28 CMAMCal L4.d	Cocaine	6	2.449	50703	25.2713	Pass	25.0000	101.09	Concentration is below the	
<ul> <li>29 CMAMCal_L5.d</li> </ul>	Cocaine	6	2.448	199967	125.0735	Pass	125.0000	100.06		
<ul> <li>30 CMAMQC_L2.d</li> </ul>	Cocaine	6	2.453	9246	4.2837	Below limit	5.0000	85.67	Limit. It contains the word	
<ul> <li>31 CMAMQC_L4.d</li> </ul>	Cocaine	6	2.455	48582	24.5172	Pass	25.0000	98.07		
<ul> <li>32 CMAMSam_02.d</li> </ul>	Cocaine	6	2.460	9735	4.3730	Below limit			"Pass" if the Final	
<ul> <li>33 CMAMSam_03.d</li> </ul>	Cocaine	6	2.446	24841	10.9296	Pass			Concentration is not less than	
- 34 · 35 MDMA										
36 Data File	Compound	Limits	RT	Resp	Final Conc	Limit Check	Exp Conc	Accuracy	the Limit.	
37 CMAMBIk 01.d	MDMA	8	2,466	26	6,9547	Below limit	Exp cone	Accuracy		
· 38 CMAMCal L1.d	MDMA	8	2.276	3794	2.2766	Below limit	2.5000	91.07		
· 39 CMAMCal_L2.d	MDMA	8	2.277	7432	4.6439	Below limit	5.0000	92.88		
40 CMAMCal_L3.d	MDMA	8	2.277	17023	11.2481	Pass	12.5000	89.98		
41 CMAMCal_L4.d	MDMA	8		33212	24.8217	Pass	25.0000	99.29		
42 CMAMCal_L5.d	MDMA	8	2.271		125.1796	Pass	125.0000	100.14		
Summary 🖓										
Ready 🛅							100% (-)-			

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
  - 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\_Su mmary.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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