

# Agilent MassHunter Workstation Software Reporting

# **Familiarization Guide**



## Notices

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#### **Manual Part Number**

G3335-90159

#### **Edition**

July 2013

Printed in USA

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

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### In This Guide...

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

#### **Exercise 1** Creating Reports

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

#### **Exercise 2** Customizing a template

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

#### Exercise 3 Customizing a table

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

#### **Exercise 4** Additional ways to customize a table

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

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

#### **Exercise 5** Graphics

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

#### **Exercise 6** Advanced topics

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

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

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Agilent MassHunter Workstation Software Reporting Familiarization Guide

## 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 you create a report method.
- In Task 7 you generate a Quantitative report using the report method.



Each exercise is presented in a table with three columns:

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

## **Creating Reports in the Qualitative Analysis Program**

### **Increasing Speed of Qualitative Analysis Report Generation**

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

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

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

1

## Task 1. Open the Qualitative Analysis program

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

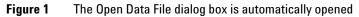
Task 1. Open the	Qualitative Ana	alvsis program	with multiple	data files
		, p		

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,</li></ul>	<ul> <li>The sulfas-PosMS.d file contains MS (TOF or Q-TOF) data. The sulfas-PosAutoMSMS.d and sulfas-PosTargetedMSMS.d files contain both MS and MS/MS (Q-TOF) data.</li> <li>You can get help for any window, dialog box, or tab by pressing the F key when that window is active.</li> </ul>	

Task 1. Open the Qualitative Analysis program

Steps	Detailed instru	ctions	Comment	S
	Dpen Data File	1-	- O 🕫 e	
		_	d	Open Cancel
	Options Load worklist meth Ouse current methu Load results meth Load results meth Load result data Run 'File Open' a selected method	od od	Sample Information Sample Name : User Name : Sample Position : Description :	

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



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

C	Press and hold the <b>Shift</b> key while you click <b>sulfas_PosAutoMSMS</b> , <b>sulfas_PosMS.d</b> and		If you press the <b>Ctrl</b> key instead, you can pick files which are not directly next to each other in the
	sulfas-PosTargetedMSMS.d.		list.
d	Click <b>Open</b> .	•	What you see in the main window
	All three data files are displayed in		at this point depends on the
	Data Navigator, and three		method, layout, display, and plot
	chromatograms are displayed in the		settings used before you opened
	Chromatogram Results window.		these files.

Task 1. Open the Qualitative Analysis program

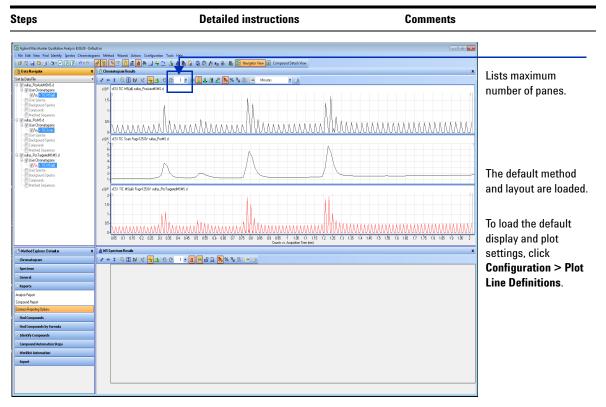


#### Task 1. Open the Qualitative Analysis program with multiple data files (continued)

Figure 2 Qualitative Analysis main window

- 2 Return the main window to its default workflow, **General**. The default method and layout are loaded.
  - Make sure you can see all three chromatograms.
- a If necessary, click Configuration > Configure for Workflow > General.
- **b** In the **Workflow Configuration** dialog box, mark:
  - Load workflow's default method
     Load workflow's default layout
- c Click the down arrow next to the Maximum number of list panes list in the Chromatogram Results toolbar, and select 3.
- The display and plot settings will remain the same even after you switch to the General workflow. These settings differ depending on your specific situation.
- You can change the layout by clicking Configuration > Window Layouts > Load Layout.

Task 1. Open the Qualitative Analysis program



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

Figure 3 Qualitative Analysis main window with the General Workflow selected

Task 2. Print an analysis report

## Task 2. Print an analysis report

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

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

S	teps	Detailed instructions	Comments	
1	Save the intermediate report files.	<ul> <li>a Click Configuration &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>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 Reports &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>	<ul> <li>A section in a report is only included if:</li> <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 integrated the chromatogram, the peak table cannot be included.</li> <li>If you are keeping the intermediate report directories to customize a template, mark all of these check boxes. You also need to generate al of these results. Then, all results are available when you are customizing a template.</li> </ul>	

#### Task 2. Print an analysis report

Task 2. Print an analysis report

Steps	Detailed instructions	Comments
Method Explorer: Default.m  Chromatogram  Spectrum  General  Reports  Analysis Repot  Compound Repott  Compound Repott  Gompounds  Find Compounds  Find Compounds  Find Compounds  Find Compounds  Find Compounds	Image: Show user spectra     Image: Show user spectra       Image: Show user spectra     Image: Show user spectra       Image: Show user spectra     Image: Show user spectra       Image: With ibray spectrum     Image: With ibray spectrum	Before printing the analysis report, you generate the results that you want to include. For example, if you want to include compound chromatograms, you need to run one of the <b>Find</b> <b>Compounds</b> algorithms.
Identify Compounds  Compound Automation Steps  Worklist Automation  Export	With difference spectrum Compounds Show compound chromatograms With peak tables V Ahn peak tables V With peak tables	If you want to increase the speed of printing a report, remove any unnecessary graphics. Including graphics in a report slows down report generation.

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

Figure 4 Analysis Report section in the Method Editor

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

Task 2. Print an analysis report

Steps	<b>Detailed instructions</b>		Comments
Method Explorer: Default.m ×     Orromatogram	Method Editor: Common Reporting Options           O         Print Compound Report         Image: Second Report	× ₅• (2) (3)	
Spectrum  General  General  Compound Report  Compound Report  Find Compounds  Find Compounds	Templates         Options           General         Page orientation           Page orientation         Italies           Italie empty columns in tables         Show sample information           Peak table limits (include all peaks unless limits are specified)         Chromatogram peaks           Italies meaks         10           Italies meaks         10           Italies meaks         10           Italies specified)         Chromatogram peaks           Italies specified)         Custom politinis (autoccaled unless limits are specified)		Mark this check box if you do not want to include empty columns in any table in the report.
<ul> <li>Identify Compounds</li> <li>Compound Automation Steps</li> <li>Worklist Automation</li> <li>Export</li> </ul>	User Anna Gamma Gamma 2 2000-10.000     Compound chromatograms     MS spectra     MS/MS spectra     Deconvoluted spectra     UV spectra     UV spectra	min min m/z Da m	You can specify the plot limits to use in the report for each type of graphic.

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

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

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

## Task 3. Print a compound report

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

S	tep	Detailed instructions	Comments	
1	Save the intermediate report files.	<ul> <li>a Click Configuration &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 made 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>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>	<ul> <li>a Click File &gt; Open Data File to load a data file.</li> <li>b Click one of the commands in the Find menu to find compounds.</li> <li>c In Method Explorer, click Reports &gt; Compound Report.</li> <li>d Mark the check boxes for any additional sections you want to print.</li> <li>e Clear any chromatogram and spectra choices you do not want to print.</li> </ul>	<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 are customizing a template.</li> </ul> </li> </ul>	

Task 3. Print a compound report

Step	Detailed instructions	Comments	
Method Explorer: Defaxt.m   Chromatogram   Spectrum   General   Reports   Analysis Report   Compound Report   Compound Seport   Find Compounds   Find Compounds   Compound Automation Steps   Worklist Automation   Export	Method Editor: Compound Report         > Print Compound Report         > Show Compound Report         > Show compound table         Sort order:       Increasing         > Stow compound table         Sort order:       Increasing         Exclude details for unidentified compounds         Hornalograms         Show user chromatogram(s)         Show user chromatogram(s)         Overlay compound chromatogram(s)         Overlay compound chromatogram(s)         Show MS spectrum         Overlay predicted isotope distribution         ompound spectrum (MS/MS)         Show MS/MS spectrum         Overlay predicted isotope distribution         ompound spectrum (MS/MS)         Show MS/MS spectrum         Show MS/MS spectrum	To increase the speed of creating a report, remove any unnecessary graphics. Including graphics in a report slows down the creation of reports.	1

#### Task 3. Print a compound report (continued)

Figure 6 Compound Report tab in the Method Editor

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

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, select the printer in this dialog box.</li> <li>f Click OK.</li> </ul>	<ul> <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 Compound</li> </ul>
Print Page Zoom Clos	CompoundReport1 - Excel ? 🖻	This button closes the <b>Print</b> <b>Preview</b> window without sending the report to the printer.

#### Task 3. Print a compound report (continued)

**Figure 7** The Print Preview window showing the Compound Report

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

Task 4. Generate a graphics report

## 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.

Step	Detailed instructions	Comments
<b>1</b> Save the intermediate report files.	<ul> <li>a Click Configuration &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 made 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 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 or graphicfullpage.</li> </ul>	<ul> <li>a In Method Explorer, click Reports &gt; Common Reporting Options.</li> <li>b Verify that the correct Report template folder is selected.</li> </ul>	• The report templates shipped with the software are separated into two folders. One folder contains reports formatted to print on Letter size paper. The other folder contains reports that print on A4 size paper.
<b>3</b> 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 <b>graphicfullpage</b> template is used.</li> </ul> </li> </ul>

#### Task 3. Print a graphics report (continued)

Step		Detaile	l instructions	Comments
Print Print Options Contents V Include header V Include footer	Orientation Potrait Candocape		Print       Options         Report contents       All spectra         Only highlighted spectra       Only visible spectra         Report options       On spectrum per page         Report destination       Printer name:         Ø Print Preview       Ø Print Preview	
	OK	Cancel		OK Cancel

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

■ S· C· ÷ FL: PRINT PREVIEW	GraphicFul	IIPage2 - Excel		? • – • × • •	
Print Page Print Zoom Com Show M	Page Close Print			^	This button closes the <b>Print</b> <b>Preview</b> window without sending the report to the printer.
Sample Name 1 ng sufiz Ing Vol 1 Date Flemane sufice, powers/MSd 2 10 5 Court 7 0 0021 + 23 CEC 3 2 0 0 0021 + 23 CEC 2 0 0 0 201 + 23 CEC 2 0 0 0 201 + 23 CEC 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	InjPosition Sar	mpleType Sample nument	Isor Name Regulation Status Acquired Time	Screes 8/5/2000 11:00-41	
Figure 9 The Pr 4 Close the Print Pre	rint Preview windov eview window. C	w showing the ( lick <b>Close Print P</b>	•	•	<ul> <li>If you want to print the report, click Print. The report is printed on the printer selected in the Print Compound Report dialog box.</li> </ul>

### Creating Reports 1

Task 4. Generate a graphics report

## **Creating Reports in the Quantitative Analysis Program**

### **Increasing Speed of Quantitative Analysis Report Generation**

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

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

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

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

1

key when that window is active.

## 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 Move to the folder \ Your Directory \DrugsOfAbuse\.</li> <li>d Select a batch. You can select either DrugsOfAbuseDemo.batch.bin or <i>iii_</i>Test_01.</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 Formation of the set of</li></ul>	



Figure 10 Open a batch file

1

Task 5. Open a batch in the Quantitative Analysis program

#### Task 5. Open the Quantitative Analysis program (continued)

Steps	Detailed instructions	Comments	
<ul> <li>2 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> </ul>	<ul> <li>a Click 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 two 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>	

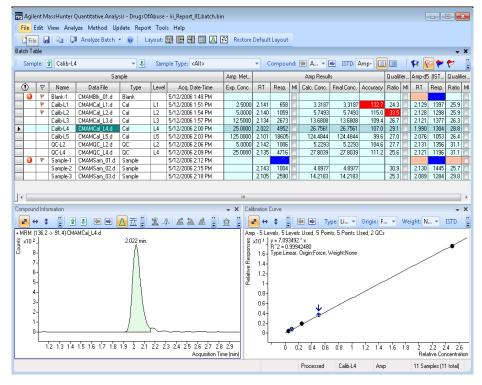


Figure 11 Quantitative Analysis program after analyzing batch

### Task 6. Create a quantitation report method

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

Task 6. Create a quantitation report method
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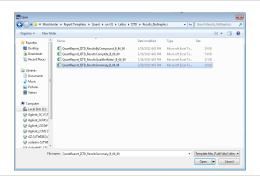
Steps	Detailed instructions	Comments
<ol> <li>If necessary, open the batch file <i>iii</i>_Report_01.batch.xml.</li> <li>If the batch is already open, skip to step 2.</li> </ol>	<ul> <li>a To start the Quantitative Analysis program, click the Quantitative Analysis (QQQ) icon on your desktop.</li> <li>b Click Open Batch and provide the open Batch dialog box.</li> <li>c Move to \ Your Directory \ DrugsOfAbuse and select iii_Test_01.batch.bin.</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 Default Layout</li> </ul>
2 Select report template.	<ul> <li>a Click Report &gt; Generate. The system displays the Generate Report dialog box.</li> <li>b Select New The Report Method Edit window opens.</li> </ul>	The Batch folder and file from your batch is displayed under Batch file. For faster report generation, choose a PDF template at \MassHunter\ Report Templates\Quant\ PDF-Reporting
		See the Quant DA online help for more details on configuring reports.

Report Method Edit			
File Edit			
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Templates Results Graphics settings			
Template	Report mode	Destination file	Publish forr
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Task 6. Create a quantitation report method

Task 6. Create a quantitation	report method	(continued)
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Steps	Detailed instructions	Comments
	<ul> <li>c From the Template tab, select Add Template The Open dialog box opens.</li> <li>d Navigate to and select \MassHunte Report Templates\Quant\en-US\ Letter\ISTD\Results_NoGraphics` QuantReport_ISTD_ResultsSumma</li> </ul>	λ



e Select Open. The template is added to the **Report Method Edit** window.

Report Wethod Edit									08
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### Task 7. Generate quantitation reports using a report method

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

Steps	Detailed instructions	Comments
<ol> <li>If necessary, open the batch file <i>iii_Report_01.batch.bin</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 Move to \Your Directory\ DrugsOfAbuse and select iii_Test_01.batch.bin.</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> </ul>
<b>2</b> Select options for your report.	<ul> <li>a Select Report &gt; Generate</li> <li>b Under Report folder use the default location or select Browse to use another location.</li> <li>c Under Report method, select Choose</li> <li>d In the Open window, navigate to and select the method you created in "Task 6. Create a quantitation report method" on page 25. The method is displayed under Report method.</li> <li>e Select All samples and All compounds or use Choose samples or Choose compounds to select the items you want in your report.</li> <li>f Under Generate, select Generate reports now.</li> </ul>	<ul> <li>Under Generate, you may choose Queue report task and Start Queue Viewer to view the report status as it is generated.</li> </ul>

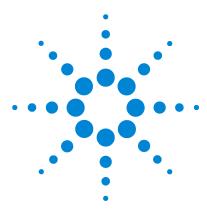
1

Task 7. Generate quantitation reports using a report method

Steps	Detailed instructions	Comments
	r	
	Generate Report	8
	Batch file:	
	Batch folder:	C:\MassHunter\Data\DrugsOfAbuse\
	Batch file:	iii_Report_01.batch.bin Browse
	Report folder:	
	C:\MassHunter\Data\D	rugs0fAbuse\QuantReports\iii_Report_01 Browse
	Report method:	
	C:\Users\lh\Desktop\te	est\test.m
		Choose New Edit
	Samples/Compounds:	
	All samples	Choose samples
	☑ All compounds	Choose compounds
	Generate:	
	Generate reports not	w
	Queue report task	
	Start Queue V	Viewer
		OK Cancel

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

Progress	
Genera	ing report(s). Please wait
	Cancel



Agilent MassHunter Workstation Software Reporting Familiarization Guide

## **Exercise 2 Customizing a template**

Task 1. Open a Qualitative Analysis template 30
Task 2. Customize the footer of the Qualitative Analysis template 32
Task 3. Use the new template in the Qualitative Analysis program 37
Task 4. Open a Quantitative Analysis Excel template 40
Task 5. Customize the footer of the Quantitative Analysis Excel template 42
Task 6. Use the new Excel template in the Quantitative Analysis program 46

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.

Step	Detailed in	nstructions		C	omments
Make a copy of the Analysis Microsoft Excel Template file rename the file iii_CustomAnalysisReport	e and b Move t folder in the dat c Move t d Right-c Micros Copy. e Click Ed report t f Right-c	o the Letter or A4 lick the Analysis oft Excel Template lit > Paste to add emplate to the cu lick the new file, isReport-Copy an	plates \ e you in folder <b>Report</b> e file an l a copy urrent fo	<b>.Qual</b> stalled nd click y of the	You do the same steps to open a <b>Quantitative Analysis</b> template.
	<b>g Type</b> iii_C	CustomAnalys	isRe	port	
	• • •	CustomAnalys	isRe	port	
	iii_0	■ 8.05.01 → en-US → Letter →	· 14 Search	ietter f	
	iii_0	■ B05/II + en-US + Letter + ■ Print E-mail New folder	• <b>49</b> Search	Letter F	
	iii_C	B05/II + en-US + Letter + Print E-mail New felder Name	• • • Search	Letter F III • I @ Type Sax	
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	iiiC	BOURD + cn-OS + Letter +  Print E-mail New Folder Name Coding Co	<ul> <li>49 Search</li> <li>Date modified</li> <li>4/18/2813 3:18 PM</li> <li>4/18/2013 3:18 PM</li> <li>10/15/2012 12:00</li> </ul>	Letter F Type Size File folder File folder File folder RLC File	
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Figure 12 Report Templates\Qual\Letter folder

Task 1. Open a Qualitative Analysis template

Step	Detailed instructions	Comments
2 If needed, remove the <b>Read-only</b> attribute from the new template.	<ul> <li>a Right-click the new file and click Properties.</li> <li>b Clear the Read-only check box in the Attributes section.</li> <li>c Click OK.</li> </ul>	<ul> <li>If a template is read-only, you cannot save any changes to the template.</li> </ul>
	Image: CustomAnalysisReport Properties         General Security Details Previous Versions         Image: CustomAnalysisReport         Type of file:         Microsoft Excel Template (x8x)         Deners with:       Excel (desktop)         Location:       C:MassHunter/Report Templates/QuarkB.06.00/ver         Size on disk:       56.0 KB (57.344 bytes)         Created:       Today, May 14, 2013, 8 minutes ago         Modified:       Saturday, August 11, 2012, 519,28 PM         Accessed:       Today, May 14, 2013, 8 minutes ago         Attribute:       Readonly         Image: Cancel       Apply	Clear the <b>Read-only</b> check box.

#### Task 1. Open a Qualitative Analysis template (continued)

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 "Task 1. Open a Qualitative Analysis template" on page 30.

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

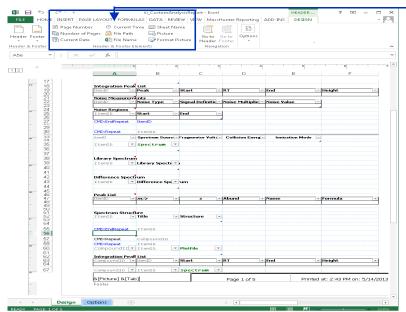
Step	Detailed instructions	Comments
<ul> <li>Switch to the <b>Design</b> worksheet if necessary.</li> </ul>	Click <b>Page Layout</b> in the Workbook Views group in the <b>View</b> tab in the Ribbon. You can also click the <b>Page Layout</b> icon ( at the bottom of the Excel program to switch to the Page 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. Click any of these sections to edit that part.</li> </ul>
Preview Zoom Workbook Views Zoom	Zoom to Zoom to Selection     Image All Presse Panes - Window     Image All Windows     Image All Windows     Image All Macros Macros       Image All Macros     Image All Window     Image All Macros     Image All Macros     Image All Macros       Image All Macros     Image All Macros     Image All Macros     Image All Macros     Image All Macros       Image All Macros     Image All Macros     Image All Macros     Image All Macros       Image All Macros     Image All Macros     Image All Macros       Image All Macros     Image All Macros       Image All Macros     Image All Macros       Image All Macros     Image All Macros       Image All Macros     Image All Macros       Image All Macros     Image All Macros       Image All Macros     Image All Macros       Image All Macros     Image All Macros       Image All Macros     Image All Macros       Image All Macros     Image All Macros       Image All Macros     Image All Macros       Image All Macros     Image All Macros       Image All Macros     Image All Macros       Image All Macros     Image All Macros       Image All Macros     Image All Macros       Image All Macros     Image All Macros       Image All Macros     Image All Macros       Image All Macros     Image All Macros	Click this button to switch to the Page Layout view.
Image: State of the state o	Tend Tript	This template has two different sheets. Make sure the <b>Design</b> worksheet is selected.
Production of the second of th	• 2 • 7 • 7 • 7 • 7 • 7 • 7 • 7 • 7	You can also click this button to switch to the <b>Page Layout</b> view.

Figure 14 Switching to the Page Layout view in Excel

Task 2. Customize the footer of the Qualitative Analysis template

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 Insert a space.</li> <li>d 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>

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



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

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

Figure 15 The Header and Footer Design Tab in Excel

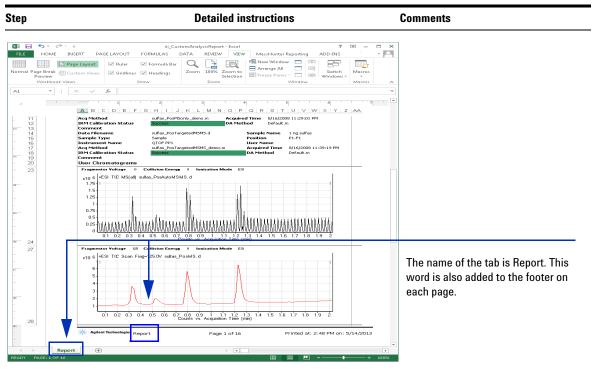
Task 2. Customize the footer of the Qualitative Analysis template

S	tep	Detailed instructions	Comments
3	Finish editing the footer.	<ul> <li>a Click in any of the cells in the spreadsheet to stop editing the fo</li> <li>b Click Normal in the Workbook Vingroup in the View tab in the Ribbo</li> </ul>	ews
4	Test the changes to the template.	<ul> <li>a Click the MassHunter Reporting to Click Process Report.</li> <li>c Click Browse.</li> <li>d Move to the \MassHunter\reporter temp folder.</li> <li>e Double-click one of the folders the contains analysis results.</li> <li>f Select Report.</li> <li>g Click Open.</li> <li>h Click OK.</li> <li>i After the report is processed, click Page Layout in the Workbook Vie group in the View tab in the Ribbo</li> <li>j Scroll to the bottom of the page to the change. The name of the tab in added after the Agilent logo.</li> </ul>	<ul> <li>part of the MassHunter toolbar in the MassHunter Reporting 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 (continued)

Task 2. Customize the footer of the Qualitative Analysis template





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

- 5 Save the changes to the template.
  - You have to clear the results first.
- Reporting tab in the Ribbon.
- **b** Click **File > Save**.
- a Click Clear Results in the MassHunter You can click Save As if you want to change the name of the template.
  - The Save as type is Excel Template.

You can either save the template to the same name or to a new name.

Task 2. Customize the footer of the Qualitative Analysis template

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لدودal Disk (C:) کی Agilent_GC (۱/۱۲۷ کی Agilent_GCMS (۱/ کی Agilent_LSGSW (۱/ کی Agilent_LCMS (۱/	GraphicFullPageNoHeader     III_custornAnalysisReport     QualitativeMethodReport	7/10/2012 2:12 AM 5/14/2013 2:54 PM 3/30/2010 12:34 PM 4/29/2010 12:40 PM 2/10/2011 2:14 PM	Microsoft Excel Te Microsoft Excel Te Microsoft Excel Te	20 K8 80 K8 34 K8 46 K8 62 K8
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Task 2. Customize the footer of the Qualitative Analysis template (continued)

## 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 Reports &gt; Common Reporting Options.</li> <li>b Select the template <i>iii</i>_CustomAnalysisReport as the Analysis report template, where <i>iii</i> 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>Click the button next to the Report template folder.</li> </ul>		
			<b>b</b> Click <b>OK</b> . Do not change the folder that is selected.		

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

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

Steps	Detailed instructions	Comments
Steps         Image: Chromatogram         Image: Chromatogram </th <th>Detailed instructions</th> <th>You select the new report template</th>	Detailed instructions	You select the new report template
Figure 18 Analysis Report sect	ion in the Method Editor	

- 3 Select the template to use when a In Method Explorer, click Reports > printing this report. **Common Reporting Options**. **b** Verify that the correct **Report template** folder is selected. c Verify that the correct Analysis report
  - template is being used.
  - d Click Options.
  - Verify the settings on this tab. е
- · The report templates shipped with the software are separated into two folders. One folder contains reports that are formatted to print on Letter size paper. The other folder contains reports that print on A4 size paper.
- Three different analysis report ٠ 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>Select Print Analysis Report from the list, printer icolbar.</li> <li>Right-click the Analysis Report section in the Method Editor, and click Print Analysis Report.</li> <li>Select the data file in the Data Navigator, and click Print Analysis Report.</li> <li>Click Generate Analysis Report in the Actions menu.</li> </ul> </li> </ul>	The Run icon in the Method Editor toolbar sometimes allows you to choose an action from a set of possible actions. For example, if you switch to the Reports > Common Reporting Options section, four different actions are possible when you click Run. If you click the arrow, a list of possible actions is shown, and you can choose which action to do. Choosing a different action from the list changes the default action. If you simply click Run, the default action is performed.		

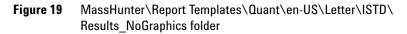
#### Task 3. Use the new template in the Qualitative Analysis program (continued)

## Task 4. Open a Quantitative Analysis Excel template

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

Task 4. Open a Qu	antitative Analysis Excel template
-------------------	------------------------------------

St	eps	De	etailed instru	ctions	C	omments
1	Make a copy of the QuantReport_ISTD_Summary_ <i>B_0</i> <i>4_00</i> Microsoft Excel Template file and rename the file <b>iii_Custom_ISTD_Summary</b> .	a b c d e f g	Open the <b>Re</b> en-US folder installed the Move to the <b>ISTD/Result</b> Right-click th <b>ResultsSum</b> click <b>Copy</b> . Click <b>Edit</b> > I report templa Right-click th <b>QuantReport</b> _ <b>B_06_00</b> -	Letter or A4 folder. ts_NoGraphics folder. ne QuantReport_ISTD_ mary_B_06_00 file and Paste to add a copy of the ate to the current folder.		You do the same steps to open a Qualitative Analysis template. In the <b>Report Templates\Quart\</b> <b>en-US\Letter or A4</b> folder, the templates are separated into additional folders, including <b>ESTD</b> and <b>ISTD</b> .
			Organize	en-US > Letter > ISTD > Results_NoGraphics  Print E-mail New folder Name batch.results.ad  G in Custom JSTD_Summary Q QuantReport_ISTD_ResultsQcompound_B.06.0  Q QuantReport_ISTD_ResultsQcompound_B.08.0  Q QuantReport_ISTD_ResultsQuantmary_B.06.00		<ul> <li>4y Search Resu</li> <li>Date modified</li> <li>2/20/2013 402 PM</li> </ul>



Task 4. Open a Quantitative Analysis Excel template

		Comments		
Remove the <b>Read-only</b> attribute from the new template.	<ul> <li>a Right-click the new file and click</li> <li>Properties.</li> <li>b Clear the Read-only check box in the Attributes section.</li> <li>c Click OK.</li> </ul>	<ul> <li>If a template is read-only, you cannot save any changes to the template.</li> </ul>		
	Image: Custom_JSTD_Summary Properties         General       Geounity       Details       Previous Versions         Image: Custom_JSTD_Summary       Image: Custom_JSTD_Summary         Type of file:       Microsoft Excel Template (xikk)         Opens with:       Excel (desktop)       Change.         Location:       C:WastHurtlerARpool       Change.         Created:       Today. May 15, 2013, 15 minutes ago         Modified:       Thrusday. February 28, 2013, 402 24 PM         Accessed:       Today. May 15, 2013, 15 minutes ago         Attributes:       Readonty       Hidden         Advanced       DK       Cancel	Clear the <b>Read-only</b> check box. This check box may already be clear.		

Task 4. Open a Quantitative	Analysis Excel	template	(continued)
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- Figure 20 Properties dialog box
- 3 Open the template. Right-click the **new file** and click **Open**.

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

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

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

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

iteps	Detailed instructions	<ul> <li>Comments</li> <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 any of these sections to edit that part.</li> </ul>		
Switch to the <b>Page Layout</b> view.	Click <b>Page Layout</b> in the Workbook Views group in the <b>View</b> tab in the Ribbon. You can also click the <b>Page Layout</b> icon ( ) at the bottom of the Excel program to switch to the Page Layout view.			
HOM DEET PAGE LAYOUT PORMULAS DATA BECKIV      Morrison Page To P	Image Frazz     Utwee Set by Set     Image Frazz     Image Frazz <td< th=""><th>Click this button to switch to the Page Layout view.</th></td<>	Click this button to switch to the Page Layout view.		
6 Compared to the second of th	Tormula Name Categorantine 2 Target Composited Target Composited T	This template has two different sheets. Make sure that the Design Summary worksheet is visible.		
33         34           34         34           35         37           37         37           37         37           40         42           Options         Design Summary           FAMO         FAMO		You can also click this button to switch to the Page Layout view.		

Figure 21 Switching to the Page Layout view in Excel

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

Steps	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 Insert a space.</li> <li>d 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:         <ul> <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> </li> </ul>		

	-		iii_Custom_ISTD_Su	mmary - Excel			HEADER & FOOTER	TOOLS	2 10
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#### The Header & Footer Elements are

shown in the Design tab when you click one of the sections in the header or footer. You can click these buttons to quickly add these items to the header or footer.

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

#### Figure 22 The Header and Footer Design Tab in Excel

**3** Finish editing the footer.

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

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

Steps	Detailed instructions	Comments	
<b>4</b> Test the changes to the template.	<ul> <li>a Click Process Report.</li> <li>b Click Browse.</li> <li>c Move to the \MassHunter\Data\DrugsOfAbuse\QuantReports\DrugsOfAbuseDemo folder.</li> <li>d Select report.results.</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> </ul>	<ul> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in the Ribbon.</li> <li>You can only see the header and the footer in the Page Layout view.</li> </ul>	

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Task 5. Change th	e tooter of the	Quantitative Analy	ysis excel tem	plate (continued)

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14	CMAMCal L5.d		allo-L9 allo-L5	P1-C17		5	LS	Calibration	APCIautotune.m					
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16	CMAMQC_L4.d	9	C-L4	P1-C15		5	L4	QC .	APCIautotune.m					
17	CMAMSam_01.d		ample-1	P1-C22		5		Sample	APCIautotune.m	_				
18	CMAMSam_02.d		ample-2	P1-C8		5		Sample	APCIautobune.m					
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38	CMARCal_L2.d		eth	Meth-d5		1460	2709			1011	5.0000	102.02		
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40	CMARCALL4.d		eth	Meth-d5		1035	2751			25/4 2764	125.0000	109.03		
41	CMAMQC_L2.d		eth	Meth-d5		1375	2483			2414	5.0000	104.83		
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	Summary	+	-				4						E E	

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

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

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

Steps	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>	a Click Clear Results in the MassHunter Reporting tab in the Ribbon.	<ul> <li>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 for most reports.</li> </ul>		

Agilent MassHunter Workstation Software Reporting Familiarization Guide

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

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

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

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 23.	<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 Generate Report dialog box.</li> <li>Verify the default destination directory for reports is \Your Directory\DrugsofAbuse\QuantReports.</li> <li>The default file name is iii_Test_01, where "iii" are your initials.</li> </ul>	<ul> <li>a Click Report &gt; Generate. The system displays the Generate Report dialog box.</li> <li>b Click</li> <li>c Specify the Report folder for example, \ Your Directory\DrugsOfAbuse\ QuantReports\iii_Test_01.</li> </ul>		

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

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

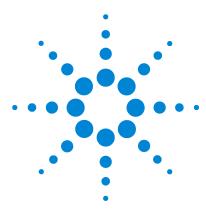
Task 6. Use the new Excel template in the Quantitation	ve Analysis program (continued)

Generate Report	
Batch file:	
Batch folder: C:\MassHunter\Data\DrugsOfAbuse\	The new template is shown here.
Batch file: DrugsOl/AbuseDemo.batch.bin Browse	The new template is shown here.
Report folder:	
C:\MassHunter\Data\L rugsDlAbuse\QuantReports\ii_Test_01 Browse	
Report method:	
C: \MassHunter\reports\temp\ii_Custom_ISTD_ResultsSummary.m	
Choose New Edit	
Samples/Compounds:	
All samples Choose samples	
All compounds Choose compounds	
Generate:	
Generate reports now	
Queue report task	
V Start Queue Viewer	
OK Cancel	
UK Lancei	

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

Steps	Detailed instructions	Comments	
<ul> <li>Generate the report.</li> <li>View the status of the report generation in the Task Queue Viewer.</li> </ul>	<ul> <li>a Click OK in the Generate Report dialog box to generate the report. Select All samples and All compounds or use Choose samples or Choose compounds to select the items you want in your report.</li> <li>b Under Generate, select Queue report task and Start Queue Viewer to view the report status as it is generated.</li> <li>c Watch the progress of the report in the Status column.</li> </ul>	<ul> <li>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.</li> </ul>	

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



Agilent MassHunter Workstation Software Reporting **Familiarization Guide** 

## **Exercise 3 Customizing a table**

Task 1. Rename a column header in a table 51 Task 2. Delete a column from a table 54 Task 3. Change the width of a column in a table 57 Task 4. Move a column in a table 61 Task 5. Add a column to a table 64 Task 6. Add a mapped column to a table 68 Task 7. Add a filter to a table 73 Task 8. Move or delete a column in a filtered table 78

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.

Step	Detailed instructions	Comments	
1 Open the Quantitative Analysis template \MassHunter\Report Templates\Quant\en-US\Letter\ ISTD\Results_NoGraphics\ <i>iii_</i> Custom_ISTD_Summary template, where " <i>iii</i> " are your initials.	<ul> <li>Follow the instructions in "Task 4.</li> <li>Open a Quantitative Analysis Excel template" on page 40 to open the template, iii_Custom_ISTD_Summary, where "iii" are your initials.</li> </ul>	<ul> <li>If you did not do the previous tas example templates are available the Agilent Technologies MassHunter Reporting User Information DVD in the Familiarization Templates folder</li> </ul>	
2 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 the cell containing the words Data File. This column is the second column in the table.</li> </ul>		
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	WIEW     MassHunter Reporting     ADD-INS     DESIGN     ▼       Text     ▼     Conditional Formatting ×     Image: State = 1     Image: State = 1       \$ - %     >     Format vs Table *     Image: State = 1     Image: State = 1       \$%     \$%     Image: State = 1     Image: State = 1     Image: State = 1       \$%     \$%     Image: State = 1     Image: State = 1     Image: State = 1	The contents of the current cell are shown here in the Formula bar.	
1 Batch Data Path     2 Analysis Time     Analysis Name     Reporter Name     Reporter Name     Last Calib Update     Quart Ratch Version     G     SampletD     Pata File     Sample Name     P	sition v Inj tv Level v Sample Type v Acq Metho(v Samplef	Click this cell in the <b>Sequence Table</b> . One of the column headers in a table in	
	rmula v Name v RetentionTime v <i>arget Compound</i> AND v CompoundT v Data File v Compound v ISTD v	the <b>Quantitation Results</b> section also is called <b>Data File</b> . Columns in differen tables can have the same name.	
21 22 ← Options Design-Summary ④	· · · · · · · · · · · · · · · · · · ·		

Figure 24 Selecting the Data File cell in Excel

Task 1. Rename a column header in a table

tep	Detailed instructions	Comments		
	<b>c</b> Type <i>Acquisition File.</i> You can also click in the <b>Formula Bar</b> to overwrite only part of the name.	• Two columns in the same table cannot have the same name. Excel automatically changes the name of the column that appears second in the table if two column names are the same.		
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B8 I I X I Acquisition		×		
2     Analysis Time     Anal       3     Report Time     Report       4     Last Calib Update     Batc	lyst Name Arter Ar	The column header has been changed to Acquisition File.		
7 Sequence Table 8 SampleID Acquisition File Samp 9	ple Name v Position v Inj v Level v Sample Type v Acq Metho(v SampleF			
10 11 12 Quantitation Results 13 CMD:Repeat CompoundID				
15	oundType v formula v Name v RetentionTime v Target Compound CompoundID v PedID v CompoundT Data File v Compound v ISTD v			
18 19 20 CMD:EndRepeat CompoundID 21				
22	(+) : (	Ŧ		

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

Figure 25 Changing the header of the column to Acquisition File

**3** Test the changes to the template.

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

Task 1. Rename a column header in a table

Task 1. Change the column	header in a Q	uantitative Anal	vsis table	(continued)

Step		D	Detailed instructions					Comments			
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FILE HOME	INSERT PAGE LAYOUT	FORMULAS DAT	A REVIEW	VIEW	MassHunter Rep	orting ADD-INS		- 0			
Process Clear Add Report Results Data	Add Add Advan Graphics Formatting Proper	ced Validate About Hel									
	MassHunter Reporting							^			
A1 - :	× √ ƒ <sub>×</sub> Bat	ch Data Path						~			
A 1 Batch Data Path		C uantExamples\QQQ\Drugs			F psOfAbuseDemo.b	G atch.bin	Н	-			
2 Analysis Time 3 Report Time 4 Last Calib Update 5 Quant Batch Vers 6 7 Sequence Table		Anaiyst Name Reporter Name Batch State Quant Report Vers	Quantswitest- QuantSWtest- Processed ion B.05.02						The column header is now Acquisition File.		
Acquisition File	Sample Name	Position	Inj ¥ol	Level	Sample Type	Acq Method File					
CMAMBIk_01.d	Blank-1	P1-C1	5		Blank	APCIautotune.m					
) CMAMCal_L1.d CMAMCal_L2.d	Calib-L1	P1-C6	5	L1	Calibration	APCIautotune.m					
	Calib-L2	P1-C10	5	L2	Calibration	APCIautotune.m					
CMAMCal_L3.d CMAMCal_L4.d	Calib-L3 Calib-L4	P1-C11 P1-C14	5	L3 L4	Calibration Calibration	APCIautotune.m APCIautotune.m					
CMAMCal_L4.d	Calib-L5	P1-C17	5	L4 L5	Calibration	APCIautotune.m					
CMAMQC_L2.d	QC-L2	P1-C9	5	L2	QC	APCIautotune.m					
CMAMQC_L4.d	QC-L4	P1-C15	5	L4	oc	APCIautotune.m					
7 CMAMSam_01.d	Sample-1	P1-C22	5		Sample	APCIautotune.m					
8 CMAMSam_02.d	Sample-2	P1-C8	5		Sample	APCIautotune.m					
9 CMAMSam_03.d	Sample-3	P1-C12	5		Sample	APCIautotune.m		*			
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READY					E	8 8		+ 100%			

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

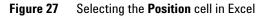
4	<ul> <li>Save the changes to the template.</li> <li>You have to clear the results first.</li> <li>You save the template to the</li> </ul>	b	Click Clear Results in the MassHunter Reporting tab in the Ribbon. Click File > Save As. In the Save As dialog box, type	•	The <b>Save as</b> type is <b>Excel Template</b> .
	new name, iii_1_Custom_ ISTD_Summary.		<pre>iii_1_Custom_ISTD_Summary. Verify the folder selected in Save in is correct. Click Save.</pre>		

## Task 2. Delete a column from a table

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

Task 2. Del	ete a columr	ı from a	Quantitative	Analysis table
-------------	--------------	----------	--------------	----------------

	ер	Detailed instructions	Comments
1 Open the Quantitative Analysis template \MassHunter\Report Templates\Quant\en-US\Letter\ ISTD\Results_NoGraphics\ iii_1_Custom_ISTD_Summary.		<ul> <li>Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template,</li> <li>iii_1_Custom_ISTD_Summary, 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>
2	Delete the column <b>Position</b> in the <b>Sequence Table</b> .	<ul> <li>a Find the table labeled Sequence Table.</li> <li>b Click the cell containing the words Position. This column is the fourth column in the table.</li> </ul>	
X		Custom JSTD_Summary.ubc - Excel ? 🗉 🗧	
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1 2 3 4 5 6 7	IB Cory     If U + □ + ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓	Interface         Description         Present         Description         Present         Constraint         Soft Field &	Click this cell in the Sequence Table
1 2 3 4 5 6 7 8 9 10 11 12	ID Copy     If IP + IP	Interface         Description         Present         Description         Description <thdescripant< th=""> <thdescripant< th="">         Des</thdescripant<></thdescripant<>	Click this cell in the Sequence Table
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19	B C cyn     I     II     II	Al 2 Generation Formula (Good Neutral )     Mar Shall      Ma	Click this cell in the Sequence Table
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24	IP Copy     IF IP + IP	Al 2 Generation Formula (Good Neutral )     Defermine (Columnation (Good Neutral )     Defermine (Good Neutra)     Defermine (Good Neutral )     Defermine (Good Neutral )	Click this cell in the Sequence Table
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19	B C cyn     I     II     II	Al 2 Generation Formula (Good Neutral )     Defermine (Columnation (Good Neutral )     Defermine (Good Neutra)     Defermine (Good Neutral )     Defermine (Good Neutral )	Click this cell in the Sequence Table



Task 2. Delete a column from a table

ер		Detailed instructions Comments	
		Table Columns.keyboard totable. If youthe column h	the <b>Delete</b> key on the delete a column in a press the <b>Delete</b> key, neader is changed and s not deleted.
I → · · · Q. A. · · TE HOME INSERT PAGE LAW M → · · · · · · · · · · · · · · · · · ·	DUT FORMULAS DATA A = = = ≫ + ₽ A = = = € € € € G Alignment	Custom, ISTD_Summary1 - Excel REVIEW VIEW MassHunter Reporting DEVELOPER DESIGN Wrap Text Merge & Center - G Number G Conditional Format as Cell Number G Styles Styles Center Format Styles Center Format Styl	
A B Batch Data Path Analysis Time Report T	C Analyst Name Reporter Name Batch State Quant Report Version Sample Name	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	You can also click Delete > Table Columns in the Cells group in the Home ta in the Ribbon.
Quantitation Results (Compound D SampleD Compound D SampleD Compound D CMD:EndRepeat Compound D			In the shortcut menu, click the command Delete > Table Columns.
options Design-Sum gure 28 Deletin	mary ⊕ g the <b>Positio</b> r	Image: Second	
Test the changes to	the template.	b Click Browse. part of the N	Report command is lassHunter toolbar in <b>nter Reporting</b> tab in

g Find the Sequence Table. The Sample Name column and the Volume column are adjacent.

Task 2. Delete a column from a table

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

Step	Det	tailed	instruct	ions		Comments		
🚺 🗄 S- 0	:	iii_1_Custor	n_ISTD_Sun	nmary - Excel			? 🗉 – 🗆 X	
FILE HOME IN	SERT PAGE LAYOUT F	ORMULAS DATA	REVIEV	V VIEW	MassHunter Reporting	ADD-INS	- 0	
Process Clear Add A Report Results Data Gra	phics Formatting Properties D MassHunter Reporting							
A1 • : :	X 🗸 🏂 Batch Dat	a Path					*	
2 Analysis Time 3 Report Time	10/10/2012 9:51 AM R 3/8/2012 11:58 AM B	amples\QQQ\DrugsOf nalyst Name eporter Name atch State uant Report Version	QuantSW QuantSW Processed	test-PC\admin test-PC\admin	ysOfAbuseDemo.batch.bin			The Position column is no longer included in this table in the report.
7 Sequence Table	c . I.N.							
8 Acquisition File 9 CMAMBIk_01.d	Sample Name Blank-1	Inj Vo		Sample Typ Blank	e Acq Method File APCIautotune.m			
10 CMAMCal_L1.d	Calib-L1	5		Calibration	APCIautotune.m			
11 CMAMCal L2.d	Calib-L2			Calibration	APCIautotune.m			
	Calb-L3			Calibration	APCIautotune.m			
	Calib-L4	5		Calibration	APCIautotune.m			
	Calib-L5	-		Calibration	APCIautotune.m			
	QC-L2	5		QC	APCIautotune.m			
16 CMAMQC_L4.d	QC-L4	5		QC.	APCIautotune.m			
17 CMAMSam_01.d	Sample-1	5	5	Sample	APCIautotune.m			
18 CMAMSam_02.d	Sample-2	5	5	Sample	APCIautotune.m			
19 CMAMSam_03.d	bampie-b		,	Sample	APCIautotune.m			
⊃∩ ∢ → Summa	ary (+)			: 4				
	-							

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

4	Save the changes to the template
	<ul> <li>You have to clear the results</li> </ul>
	first.

- You save the template to the new name, iii\_2\_Custom\_ ISTD\_Summary.
- te. a Click Clear Results in the MassHunter The Save as type is Excel Template. Reporting tab in the Ribbon.
  - **b** Click **File > Save As**.

  - d Verify the folder selected in **Save in** is correct.
  - e Click Save.

## 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

St	ep	Detailed instructions	Comments <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>	
1	Open the Quantitative Analysis template C:\MassHunter\Report Templates\Quant\en-US\Letter\ ISTD\Results_NoGraphics\ iii_2_Custom_ISTD_Summary.	<ul> <li>Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template,</li> <li>iii_2_Custom_ISTD_Summary, where "iii" are your initials.</li> </ul>		
2	Change the width of the <b>Level</b> column to 10.	<ul> <li>a Find the table labeled Sequence Table.</li> <li>b Click the cell containing the word Level. This is the fifth column in the table.</li> </ul>		
Þ				
	FILE HOME INSERT PAGELAYOUT FORMULAS DATA	REVIEW VIEW Markhunker Reporting ADD-INS DESIGN	Changing the width of an entire column in Excel does not change the width of the	
E	8 🔻 : 🗙 🗸 $f_{\rm x}$ Level	•	<ul> <li>column in a table.</li> </ul>	
1 2 3 4	Last Calib Update Batch State	D E F G H	Click the Level column in the	
567		rsion	Sequence Table.	
9 10	SampleID  Acquisition File  Sample Sample Name	Inj      Level      Sample Type      Acq Method File      SamplePositit      Ti		
111111	2 Quantitation Results			
1	4 SampleID  CompoundID  CompoundType	v Formula v Name v RetentionTime v		
18	SampleID CompoundID ISTDCompoundID	Target Compound PealdD Compound Data File Compound I ISTD V		
17				
17 18 18	CMD:EndRepeat CompoundID			

Figure 30 Selecting the Level column in Excel

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

ep	Detailed instructions	Comments	
	<ul> <li>c Click Advanced Properties in the MassHunter Reporting tab in the Ribbon.</li> <li>d Type 10 in the Text width box.</li> <li>e Click Close.</li> <li>f Move the cursor over the Level column header to see the comment that has been added to this column.</li> </ul>	<ul> <li>The Advanced Properties dialog box allows you to change the table in many different ways.</li> <li>Any changes that you make in this dialog box take effect immediately. You can make many changes before closing this dialog box.</li> </ul>	
Vanced Properties  Table properties  Associate with the following table or graphics  Hide header row Hide table body Hide empty cels Hide empty cels Columns C	Table column properties     Filter       Column     Width     Properties       SampleID     Hidden       Acquisition File     22.0       Sample Name     20       In Vol     10       Sample Name     20       Sample Name     20       Sample Name     20       Sample Name     20       Sample Name     10       Sample Position     Hidden       ✓ Text     Text width 10	You can specify a column width for each column in a table. Several columns already have the width entered.	
Combine table rows starting at column Copy rows x times across page Copy cove x times across page Copy rows x times across page Copy cove  Continue graphics layout Continue graphics across the page	C Graphic Graphic size relative to page width C Grambic Graphic size relative to page width C Formula Preset graphics row height C Hidden C Hidden Column sost order Uncosted  C Ascending C Descending Filter value Set Filter	Type the new column width for the selected column here.	

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

Figure 31 Changing the width of the Level column

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

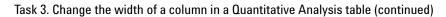
Step	Detailed instructions	Comments
🕅 🖬 S' ở' Ŧ	iii_2_Custom_ISTD_Summary - Excel	TABLE ? 🗉 — 🗆 🗙
Report Results Data Graphics Formatting Pr MassHunter Report	dvanced Validate About Help porties Design	A Width comment has been added to the Level column. The Report Designer add-in reads these comments when the report is being processed and adjusts the width of the column automatically.
o         p           0         Sequence Table           8         Sequence Table           10         Acquisition File           10         Compared to the sequence of the seque	Sample Name     Inj      Level     Se     Writh(10)     Se     Virith(10)     Se     Virith(10)     Se     Se     Virith(10)     Se     Se     Virith(10)     Se     Se     Virith(10)     Se     Se	File SamplePosts TreyNar 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.

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

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

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

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



correct. e Click Save.

Step			Detail	ed instr	uctions		Comme	ents
Process Clear Add	NSERT PAGE LAYOUT	FORMULAS D	REVI	ummary - Excel EW VIEW	MassHunter Reporting	a ? 2NI-DDA	× - •	
A1 • I Batch Data Path 2 Analysis Time 3 Report Time 4 Last Calib Update	K     K	Data Path C htExamples\QQQ\Dr. Analyst Name Reporter Name Batch State	QuantS	Wtest-PCladmin Wtest-PCladmin		G H	×	The width of this column in
Quant Batch Version           Sequence Table           Acquisition File           (CMAY86, Ol.d)           (CMAY61, I.d.d)           (CMAY61, I.d.d)           (CMAY62, I.d.d)           (CMAY62, I.d.d)           (CMAY62, I.d.d)           (CMAY63, Ol.d)           (CMAY64, Ol.d)	n B.05.01 Blark-1 Calb-1 Calb-1 Calb-12 Calb-13 Calb-14 Calb-15 QC-14 Sample-1 Sample-2 Sample-3	Quant Report Ve	nj Vol Leve 5 L1 5 L2 5 L3 5 L4 5 L5 5 L4 5 L2 5 L4 5 L5 5 L4 5 5 5	•	pe Acq Method File APClautoture.m APClautoture.m APClautoture.m APClautoture.m APClautoture.m APClautoture.m APClautoture.m APClautoture.m APClautoture.m APClautoture.m			the table is slightly wider.
∢ → Summ		naes in th	ne widt	ा जा h of the	e column afti	er using the <b>I</b>	Process F	Report command
Save the ch	anges to the to m_ISTD_Sum to clear the re	emplate <b>mary.</b>	a Clia Re b Clia c Int ii	ck Clear porting t ck File > the Save i_3_Cu		e MassHunter bon. k, type Summary.		Save as type is Excel Template

## Task 4. Move a column in a table

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

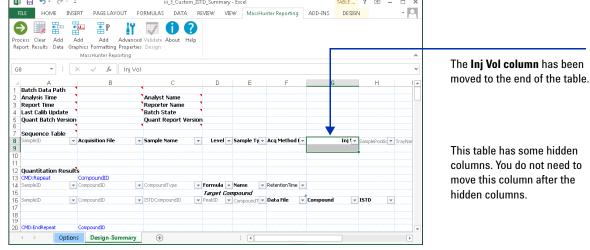
tep		Detailed instructions Comments
template Template ISTD\Re	e Quantitative Analysis \MassHunter\Report es\Quant\en-US\Letter esults_NoGraphics\ stom_ISTD_Summary.	<ul> <li>Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, iii_3_Custom_ISTD_Summary, where "iii" are your initials.</li> <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>
end of th • Move t	the cursor to the edge of Il until it changes to the	<ul> <li>a Find the table labeled Sequence Table.</li> <li>b Click the cell containing the word Inj Vol. This column is the fourth 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>* The shape of the cursor changes depending upon where the cursor pointing.</li> </ul>
FILE HOME		Sustom JSTD_Summary - Excel TABLE ? I - X ATA REVIEW VIEW MassHunter Reporting ADD-INS DESIGN -
FILE HOME	INSERT PAGE LAYOUT FORMULAS D	ATA REVIEW VIEW MassHunter Reporting ADD-INS DESIGN
FILE HOME	INSERT PAGE LAYOUT FORMULAS D	ATA     REVIEW     VIEW     MassHunter Reporting     ADD-INS     DESIGN     ►       ••     ●     ●     ●     ●     ●     ●     ●       ••     ●     ●     ●     ●     ●     ●     ●       ••     ●     ●     ●     ●     ●     ●     ●       ••     ●     ●     ●     ●     ●     ●       ••     ●     ●     ●     ●     ●       ••     ●     ●     ●     ●     ●       ••     ●     ●     ●     ●     ●

Figure 34 Selecting the Inj Vol column in the Sequence Table

Task 4. Move a column in a table

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

Step	Detailed instructions	Comments
	<ul> <li>d Click and drag the cursor to the end of the table. You only move a column within the same table. As you drag the cursor, you can see where the column would be placed. The location between the columns changes to a hatched line. Release the mouse button when the hatched line appears between two cells.</li> <li>e Release the cursor at the end of the table.</li> </ul>	<ul> <li>If you try to move the column outside of the table, the cursor changes to outline the cell where the column would be placed. If you release the mouse button when the cursor is not within the same table, two things happen. First, the label of the cell is placed in the new location. Second, the label of the column in the table is changed. You cannot undo this action. You have to rename the cell in the table and also delete the cell that was added.</li> </ul>
K → ↔ ↔ ↔	iii_3_Custom_JSTD_Summary - Excel TABLE ? I — DUT FORMULAS DATA REVIEW VIEW MassHunter Reporting ADD-INS DESIGN	





Step	Detailed instructions	Comments	
<b>3</b> Test the changes to the template.	<ul> <li>a Click Process Report.</li> <li>b Click Browse.</li> <li>c Move to the \MassHunter\Data\ 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 InjVol.</li> </ul>	<ul> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in the Ribbon.</li> </ul>	

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

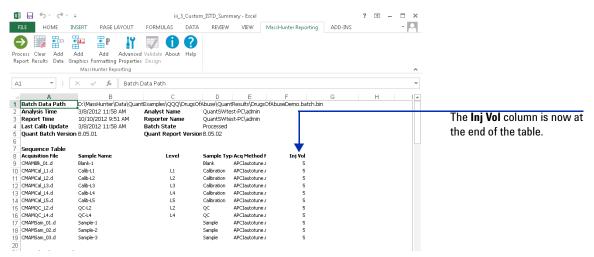


Figure 36 Verifying changes in the column header after using the Process Report command

4 Save the changes to the template iii_4_Custom_ISTD_Summary.	а	Click <b>Clear Results</b> in the <b>MassHunter</b> <b>Reporting</b> tab in the Ribbon.	•	The <b>Save as type</b> is <b>Excel Template</b> .
<ul> <li>You have to clear the results</li> </ul>	b	Click File > Save As.		
first.	C	In the Save As dialog box, type		
		iii_4_Custom_ISTD_Summary.		
	d	Verify the folder selected in Save in is		
		correct.		
	е	Click Save.		

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	column to	) a	Quantitative	Analy	sis table
---------	-------	-----------	-----	--------------	-------	-----------

S	tep	Detailed instructions	Comments	
1	Open the Quantitative Analysis template \ <b>MassHunter\Report</b> <b>Templates\Quant\en-US\Letter\</b> ISTD\Results_NoGraphics\ iii_4_Custom_ISTD_Summary.	Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, iii_4_Custom_ISTD_Summary, where "iii" are your initials.	<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>	
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>	<ul> <li>a Find the table labeled Sequence Table.</li> <li>b Click the cell containing the words Acquisition File. This column is the second column in the table.</li> </ul>	<ul> <li>The Data File column was renamed to Acquisition File in "Task 1. Rename a column header in a table" on page 51.</li> </ul>	

x∎	₽ 5· ¢	<del>-</del>			iii_4_Custorr	_ISTD_Sumi	nary - E	<cel< th=""><th></th><th></th><th>TABLE</th><th>? 📧 –</th><th></th><th>×</th></cel<>			TABLE	? 📧 –		×
FI	ILE HOME	INSERT	PAGE LAYOUT	FORMULAS	DATA	REVIEW	VIEW	MassHu	inter Reporting	ADD-INS	DESIGN		- 0	4
Ę	) 💷 🖶				00									
	cess Clear Add ort Results Data		Add Advani s Formatting Proper assHunter Reporting	ties Design	About He	lp								
B8	<b>*</b> :	$\times$		uisition File	2									•
al	А		в		С	D		Е	F	G		н	l i	
1	Batch Data Path													
	Analysis Time	1		`Analyst		1								Click this cell in the Sequen
	Report Time			Report										Click this cell in the Sequen
	Last Calib Updat			Batch S										Table.
	Quant Batch Vei	sion		Quant I	Report Ver	sion								Table.
6														
	Sequence Table SampleID	- 00	quisition File	✓ Sample	Name	- Lev	ol _ 6 a	mole Tr -	Acg Method I	_	Ini!-	SamplePositic 🔻	7	
9	Dampiero		quisición i ne	* Sample	Hame	re4	ci 👔 30	inpie i y •	Acq Hechodi		Tul L	sampiePosiciq *	Trayivar	
10														
11														
12	Quantitation Re	sults												
13	CMD:Repeat	Co	mpoundID											
	SampleID	▼ Co	mpoundID	▼ Compoun	idType	- Formul	a 🔻 Na	me 🔻	RetentionTime	-				
15							Comp							
	SampleID	✓ Co	npoundID	▼ ISTDCom	poundID	▼ PeakID	▼ Co	mpoundT 💌	Data File	<ul> <li>Compound</li> </ul>	- J	ISTD 🔻		
17														
18														
19														

Figure 37 Selecting the Acquisition File cell in Excel

Task 5. Add a column to a table

Step	<b>Detailed instructions</b>	Comments
	c Right-click this cell and click Ins Table columns to the left.	<ul> <li>You click the column to the right of the location where you want to add a column.</li> </ul>
III III IIIIIIIIIIIIIIIIIIIIIIIIIIIII	mc.DF Summing-the-Eost INBU-Food EXEM VEW Mass-Interc Reporting EXELOPER DESIZON	Click this command. The new column is added to t
9         K         Cd.           9         Fig. Corp.         Fig. Corp.           12         Quantification Result.         Parts Option:           13         Orderate:         Parts Option:           14         Orderate:         Orderate:           15         Orderate:         Parts Option:           16         Orderate:         Parts Option:	pet to pound	M N O P
Coptions Design Summary		

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

- d Follow the instructions in "Task 1. Rename a column header in a table" on page 51 to rename the column to **Location**.
- e Type = "Laboratory 1" in the cell directly below the cell Location.
- f Select the cell **Location**. Right-click the cell and click the **B** icon and click the **A** icon in the shortcut menu.
- To add a word to a table, you first type = and then type the words inside of quotation marks. You are actually entering a simple formula.
- Headers in a table are black and bold.
- You can also change the font by using the icons in the **Font** group in the **Home** tab in the **Ribbon**.

Task 5. Add a column to a table

tep		Detailed instructions	Con	nments
FILE HOME INSERT PAGE LAV Ocess Clear Add Add Add Apport Results Data Graphics Formatting MassHunter Rej	Advanced Validate About Hei g Properties Design	ISTD_Summary - Excei REVIEW VIEW MassHunter Reporting ADD-INS P	DESIGN	You can also use the icons in the Font group.
B A B Batch Data Path Analysis Time Last Calib Update Quant Batch Version Laborstory 1 Quantitation Results	B I = 2 A · · · · · · · · · · · · · · · · · ·	D E F C	3 H I A	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.
CMD:Repeat Comfecuents SampletD CompoundID SampletD CompoundID CMD:EndRepeat CompoundID GMD:EndRepeat CompoundID	Paste Special Paste	vula Vame v Retention Time v ret Compound D v compound v Data File v compound ) he Location column header		="Laboratory 1" is added to this cell.
Test the changes to	the template.	<ul> <li>a Click Process Report.</li> <li>b Click the Browse button.</li> <li>c Move to the \MassHunte DrugsOfAbuse\QuantRep DrugsOfAbuseDemo folde</li> <li>d Select report.results.xml.</li> <li>e Click Open.</li> <li>f Click OK.</li> <li>g Find the Sequence Table. To column is now Location.</li> </ul>	p r\Data\ ti ports\ ti er.	he Process Report command is art of the MassHunter toolbar in he <b>MassHunter Reporting</b> tab in he Ribbon.

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

Task 5. Add a column to a table

itep	Detailed instructions	Comments
FLE     HOME     INSERT     PAGE LAVOI       Image: State of the stat	reed Validate About Help refes Design	
A B	tch Data Path  C D E F G QuantExamples(QQQ)DrugsOfAbuseDemo.batch.bin Analyst Name QuantSWtest-PC.ddmin Reporter Name QuantSWtest-PC.admin Batch fistate Processed Quant Report VersionB.05.02	The first column is now Location.
O         Sequence Table           6         Location         Acquisition File           1         Laboratory 1         CHAMBL_D1.d           10         Laboratory 1         CHAMBL_D1.d           11         Laboratory 1         CHAMCal_L1.d           12         Laboratory 1         CHAMCal_L3.d           13         Laboratory 1         CHAMCal_L3.d           14         Laboratory 1         CHAMCal_L3.d           15         Laboratory 1         CHAMCal_L3.d           16         Laboratory 1         CHAMCal_L4.d           16         Laboratory 1         CHAMGC_L4.d           16         Laboratory 1         CHAMSam_D1.d           16         Laboratory 1         CHAMSam_D2.d           19         Laboratory 1         CHAMSam_D3.d           19         Laboratory 1         CHAMSam_D3.d	Sample Name         Level         Sample Type Acq Method File           Blank:         APCLastotune.m           Calb-L1         L1         Calbration           Calb-L2         L2         Calbration           Calb-L3         L3         Calbration           Calb-L4         L4         Calbration           Calb-L5         L5         Calbration           Calb-L4         L4         Calbration           QC-L2         L2         QC           QC-L4         L4         QC           Sample-1         Sample         APCLastotune.m           Sample-2         Sample         APCLastotune.m           Sample-3         Sample         APCLastotune.m	When you <b>Clear Results</b> , the formula <b>= "Laboratory 1</b> " is not visible. However, it is sti used whenever you process the report.
igure 40 Verifying a Save the changes to the iii_5_Custom_ISTD_Su • You have to clear the first.	mmary. <b>Reporting</b> tab in the Ribbon.	De mary.

Agilent MassHunter Workstation Software Reporting Familiarization Guide

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	l column to a	Quantitative A	nalysis table
--	----------------------	---------------	----------------	---------------

Step	Detailed instructions	Comments			
1 Open the Quantitative Analysis template \MassHunter\Report Templates\Quant\en-US\Letter\ ISTD\Results_NoGraphics\ iii_5_Custom_ISTD_Summary.	Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, iii_5_Custom_ISTD_Summary, where "iii" are your initials.	<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>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 File &gt; Options &gt; Customize Ribbon.</li> <li>b Under Main tabs, mark Developer.</li> <li>c Click OK.</li> </ul>			
Image: Second Macro     Image: Second Macro       Imag	erties Code Source 22 Expansion Packs & Export XAIL E F G XML Source XML source XML source XML source XML source XML source	if the <b>Developer</b> tab in the Ribbon is visible, you can also click the <b>Source</b> icon in the XML			
	Inj v Level Sample Type     Type	spike ate Source. You can right-click any mapped cell to select this command. dTimeStamp webigin ubtraction			

Figure 41 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 (continued)

Step				Detailed in	nstructions			Comments			
}	end of the • Hint: clic Sequence	lumn <b>Barcode</b> Sequence Tabl :k two items in :e Table to iden section of the X	e. the tify the	b Click th	e table labele e <b>Acquisitio</b> e <b>Level</b> colu	n File col		the table XML So If the ele Bold let mapped Element	click the mapped columns in e, the list of elements in the urce window also changes. ement in the list is shown in ters, that item is already or used in the worksheet. ts in the same map cannot more than once.		
X			iii_5_ ORMULAS DATA	Custom_ISTD_Summary REVIEW VIEW M		DEVELOPER AD	TABLE 2		When you click the Level		
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	A Batch Data Path	В	С	D	E F	G 🔺		×	nightighted.		
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7 8 9	Sequence Table	▼ Location	<ul> <li>Acquisition File</li> </ul>	▼ Sample N ▼	evel 👻 Sample Type	- Acq Method		Expected Barcode Graphic Sample CR Injections Per Posit Injector Volume	<b>ns1:</b> is part of the syntax o		
11							- 🗐 nsl	:InstrumentName	the element in the <b>XML</b>		
	Quantitation Resu CMD:Repeat	ult's CompoundID						strumentType ISTDDilution	Source window. Every iten		
4			<ul> <li>CompoundType</li> </ul>	🔻 Formula 👻 Nam		•	🗐 ns1	:LevelName	in the XML Source window		
56	SampleID	▼ CompoundID	▼ ISTDCompoundID	Target Compou		- Compound	<	I orked			
7		pouroace			ourse plant back the	Suboard	To map repeating e elements from the		starts with <b>ns1:.</b>		
18							worksheet where y headings to appea	ou want the data			
10 19	CMD:EndRepeat	CompoundID									
19 20							To import XML data mapped cell, point	, right click an XML to XML, and then click			
19 20 21 22							Import				
19 20 21							Import.	IL Maps			

Figure 42 Selecting the Level column in Excel

Task 6. Add a mapped column to a table

Step	Detailed instructions	Comments
	<ul> <li>d Scroll until the column after the end of the Sequence Table is visible.</li> <li>e In the XML Source window, scroll up to display the element ns1:Barcode.</li> <li>f Click and drag the element ns1:Barcode to the cell that is next to the Vial column.</li> <li>g Click the cell Barcode.</li> <li>h Right-click the cell and click the B icon in the shortcut menu.</li> </ul>	<ul> <li>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.</li> <li>If you drag the element to a location that is not at the end of the table, ar error is displayed. Right-click this column and click <b>Delete &gt; Table Columns</b> to remove the column. Then, click and drag the element again to the end of the table.</li> </ul>

FILE HO	ME INSER Record Ma Use Relativ Macro Secu Code	cro e References A urity	OUT FORMU	LAS DATA	5_Custom_IST REVIEW Properties Q View Code Run Dialog rols	VIEW	y - Excel MassHunter R Map Propert Expansion P Refresh Data XML	ties 📑 Impor acks 🔍 Export			When you click a column in a table the Table Tools Design tab is added to the
E 1 2 3 4 5 5 6 7 8 4 Level 9 0 1	F Sample Typ	G		H I	ysib TrayNar	J ne 💌	K Vial V	L Barcode V		XML Source XML maps in this workbook: QuantitationDatsEt Map ns15AcqDateTime ns15AcqDateTime ns12AcqDateTime ns12AcqDetationame ns12AcqDeta	<ul> <li>Ribbon. You can change the Table</li> <li>Style using this group.</li> </ul>
2 3	r RetentionTim	5 v v Compound	v ISTD	Y	Re	ISTD Re	Resp Ra 👻	Final Cc ≠	E	In L3arcode     nol.CalibrationReferenceSample     nol.Comment     nol.Comment     nortComment     mortComment     mortCo	column is added after the Vial column. You can

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

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

Task 6. Add a mapped column to a table

Step	Detailed instructions	Comments
Test the changes to the template.	<ul> <li>a Click Process Report.</li> <li>b Click the Browse button.</li> <li>c Move to the \MassHunter\Data\ 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.</li> <li>h Scroll to the end of the Sequence Table. The Barcode column is now the last column in the Sequence Table.</li> </ul>	<ul> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in the Ribbon.</li> </ul>
FILE     HOME     INSERT     PAGE LAYOUT     FORMULAS     DATA     F       Process     East     Eas	gsOfAbuseQuantResults)DrugsOfAbuseDemo.batch.bin QuantSWtest-PC\admin QuantSWtest-PC\admin Processed	
ELE     HOME     INSERT     PAGE LAYOUT     FORMULAS     DATA     F       Process     Clear     Add     Add     Advanced Validate     About     H       Process     Clear     Add     Add     Advanced Validate     About     H       Image: Add     Add     Add     Advanced Validate     C     C       Image: Add     Add     Advanced Validate     Amagee     C     C       Image: Add     Add     Add     Advanced Validate     Amagee     C       Image: Add     Add     Add     Advanced Validate     Amagee     Amagee       Image: Add     Add     Add     Add     Advanced Validate     Amagee       Image: Add     Add     Advance	EVIEW VIEW MassHunter Reporting DEVELOPER ADD-INS	The last column in the Sequence Table is now the Barcode column.

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

- You have to clear the results first.
- b Click File > Save As.
  c In the Save As dialog box, type
  - iii\_6\_Custom\_ISTD\_Summary.
- d Verify the folder selected in **Save in** is correct.
- e Click Save.

Task 6. Add a mapped column to a table

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

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

# Task 7. Add a filter to a table

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

<ul> <li>template \MassHunter\Report Templates\Quant\en-US\Letter\ ISTD\Results_NoGraphics\ iii_6_Custom_ISTD_Summary.</li> <li>Add a filter to the Quantitation Results table using the Advanced Properties dialog box.</li> <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> <li>Find the second table in the section Quantitation Results.</li> <li>Click Advanced Properties.</li> <li>From the Table tab, select NonBlanks in the Filter value box when the Exp Conc column is selected.</li> <li>Click Set Filter.         <ul> <li>Click Close.</li> </ul> </li> </ul>		Detailed instructions	Comments
Results table using the Advanced Properties dialog box. • Only include data files that have an expected concentration. • Click Advanced Properties. • Click Advanced Properties. • Click Advanced Properties. • Click Advanced Properties. • Click Set Filter. • Click Set Filter. • Click Close. • Click Close.	ate \MassHunter\Report ates\Quant\en-US\Letter\ Results_NoGraphics\	Open a Quantitative Analysis Excel template" on page 40 to open the template, iii_6_Custom_ISTD_Summary, where	<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>
Advanced Properties Template   Design Worksheet   Cell Table    Table properties Associate with the following table or graphics Hide header row Hide table body Table control transposed to column in the Table column in the Tabl	ts table using the Advanced erties dialog box. ly include data files that have expected concentration.	<ul> <li>Quantitation Results.</li> <li>b Click the column labeled Exp Conc This column is column M in the table.</li> <li>c Click Advanced Properties.</li> <li>d From the Table tab, select NonBlanks in the Filter value box when the Exp Conc column is selected.</li> <li>e Click Set Filter.</li> </ul>	<ul> <li>The Advanced Properties icon is part of the MassHunter toolbar in the MassHunter Reporting tab in the Ribbon.</li> </ul>
Template   Design Worksheet   Cell Table   Column in the Table colum Properties Associate with the following table or graphics Hide header row Hide table body Table columns in the Table column properties Filter Column in the Table column Properties STD 12.5 Compound 12.5 STD 2 15TD 2 15			_ The filter is shown in the Filter
Table codum repretes Filter  Table rooking table or graphics  Hde header row  Hde header row  Column  Table codum properties			column in the Table column
Associate with the following table or graphics     Column     With Properties     Filter     FIOPELLIES IISL.       Hide header row     Data File     12.5     Data File     Properties       Hide table body     ISTD     ISTD     Properties			1
Hide header row     Compound 12.5     IST0     Hide table body     IST0     Resp     IST0     Table codet the supposed to     columns     IST0 Resp     IST0	sign Worksheet   Cell Table	n properties	
Table context transport to columns ISTO Resp ISTO	sign Worksheet   Cell Table   Titles Table column with the following table or graphics Column	Width Properties Filter	Properties list.
	sign Worksheet   Cell Table   Table colum tities with the following table or graphics der row	Width Properties Filter	Properties list.
Resp Ratio	sign Worksheet   Cell Table   Table column  vints the following table or graphics  for row  s body	Width Properties Filter	Properties list.
Even Const ANOVELANIZES	sign Worksheet   Cell Table   Table column tites with the following table or graphics der row body tents transposed to columns tents transposed to columns	Width Properties Filter	Properties list.
Text width	aign Worksheet   Cell Table   Table column trites with the following table or graphics der row body body retris transposed to pty cells	Width Properties Filter	Properties list.
Combine table rows starting at column 1 Graphic Size relative to page with Height	sign Worksheet   Cell Table   Table column Column Column Columns body tents transposed to columns phy cells mms across page 2 columns	Width Properties Filter	Properties list.
Copy rows x times across page 2 C Formula Preset graphics row height	sign Worksheet   Cell Table   Table column switch the following table or graphics ser row s body terts transposed to pty cells mins across page 2 columns table rows starting at column 1 Table column Column Compound STD Resp ISTD Resp ISTD Resp Columns Compound ISTD Resp ISTD Resp Columns Compound ISTD Resp ISTD Resp	Width Properties Filter	Properties list.
Use sper-header C Hidden Select NonBlanks as th	sign Worksheet   Cell Table   Trites	Width Properties Filter	Properties list.
	sign Worksheet Cell Table Table Columns view the following table or graphics der row body texts transposed to columns body texts transposed to columns unns across page 2 columns table rows starting at column 1 columns colu	Width Properties Filter	
Column sort order Unsorted C Ascending	sign Worksheet   Cell Table   Table column with the following table or graphics der row a body terts transposed to columns by cols mms across page 2 columns table rows starting at column 1 out columns	Width Properties Filter	Select NonBlanks as the Filter Value and then click Set Filter.

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

Task 7. Add a filter to a table

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 the arrow in the cell labeled Acquisition File. This column is column C in the table.</li> <li>c Open the list, and click Text Filters &gt; Contains. The Custom AutoFilter 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>	

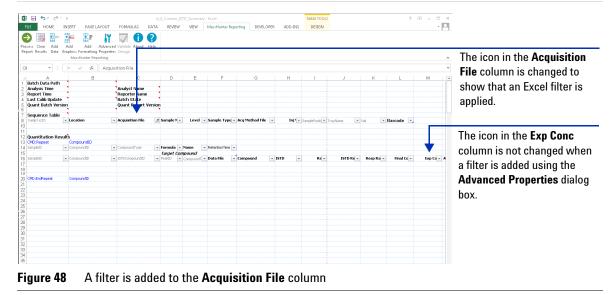
×∎	5.0.	÷			iii_6_C	ustom_ISTD_	Summary	- Excel			TABLE	? 📧	- 0	×	
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C8	· :	$\times$	√ <i>f</i> <sub>x</sub> Acquis	ition File										~	and click <b>Text Filters</b> >
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18 19			Search		P	Does	<u>N</u> ot Equal						i 1	-	
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Figure 46Add a filter to the Sequence Table using Excel features

- **d** Type Cal in the first text field.
- e Click Or.
- $f \quad \text{Select } \textbf{contains} \text{ in the second box.}$
- **g** Type Blk in the second text field.
- h Click OK.

Step	Detailed instructions	Comments
Custom AutoFilter	In this example, only file na <b>Cal</b> or <b>Blk</b> are included.	ames that include the letters
Use ? to represent any single character Use * to represent any series of characters OK Cancel		





Task 7. Add a filter to a table

Step	Detailed instructions	Comments		
4 Test the changes to the template.	<ul> <li>a Click Process Report.</li> <li>b Click the Browse button.</li> <li>c Move to the \MassHunter\Data\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 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 MassHunter Reporting tab in the Ribbon.</li> </ul>		

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	Massmunder Reporting					^	Sequence Table contained 11
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A	в	с	DE	E	G	H	rows. Each Acquisition File
1 Batch Data Path	D:\MassHunter\Data\Quar			rugsOfAbuseDemo.batch			contains either Cal or Blk in
2 Analysis Time	3/8/2012 11:58 AM	Analyst Name	QuantSWtest-PC\adr	nin			
3 Report Time	10/10/2012 9:51 AM	Reporter Name	QuantSWtest-PC\adr	nin			the name.
4 Last Calib Update	3/8/2012 11:58 AM	Batch State	Processed				
5 Quant Batch Versio	n B.05.01	Quant Report Versio	nB.05.02				
6							
7 Sequence Table							
8 Location	Acquisition File	Sample Name		Type Acq Method File	Inj Vol Baro	code	
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13	CMAMCal_L4.d	Calib-L4	L4 Calibratio			ode12345678901234	
14	CMAMCal_L5.d	Calib-L5	L5 Calibratio	n APCIautotune.m	5 BarCo	ode12356778901234567	
15							
16 Quantitation Resu							
17 Target Compound	Amp						
18 Data File	Compound	ISTD	Resp ISTD			Exp Conc Accuracy	
19 CMAMCal_L1.d	Amp	Amp-d5	658	1397 0.4708	3.3187	2.5000 132.75	
20 CMAMCal_L2.d	Amp	Amp-d5	1059	1298 0.8157	5.7493	5.0000 114.99	
21 CMAMCal_L3.d	Amp	Amp-d5	2673	1377 1.9409	13.6808	12.5000 109.45	
Figure 49	Verifying cha	nnes in the	rows that	are included	l in the filte	ered tables	
i igui e to	vernying end	inges in the	iowo that				

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

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

# 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\en-US\Letter\ ISTD\Results_NoGraphics\ iii_7_Custom_ISTD_Summary.	<ul> <li>Follow the instructions in "Task 4.</li> <li>Open a Quantitative Analysis Excel template" on page 40 to open the template,</li> <li>iii_7_Custom_ISTD_Summary, where</li> <li>"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>2 Delete the Inj Vol 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 Inj Vol and the cell beneath it. This column is column H in the table.</li> <li>c Right-click the Inj Vol 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 Inj Vol.</li> <li>e Right-click the Inj Vol 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 column K 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 move the column between two columns. 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

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

tep	Detailed instructions							Comments			
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Quant Batch Vers	ion	Quant Report V	ersion								Barcode column, Excel
Sequence Table	•										1 A.1
SampleID	<ul> <li>Location</li> </ul>	<ul> <li>Acquisition File</li> </ul>	JT Sample N -	Level	Sample Type	<ul> <li>Acq Method File</li> </ul>	▼ SamplePo	ibic 💌 TrayName 🚺 🚺	Barcode		shows you this error or a
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6											
7											
<ul> <li>Opt</li> </ul>	tions Design-Summ	nary (+)								F.	

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

Figure 50 A filter is added to the Acquisition File column

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

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

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

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

tep	Detailed instructions	Comments
ELE HOME INSERT PAGE LAYOUT FORMULAS DATA	Formatting = Table = Styles = = =	mat Sort & Find &
I X X K Barcode      Barcode      Barcode      Barcode      Analysis film      Report film      Report film      Report film      Sequence Table      Versio      Sequence Table      Versio      Versio	n c c n u i	Remove the filter from the column.
Quantitation Results         I as the second s	Formula v Name v Recensorma v <i>Farget Campound</i> Anado v Campound v Data File v Compound v IstD v Re(v	15TD Rd. – Resp Rd. – Final Cd. –
OD Erdhepax Co Esech P C Esech Ca C Esech Ca C Esech Aug		

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

Figure 51 The filter is removed from the Acquisition File column

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

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8 ▼ ! × ✓ fx Barcode	D E F G	ніј	× K L A	
Batch Data Path Analysis Time Analyst Lam Report Time Reporte Nar Last Calib Update Batch State Quant Batch Version Quant Broom	ne		Т	he <b>Barcode</b> column is now
Sequence Table SompleID V Location Acquisition Fill Duantitation Results	e 🐨 Barcode 💌 Sample Ne 💌 Level 💌 Sample Type	Acq Method     Inj     SamplePosition     Tray	Name 💌 Vial 💌	fter the <b>Acquisition File</b> olumn.
CMD:Repeat CompoundID				
SampleID  CompoundID  CompoundType	v Formula v Name v RetentionTime v			
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CMD:EndRepeat CompoundID				
Options Design-Summary (+)	÷ (		Þ	

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

Figure 52 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 column K 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 column L in the table.
- c Move the cursor to the edge of the cell until the cursor changes to a four-sided arrow, \*\*\*.
- d Click and drag the **Final Conc** column and move it after the **Exp Conc** column.

- 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 61 to move the Final Conc column.

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

tep	Detailed instructions Comments					ents						
FILE HOME	⇒ INSERT PAGE LAYOU	T FORMULAS		Custom_ISTD_Su	ummany - Excel IEW MassHunte	r Reporting DP	VELOPER /	ADD-INS DESI			×	
ste 💉 Tahoma				<b>'rap Text</b> lerge & Center	General \$ = % = Number	Conditio	nal Format as ng * Table * Styles	Cell Styles + Cells	• ↓ ↓ · · · · · · · · · · · · · · · · ·	ort & Find & ilter * Select * Editing	<u>^</u>	
.6 • : : : : : : : : : : : : : : : : : :	C Analyst Name Reporter Name Batch State Quant Report V	•	E	F	G	H	1	J	K		The <b>Barcode</b> colum the Acquisition File	
Location CompoundID CompoundID CompoundID	Acquisition File     CompoundType     ISTDCompoundID	J     Barcode       v     Formula       v     Formula       v     PoskID	Name 💌	RetentionTime	<ul> <li>Sample Type</li> <li>Compound</li> </ul>	v Acq Method v     v     ISTD v	Inj i v Re v	SamplePosition 💌	TrayName 💌 Exp Co 👻	Ţ	The Final Conc colu after the Exp Conc.	ımn is
CompoundID	ons Design-Summa	ıry 🕀				4					¥	

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

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

Test the shanges to the templete	_	Click Presses Penert	• The Presses Penert command is
rest the changes to the template.		•	• The Process Report command is
	b	Click the <b>Browse</b> button.	part of the MassHunter toolbar in
	C	Move to the <b>\MassHunter\Data</b> \	the MassHunter Reporting tab in
		DrugsOfAbuse\QuantReports\	the Ribbon.
		DrugsOfAbuseDemo folder.	
	d	Select report.results.xml.	
	e	Click <b>Open</b> .	
	f	Click <b>OK</b> .	
	g	Find the Sequence Table. The only	
		acquisition files that are included	
		contain either <b>Cal</b> or <b>Blk</b> .	
	h	Find the Quantitation Results table.	
		The only acquisition files that are	
		•	
		the blanks and samples have been	
		removed.	
	Test the changes to the template.	b c d e f g	<ul> <li>b Click the Browse button.</li> <li>c Move to the \MassHunter\Data\ 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</li> </ul>

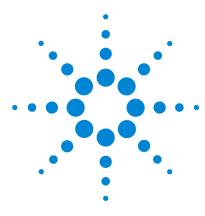
Task 8. Move or delete a column in a filtered table

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

Step	tep Detailed instructions Comme							
Process Clear Add	PAGE LAYOUT FORMUL	Validate About Help		Reporti DEV				
A1 • i A 1 Batch Data Path 2 Analysis Time 3 Report Time 4 Last Calib Update 5 Quant Batch Version 6	B D:\MassHunter\Data\Quar 3/8/2012 11:58 AM 10/10/2012 9:51 AM 3/8/2012 11:58 AM	Rep <mark>o</mark> rter Name	QuantSWtest QuantSWtest Processed	-PC\admin	F DfAbuseDemo.ba	G A	The <b>Barcode</b> column is moved to after the <b>Acquisition File</b> .	
7 Sequence Table 8 Location 9 10	Acquisition File CMAMBIk_01.d CMAMCal_L1.d	BarCode123456	<b>Sample Nan</b> Blank-1 Calib-L1	Level	Sample Type Blank Calibration	Acq Method File APCIautotune.m		
11 12 13 14 15	CMAMCal_L2.d CMAMCal_L3.d CMAMCal_L4.d CMAMCal_L5.d			L2 L3 L4 L5	Calibration Calibration Calibration Calibration	APCIautotune.m APCIautotune.m APCIautotune.m APCIautotune.m	The <b>Final Conc</b> column is moved to after the <b>Exp Conc</b>	
16 Quantitation Result 17 Target Compound 18 Data File 19 CMAMCal_L1.d 20 CMAMCal_L2.d 21 CMAMCal_L3.d 22 CMAMCal_L4.d	ts Argp Compound Amp Amp Amp	ISTD Amp-d5 Amp-d5 Amp-d5 Amp-d5	Resp 658 1059 2673 4952	<b>ISTD Resp</b> 1397 1298 1377 1304	Exp Conc 2.5000 5.0000 12.5000 25.0000	3.318 5.749 13.680	column.	
READY	hary (+)		:	III III	PT	+ 100%		

Figure 54 Verifying that columns are moved in both filtered tables

<ul> <li>7 Save the changes to the template</li> <li>iii_8_Custom_ISTD_Summary.</li> <li>You have to clear the results first.</li> </ul>	b	Click <b>Clear Results</b> in the <b>MassHunter</b> <b>Reporting</b> tab in the Ribbon. Click <b>File &gt; Save As</b> . In the Save As dialog box, type	•	The <b>Save as type</b> is <b>Excel Template</b> .
		<pre>iii_8_Custom_ISTD_Summary. Verify the folder selected in Save in is correct. Click Save.</pre>		



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)93Task 3. Add a formula column to a table96Task 4. Add an ISTD column to a Quantitative Analysis template101Task 5. Add a column that is already mapped105

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

Each exercise is presented in a table with three columns:

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



# Task 1. Add a table to a template

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

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

Task 1.	Add a table to	a Qualitative	Analysis template

S	tep	Detailed instructions	Comments		
1	Open the Qualitative Analysis template, \ <b>MassHunter\Report</b> Templates\Qual\Letter\ iii_CustomAnalysisReport.	Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 30 to open the template, iii_CustomAnalysisReport, where "iii" are your initials.	<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>		
2	<ul> <li>Add a second table to show</li> <li>additional Sample Information.</li> <li>Add the table inside the Repeat section.</li> </ul>	<ul> <li>a Find the first table in the template. The first two items are ItemID and Data Filename.</li> <li>b Click the first cell in row 5. The rows below this row are very narrow.</li> </ul>	<ul> <li>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.</li> </ul>		

Step	ep Detailed instructions Comme				
III 5× ペ× ÷	iii_CustomAnalysisReport1 - E	xcel	? [	⊡ – ⊡ ×	
FILE HOME INSERT PAGE LAYOUT FORMULAS	DATA REVIEW VIEW	MassHunter Reporting	DEVELOPER ADD-INS	- 0	
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Process Clear Add Add Add Advanced Validate Ab	out Help				
Report Results Data Graphics Formatting Properties Design					
MassHunter Reporting				^	
H27 1× √ J×				•	The current position in the
12 A B C	DE	F	G <u>H</u>	×	•
2 CMD:Repeat ItemID 3 ItemID V Data Filenam V Sample Name V Samp	nle Type y Position y In	strument Name 👻 User I	ame - Acq Methoe - Acquired	Time	template is shown here.
4				k	
	7				All of the rows between the
L · V CMD/EndRepeat ItemID					CMD:Repeat row and the
11 CMD:Repeat ItemID					CMD:EndRepeat row are
14 ItemD · ragmentor Yolt · Collision Enerc · Ioniz	ation Mod				•
16 ItemID V PlotFile V					repeated for each ItemID.
18 Integration Peak List					ItemID identifies different
19 ItemID - Peak - Start - RT 20	- End - He	eight 🔄 Area	<ul> <li>Area % Signal To</li> </ul>	Noise	data files.
21 Noise Measurements 22 ItemID - Noise Type - Signal Definiti - Noise	Multiplic - Noise Value				data mes.
23 24 Noise Regions	- Tanapar, Tonice Vulde				
25 TITEMID - Start - End -					
Design Options (+)		•		Þ	
READY III			I II	+ 100%	

Figure 55 Selecting the first cell in row 5

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

Task 1. Add a table to a template

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

Step	p Detailed instructions Comm				
FILE       HOME       INSERT       PAGE LAYOUT       FORMULAS         Image: State of the stat		ssHunter Reporting	DEVELOPER ADI	×	
User Chromatogram Peak Table User Spectrum Peak Table Compound Chromatogram Peak Table Compound Spectrum Peak Table Compound Spectrum Peak Table TitemID Y Formula Column	E • Position • Instrum	F G nent Name 💌 User Na	H M - Acq Metho	Acquired Time	The commands in the <b>Add</b> <b>Data</b> menu are different for the Qualitative Analysis and
CMD-Endlegeeat         2 stanzo	9				Quantitative Analysis Program. Different types of Qualitative Analysis
18 19 ItemID V PlotFile V 20					templates also have differen commands.
21 22 Integration Peak List 23 ItemID - Peak - Start - RT 24	End Height	_ Area	z Area %	Signal To Noise	
25 6 Noise Measurements 27 Itemiti – Noise Type – Signal Definiti – Noise Multi 28 29	pli( - Noise Value -				

### Figure 56 Add a second Sample Information table

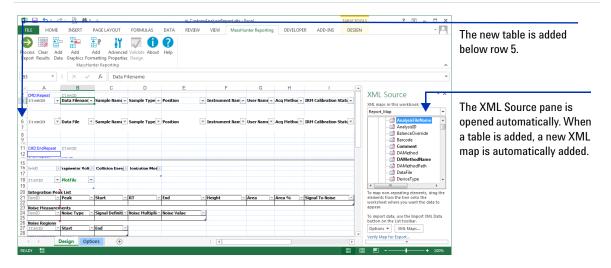


Figure 57 Add a second Sample Information table

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

Step	Detailed instructions	Comments	
<ul> <li>3 Compare the columns in the two tables.</li> <li>The XML Map changes depending on which table you are looking at.</li> <li>The names of some of the columns are different.</li> </ul>	<ul> <li>a Click the Data Filename column in the first table. The XML map is Report_Map.</li> <li>b Click the Data File column in the second table. The XML map is Report_Map1.</li> </ul>	<ul> <li>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.</li> </ul>	

cess Clear	ME INSERT		vance pertie	FORMULAS DATA	RE	VIEW VIEW	MassHunte	r Reporting	DEVELOPER	ADD-INS	DESIGN	· •	
5	• E × 4	f <sub>x</sub>	iamp	e Name								*	
A	В	С		D	Е		F	G	Н	1		XML Source • *	
CMD:Repeat ItemID	TtemID ▼ Data Filenan ▼ Data File	▼ Sample N	в	$\begin{array}{c c} & & & \\ \hline \\ \hline$	• % ‰ ₊	3 💉			Acq Metho( - IR Acq Metho( - IR			XIVIL SOUTCE XML maps in this workbook: Report_Map1	Select the columns that
CMD:EndRepe	eat ItemID		G <sub>B</sub>	Copy Paste Options:								DeviceType     DeviceType     Diution     EquilibTime     InjPosition     InjVol	you want to delete. Right-click and click <b>Delete &gt; Table Columns</b>
ItemID	∵ragmentor ¥o ▼ PlotFile	It Collision	В	Paste <u>Special</u> Refresh <b>Insert</b> Delete	Þ	Table Colum						- 📑 InstrumentN - 📑 IRMStatus - 📑 ItemID 🚰 LevelName	All of the columns that are selected are remove
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ItenID Criptonarcpo	- Start	- End		Filt <u>e</u> r Ta <u>b</u> le XML								SampleName     SampleDactit     To map non-repeating elements,	
ItemID	E Spectrum Sou	ard <sup></sup> raamento	_	Insert Comment	ŕ	lode =						drag the elements from the tree onto the worksheet where you want the data to appear. To import data, use the Import	
ItemID PeakList ItemID	▼ Spectrum	▼ × Z		Pic <u>k</u> From Drop-down List Hyperlink			- Ior		Score (DB) _ Hi	ts (DB)	×	XML Data button on the List toolbar. Options V XML Maps	
 ← →	Design O	ptions	(+)				4			1		Verify Map for Export  7 Tips for mapping XML	

Figure 58 Delete multiple columns in the second Sample Information table

Task 1. Add a table to a template

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

Step	Detailed instructions	Comments	
<ul> <li>Change the second table to include only the following columns: <ul> <li>ItemID</li> <li>Data File</li> <li>Injector Volume</li> <li>Dilution</li> </ul> </li> </ul>	<ul> <li>a Click the Sample Name column in the second table. The XML map is Report_Map1.</li> <li>b Delete all of the columns in the table that are after the Data File column.</li> <li>c Click the Data File column in the second table.</li> <li>d Add the mapped columns, Inj Vol and Dilution.</li> <li>e Rename the Inj Vol column to Injector Volume.</li> </ul>	<ul> <li>You can delete more than one table column at the same time.</li> <li>Follow the instructions in "Task 2. Delete a column from a table" on page 54 to remove the columns.</li> <li>You click one of the items in the table first to make sure that the correct XML map is selected. All or the columns in a table are mapped using the same XML map. The <b>Report_Map1</b> map is selected.</li> <li>Follow the instructions in "Task 6. Add a mapped column to a table" on page 68 to add the columns.</li> <li>Follow the instructions in "Task 1. Rename a column header in a table" on page 51 to rename the columns.</li> </ul>	
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日 ち・ご・ Q 曲・=	iii_CustomAnalysisReport.xltx - Excel	TA	BLE TOOLS	? 🗈 – 🗆 🗙	
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ess Clear Add Add Add Advan <del>ced Valuate About Tield</del>					
Kess Clear Add Add Add Advanced valuate Addd Frep kort Results Data Graphics Formatting Properties Design MassHunter Reporting				^	The Injector Volume
▼ : × ✓ f <sub>x</sub> Dilution				*	and <b>Dilution</b> column
A B C D	E F G	н і	J 🔺		are added to the
CMD:Repeat ItemID	on v Instrument Nam v User Name v A			XML Source 🔹 👻	second table.
ItemID v Data Filenam v Sample Nam v Sample Type v Positie	n v Instrument Nam v User Name v A	cq metho - IRM Calibration Stati	t - DA Meti	XML maps in this workbook:	second table.
				Report_Map1	
ItemID   Data File  Injection Vol  Dilution  ItemID				📑 Barcode 📃	You can change the
				📑 Comment 📑 DAMethod	•
				DAMethod	formatting for each
CMD:EndRepeat ItemID				📑 DAMethodPa 📑 DataFile	column using
A					standard Excel
temD ragmentor Yolt Collision Ener				4 m	Stanuaru Excer
ItemID V PlotFile V				To map non-repeating elements, drag the elements from the tree	features in the Home
				onto the worksheet where you want the data to appear.	tab.
Integration Peak List ItemID - Peak - Start - RT - End	- Height - Area - A	Area % 🔄 Signal To Noise	×	To import data, use the Import	Lab.
(→ Design Options (+)	: 4			XML Data button on the List toolbar.	



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

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

🖾 🖯 ぐ 🗟 緒・ 🗉	iii_CustomAnalysisR	eport.xltx - Excel	? 🖅 — 🗖 🗙	
	RMULAS DATA REVIEW VIEW Mas	sHunter Reporting DEVELOPER ADD-INS	- 0	The first table is transposed
Process Clear Add Add Add Add Advanced Valid Report Results Data Graphics Formatting Properties Desi MassHunter Reporting	date About Help		á	and shows the information next to the column header.
A1 • : × ✓ fx			~	
ABCDEFGHIJKLMI		Z AA AB AC AD AE AF AG AH AI AJ AK AL AM AN A		
3 Sample Type Sample Positi 4 Instrument Name QTOF PP1 User	uple Name I ng sulfas tion P1-F1 Name Calibration Status Success			
8 Diution 1 9 10 11 User Chromatograms				The second Sample
13 14 Fragmentor Voltage 125 Collision Energy 0 Ionization	n Mode ESI			
x10 € +ESI TIC Scan Frag=125.0V sulfas_PosMS.d	1.225			njector Volume and the Dilution.
5- 4- 0.325 3-				
2 0.518			*	

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

<ul> <li>6 Save the changes to the template.</li> <li>You have to clear the results first.</li> <li>You save the template to the new name, iii_1_Custom AnalysisReport.</li> </ul>	<ul> <li>a Click Clear Results in the MassHunte Reporting 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_1_CustomAnalysisReport.</i></li> <li>d Verify the folder selected in Save in is correct.</li> <li>e Click Save.</li> </ul>	1
--	--	---

Task 1. Add a table to a template

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

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

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

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

Step	Detailed instructions	Comments		
1 Open the Qualitative Analysis template, \MassHunter\Report Templates\Qual\Letter\ iii_1_CustomAnalysisReport.	Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 30 to open the template, <i>iii_1_CustomAnalysisReport,</i> where "iii" 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 a column in the second table.</li> <li>b Click Advanced Properties which is part of the MassHunter toolbar in the MassHunter Reporting 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 <b>Table</b> 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 in a Qualitative Analysis template

4

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

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

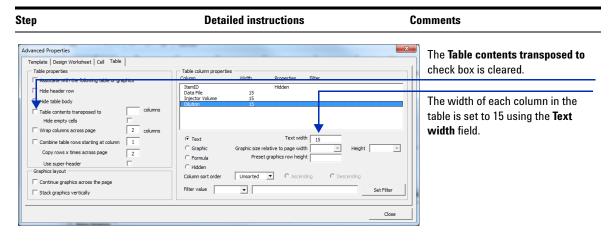


Figure 61 Changing table properties in the Advanced Properties dialog box

- 3 Format the first table.
  - Hide the header row.
- **a** Click a column in the first table.
- **b** Click the Advanced Properties dialog box.
- c Mark the **Hide header row** check box under Table properties.
- d Click Close.
- **4** Test the changes to the template.
- a Click Process Report.
- **b** Click the **Browse** button.
- c Move to the \MassHunter \Reports\Temp folder.
- **d** Double-click one of the folders that contains analysis results.
- e Select Report.xml.
- f Click Open.
- g Click OK.

- 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 MassHunter Reporting tab in the Ribbon.

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

	Task 2. Forr	nat a table in a	Qualitative Ana	lvsis template	(continued)
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Step	Detailed instructions	Comments
	iii.3.CustomAnalysisReportLatto - Escel DATA REVIEW VIEW MassHunterReporting DEVELOPER ADD-INS	×
Process Tear Add Add Add Add Addraced Validate About Report Ruuts Data Graphic Forwarding Properties Design MassHunter Reporting AB25	2   R   S   T   U   V   W   X Y Z   AA <mark>(<u>AB)</u> AC AD AE AF AG AH AI AJ AK AL AMA</mark>	The first table is transposed and the header row is hidden.
4. (COTO PP) 5. Indife, protociny_demo.m 6. Debrakzm 7. Totak File 9. Jaulies_protis_d. 1 10 11. User Chromatograms	1	The second Sample Information table is not transposed. The column
13         Fragmentor Voltage 10* Collision Energy 0         Instantion Mode E8           14         Fragmentor Voltage 10* Collision Energy 0         Instantion Mode E8           15         0         0791         1225           1         0.791         1225         0           1         0.791         1225         0           1         0.791         1225         0           1         0.791         1225         0           1         0.791         0.791         1225           1         0.791         0.791         1225           1         0.791         0.791         1.72           1         0.791         0.791         0.791           1         0.791         0.791         0.791           1         0.791         0.791         0.791           1         0.791         0.791         0.791           1         0.791         0.791         0.791           1.791         0.791         0.791         0.791           1.792         0.791         0.791         0.791           1.792         0.791         0.791         0.791           1.792         0.791         0.791	14 15 16 17 18 19 2	header is above the information.
< → Report READY	: 4	

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

5	Save the changes to the template, iii_ <b>2_CustomAnalysisReport</b> .	а	Click Clear Results in the MassHunter Reporting tab in the Ribbon.	•	The Save as type is Excel Template
	<ul> <li>You have to clear the results</li> </ul>	b	Click the Microsoft Office button and		
	first.		then click Save As and click Other		
			Formats.		
		C	In the Save As dialog box, type		
			<pre>iii_2_CustomAnalysisReport, where "iii" are your initials.</pre>		
		d	Verify the folder selected in Save in is		
			correct.		
		е	Click <b>Save</b> .		

# 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.

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

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

Task 3. Add a formula column to a table

Step	Detailed instructions	C	omments
Home Insert Pane Javout Formula: Data Revi f.x E AutoSum · Polocal · Lookup & Reference · Server & Recently Used · A Text · M Math & Trig ·	Image: Book of the sector         I	edents 📓 🗾 🗐	This tab in the Ribbon helps you add a formula to the table. For information about formulas and functions, see the online Help for Microsoft Excel.
20         20         21         kmD         27         regnerator Votis         Collision Energe         Ionization Mo           23         23         24         ItemID         ♥         PlotFile         25           26         27         Integration Peak List         28         28         29         29           29         29         Peak         ■         Start         RT         29           20         29	End PWFH P		The new column <b>PWFH</b> is to the right of the End column. The Excel comment, <b>Formula</b> is added to this column.

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

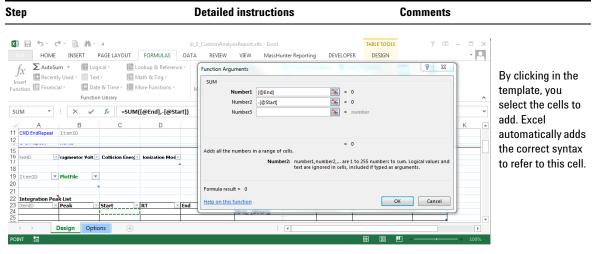


- **g** Click the **Insert Function** button in the Function Library group in the **Formulas** Tab in the Ribbon
- In the select a category list, select
   Math & Trig.
- i In the Select a function list, select SUM.
- j Click OK.
- **k** Click the **Number1** box in the Function Arguments dialog box.
- 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

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



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

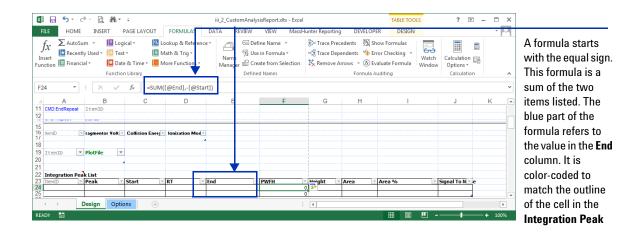
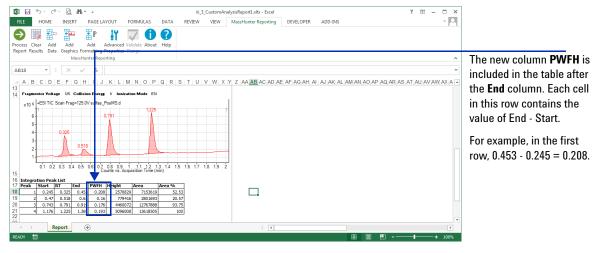


Figure 65 The formula has been added to the Integration Peak List table

Task 3. Add a formula column to a table

Step			etailed instructions	Comments		
3	<b>tep</b> Test the changes to the template.	D a b c d e f g h i	Click the MassHunter Reporting tab in the Ribbon. Click Process Report. Click the Browse button. Move to the \MassHunter \Reports\Temp folder. Double-click one of the folders that contains analysis results. Select Report.xml. Click Open.			
			difference between the <b>End</b> and the <b>Start</b> of the peak.			

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



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

Task 3. Add a formula column to a table

Step	Detailed instructions	Comments	
4 Save the changes to the template, iii_3_CustomAnalysisReport, where iii are your initials.	<ul> <li>a Click Clear Results in the MassHunter Reporting 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, 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>	• The Save as type is Excel Template.	

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

# 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.

Step	Detailed instructions			
1 Open the Quantitative Analysis template, \MassHunter\Report Templates\Quant\en-US\Letter\ ISTD\Results_NoGraphics\ Parts\iii_8_Custom_ ISTD_Summary template.	Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, iii_8_Custom_ISTD_Summary, where "iii" are your initials.	<ul> <li>If you do not have this template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the Familiarization Templates folder.</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 68 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 51 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 Alignment tab.</li> <li>f Select Right (Indent) in the Horizontal list. Click OK.</li> <li>g Click the AT 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 Paders.</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 click the Format Cells command to select the number category and to select the number of decimal places.</li> <li>(optional) You can set the width of the RT and ISTD RT column.</li> </ul>		

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

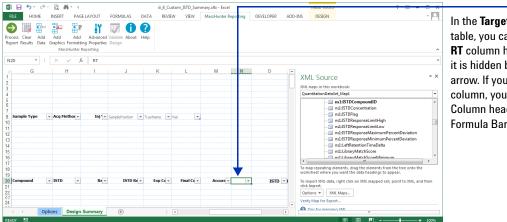
4

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

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

itep	Detailed instructions	Comments
Pick a column		with the word <b>ISTD</b> . These columns are nns. Do not select any of these columns.
SempleID CompoundID ISTOCompoundID PeekID CompoundType Data File Compound ISTD Resp ISTD Resp Exp Conc Final Conc Accuracy RT ISTD RT	column. This column is autom	) has to be part of the table to add an ISTD atically added when you add an ISTD uded. The <b>ISTDCompoundID</b> column is a
OK Cancel		





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

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

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

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 Move to the \MassHunter\Data\ 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 last column in the Sequence Table.</li> </ul>	<ul> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in the Ribbon.</li> </ul>	

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

FILE HOME INSER	_*	FORMULAS DA		om_ISTD_Summary VIEW MassHu	xltx - Excel Inter Reporting	DEVELOPER	ADD-INS	DESIGN	×	
Tahoma aste v ipboard r	- 8 - A	A = = *	>• <mark>₽</mark> ≡ #= □ •	General ▼ \$ ▼ % ≯ *.00 .00	Conditional F Format as Tai Cell Styles • Style	ormatting * ble *	Insert •	∑ - A ↓ Z Sort & ✓ Filter + Editing		The last two columns in th Target Compound Table a
1150 - E	< √ fx 2. G	.102116666666667 H	1	J	к	1	М	N	v 0	the <b>RT</b> and <b>ISTD RT</b> columns.
6		▼ ISTD ▼	Re 🔻	ISTD Re 🔻	Exp Cc 👻	Final Cc →		RT 🔻	ISTD	The <b>RT c</b> olumn is the
CMAMBk_01.d CMAMCal_L1.d	Amp Amp	Amp-d5 Amp-d5	658	1397	2.5000	3.3187		2.1021167 2.1021167	2.07778333 2.07778333	retention time of that
3 CMAMCal_L2.d 5 CMAMCal_L3.d 1 CMAMCal_L4.d	Amp Amp Amp	Amp-d5 Amp-d5 Amp-d5	1059 2673 4952	1298 1377 1304	5.0000 12.5000 25.0000	5.7493 13.6808 26.7561	109.45	2.1021167 2.1021167 2.1021167	2.07778333 2.07778333 2.07778333	compound. The ISTD RT
2 CMAMCal_L5.d ) CMAMQC_L2.d	Amp Amp Amp	Amp-d5 Amp-d5 Amp-d5	18605 1006	1053	125.0000 5.0000	124.4844	99.59	2.1021167 2.1021167 2.1021167	2.07778333 2.07778333	column is the retention tin
CMAMQC_L4.d CMAMSam_01.d	Amp Amp	Amp-d5 Amp-d5	4716	1196	25.0000	27.8039	111.22	2.1021167 2.1021167	2.07778333 2.07778333	for the internal standard f that compound.
CMAMSam_02.d ) CMAMSam_03.d	Amp Amp	Amp-d5 Amp-d5	1004 2590	1445 1284		4.8977 14.2183		2.1021167 2.1021167	2.07778333 2.07778333	
∢ → Summa	ry Design-Sum	mary (+)			•					
ADY FILTER MODE CA		. 0				▦	∎ ଅ -	—	<b>+</b> 100%	

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

4 Save the changes to the template, iii_9_Custom_ISTD_Summary.	а	Click Clear Results in the MassHunter Reporting tab in the Ribbon.	•	The Save as type is Excel Template.
<ul> <li>You have to clear the results</li> </ul>	b	Click File > Save As.		
first.	C	In the Save As dialog box, type		
		<pre>iii_9_Custom_ISTD_Summary.</pre>		
	d	Verify the folder selected in Save in is		
		correct.		
	e	Click <b>Save</b> .		

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

# Task 5. Add a column that is already mapped

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

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

Usually, you will not need to do this task.

St	tep	Detailed instructions	Comments		
1	Open the Qualitative Analysis template \MassHunter\Report Templates\Qual\Letter\ iii_3_CustomAnalysisReport, where iii are your initials.	Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 30 to open the template, iii_3_CustomAnalysisReport, where "iii" are your initials.	<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>		
2	Add the item <b>AnalysisFileName</b> to the first column in row 10.	<ul> <li>a Find the second table in the template. The items in this table are ItemID, Data File, Injector Volume and Dilution.</li> <li>b In the table, click Data File.</li> <li>c Right-click and click XML &gt; XML Source.</li> <li>d Click the Dilution column.</li> <li>e Try to add the AnalysisFileName item to the end of the table. An error message is displayed.</li> </ul>	<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 68 for instructions on adding a mapped column to a table.</li> </ul>		
	Microsoft Excel	×			

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

OK

Task 5. Add a column that is already mapped

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 Move 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>	

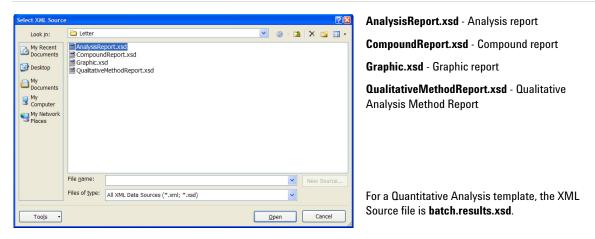
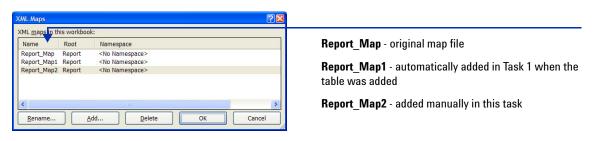
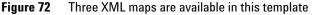


Figure 71Add another map file





Task 5. Add a column that is already mapped

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

Step	Detailed instructions	Comme	ents
	I Select <b>Report_Map2</b> Source pane. <b>m</b> Add the mapped colu <b>AnalysisFileName</b> in of row 10.	umn,	
Home Insert Page Layout Formulas Data	Review View Add-Ins Acrobat       Test     Add-Ins Acrobat       Image: State of the state o	w _ ♂ × ng * 3* Inset * * Delete * Format * Cells Editing	The <b>AnalysisFileName</b> is added to the first column in row 10. Because this cell is not part of a table, the column
A10 • 🖍 A B C Formula Bar	E F 🚔	× XML Source × ×	header is not automatically added above the value.
2 OPD.Repeat TremID 3 ItemID v Data Filenam v Sample Nam(v Sample Type v 4 J 5 TremID v Data File v Injector Volu Dilution v	Position 💽 Instrument Nam Vse 🚍	XML maps in this workbook: Report_Map2 ♥ ■	
10         10           11         CMDEndRepeat         TCmID           12         11         11           15         15         15		Acquired Time Acquired Time Analysis Tiettame Analysis D	
16 kemů Sragmentor Volt Collision Energe Ionization Moder 18 1 19 stemů V Plotřile V 20 2 21 Interration Peak List		To map non-repeating elements, drag the elements from the tree onto the worksheet where you want the data to appear. To import data, use the Import XML Data button on the List toobar. Obtions - XML Maps	
H ( ) Design Options	· · · · · · · · · · · · · · · · · · ·	-	

Figure 73 Add the AnalysisFileName item

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

Task 5. Add a column that is already mapped

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

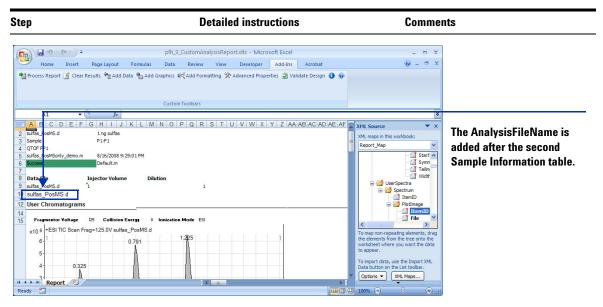


Figure 74 Verifying that the AnalysisFileName is repeated

4	Save the changes to the template. • You have to clear the results	a	Click <b>Clear Results</b> in the <b>MassHunter Reporting</b> tab in the Ribbon.	•	The Save as type is Excel Template.
	first.	b	Click the Microsoft Office button and		
	<ul> <li>You save the template to the</li> </ul>		then click Save As and click Other		
	new name, iii_4_Custom		Formats.		
	AnalysisReport, where iii are	C	In the Save As dialog box, type		
	your initials.		<i>iii_</i> 4_CustomAnalysisReport.		
		d	Verify the folder selected in Save in is		
			correct.		
		е	Click Save.		



Agilent MassHunter Workstation Software Reporting Familiarization Guide

# Exercise 5 Graphics

Task 1. Adding graphics to a template110Task 2. Display multiple graphics per row112

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.



#### 5 **Graphics**

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. Add graphics to a Quantitative Analysis template

S	tep	Detailed instructions	Comments		
1	Open the Quantitative Analysis template, \MassHunter\Report Templates\Quant\en-US\Letter\ ISTD\Results_NoGraphics\ Parts\iii_9_Custom_ ISTD_Summary template.	Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, iii_9_Custom_ISTD_Summary, where "iii" are your initials.	<ul> <li>If you do not have this template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the Familiarization Templates folder.</li> </ul>		
2	<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 125 for an explanation of repeating sections.</li> <li>Three different graphics are added in the Compound Graphics table.</li> </ul>		

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ess Clear cort Results	Add	Add Add raphics Formatting MassHunter Rep	Properties orting	Validate About	? Help								^	graphics in th template bec are shown in
	٨	В		С		D	E	F		G	н	-		the template
	-		•			, in the second s							XML Source • ×	
SampleID		- Location		Acquisition File		Deserte	Sample Na 🗸	Level	6	le Type	- Acg Me		XML maps in this workbook:	The graphics
sampreib	k	Location	×	Acquisition File	γI	barcode *	Sample na 🔹	Level	* Samp	ie rype	✓ Acq rie		QuantitationDataSet Map1	•••
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uantitat														
CMD:Repea		CompoundID											ns1:UserDefined8	CompoundI
ampleID		<ul> <li>CompoundID</li> </ul>	Ŧ	CompoundType	Ŧ	Formula 👻		RetentionTime	-				ns1:UserDefined9	
SampleID	T	CompoundID	_	ISTDCompoundID		Target Com	CompoundT -	Data File	Com	ound	▼ ISTD		ns1:Vial	
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													۰ III ۲	
													To map repeating elements, drag the elements from the tree onto the worksheet where you want the data	
													headings to appear.	
MD:EndRep	eat	CompoundID												
													To import XML data, right click an XML mapped cell, point to XML, and then click Import.	
												-	Options  XML Maps	
( )×	Optic	ons Design-Su	mmary	+		÷ 1	4				•		· · · · · · · · · · · · · · · · · · ·	

find any ise they reen in

re epeating

Select the **RT** column Figure 75

	Detailed instructions	Comments		
Test the changes to the template.	<ul> <li>a Click Process Report.</li> <li>b Click the Browse button.</li> <li>c Move to the \MassHunter\Data\ 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>	<ul> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in the Ribbon.</li> </ul>		
Image: Second		The Compound Graphics fo each data file are shown in		
30 Amp + MRM (136.2 -> 91.4 CMAMCal_L1.d		different rows. All of the graphics for the first compound are shown together.		
32 33 Amp + MRM (136.2 -> 91.4) CMAMCal_L2.d [136.2 -> 91.4],	136 2 -> 119 4 + MRM (2.077-2.278 min, 33 scans) (136			

Task 1.	Add graphic	s to a Quan	titative Anal	vsis temi	olate (	continued)	

4	Save the changes to the template,	а	Click Clear Results in the MassHunter	•	The Save as type is Excel Template.
	iii_10_Custom_ISTD_		Reporting tab in the Ribbon.		
	Summary.	b	Click File > Save As.		
	<ul> <li>You have to clear the results</li> </ul>	C	In the Save As dialog box, type		
	first.		<pre>iii_10_Custom_ISTD_Summary.</pre>		
		d	Verify the folder selected in <b>Save in</b> is		
			correct.		
		e	Click Save.		

Task 2. Display multiple graphics per row

## 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

S	tep	Detailed instructions	Comments
1	Open the Quantitative Analysis template, \MassHunter\Report Templates\Quant\en-US\Letter\ ISTD\Results_NoGraphics\ Parts\iii_10_Custom_ ISTD_Summary.	Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, iii_10_Custom_ISTD_Summary, where "iii" are your initials.	<ul> <li>If you do not have the         iii_10_Custom_ISTD_Summary         template, example templates are         available on the Agilent         Technologies MassHunter         Reporting User Information DVD in         the Familiarization Templates         folder.     </li> </ul>
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>	<ul> <li>a Click one of the graphics in the Compound Graphics table.</li> <li>b Click Advanced Properties in the MassHunter Reporting tab in the Ribbon.</li> <li>c Select 1/6 for the Graphic size relative to page width and Height boxes for each graphic.</li> <li>d Mark the Continue graphics across the page check box.</li> <li>e Click Close.</li> </ul>	• Make sure to change the width and height for each graphic.

## Graphics 5

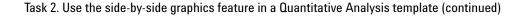
Task 2. Display multiple graphics per row

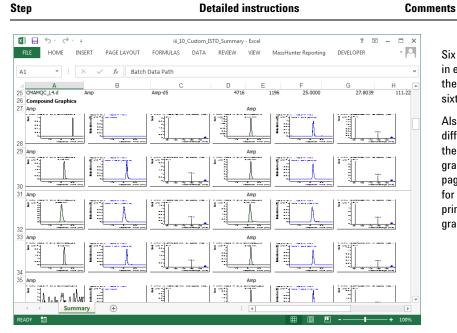
tep	Detailed instructions	Comments
dvanced Properties		
Template Design Worksheet Cell Table		Set the relative graphic width and
Table properties Tab	le column properties	height for each of the graphics.
Sa	mpleID Hiden	
	mpoundID Hidlen mpoundivame	
	aphicCompoundChromatoc Graphic(6,6) aphicCompoundQualifiers Graphic(6,6)	
Hide empty cells	aphicCompoundSpectrum Graphic(6,6)	
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	Formula Preset graphics row height	controls whether or not different
phics layout	Hidden	
Co Continue graphics across the page	lumn sort order Unsorted  C Ascending C Descending	rows of graphics can be printed on
Stack graphics vertically     Filt	er value	set Filter the same line.
		Close The Stack graphics vertically check
		box changes how the graphics are
		8 8 1
		organized on the page. If this check
		box is cleared, then the related
		graphics are printed side-by-side. If
		graphics are printed side-by-side. If
		<b>ö</b> 1 <i>,</i>
		this check box is marked, then relate
		this check box is marked, then relate graphics are printed on consecutive
		this check box is marked, then relate
aura <b>77</b> - Calact the DT colum		this check box is marked, then relate graphics are printed on consecutive
igure 77 Select the RT colum	n	this check box is marked, then relate graphics are printed on consecutive
		this check box is marked, then relate graphics are printed on consecutive rows.
i <b>gure 77</b> Select the RT colum Test the changes to the template.	a Click Process Report.	<ul> <li>this check box is marked, then relate graphics are printed on consecutive rows.</li> <li>The Process Report command is</li> </ul>
		this check box is marked, then relate graphics are printed on consecutive rows.
	a Click Process Report. b Click the Browse button.	<ul> <li>this check box is marked, then relate graphics are printed on consecutive rows.</li> <li>The Process Report command is part of the MassHunter toolbar in</li> </ul>
	a Click Process Report. b Click the Browse button. c Move to the \MassHunter\D	<ul> <li>this check box is marked, then relate graphics are printed on consecutive rows.</li> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in</li> </ul>
	a Click Process Report. b Click the Browse button.	<ul> <li>this check box is marked, then relate graphics are printed on consecutive rows.</li> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in</li> </ul>
	a Click Process Report. b Click the Browse button. c Move to the \MassHunter\D DrugsOfAbuse\QuantReports	<ul> <li>this check box is marked, then relate graphics are printed on consecutive rows.</li> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in</li> </ul>
	a Click Process Report. b Click the Browse button. c Move to the \MassHunter\D DrugsOfAbuse\QuantReports DrugsOfAbuseDemo folder.	<ul> <li>this check box is marked, then relate graphics are printed on consecutive rows.</li> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in</li> </ul>
	a Click Process Report. b Click the Browse button. c Move to the \MassHunter\D DrugsOfAbuse\QuantReports	<ul> <li>this check box is marked, then relate graphics are printed on consecutive rows.</li> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in</li> </ul>
	a Click Process Report. b Click the Browse button. c Move to the \MassHunter\D DrugsOfAbuse\QuantReports DrugsOfAbuseDemo folder. d Select report.results.xml.	<ul> <li>this check box is marked, then relate graphics are printed on consecutive rows.</li> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in</li> </ul>
	<ul> <li>a Click Process Report.</li> <li>b Click the Browse button.</li> <li>c Move to the \MassHunter\D</li> <li>DrugsOfAbuse\QuantReports</li> <li>DrugsOfAbuseDemo folder.</li> <li>d Select report.results.xml.</li> <li>e Click Open.</li> </ul>	<ul> <li>this check box is marked, then relate graphics are printed on consecutive rows.</li> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in</li> </ul>
	a Click Process Report. b Click the Browse button. c Move to the \MassHunter\Di DrugsOfAbuse\QuantReports DrugsOfAbuseDemo folder. d Select report.results.xml. e Click Open. f Click OK.	<ul> <li>this check box is marked, then relate graphics are printed on consecutive rows.</li> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in</li> </ul>
	<ul> <li>a Click Process Report.</li> <li>b Click the Browse button.</li> <li>c Move to the \MassHunter\D</li> <li>DrugsOfAbuse\QuantReports</li> <li>DrugsOfAbuseDemo folder.</li> <li>d Select report.results.xml.</li> <li>e Click Open.</li> </ul>	<ul> <li>this check box is marked, then relate graphics are printed on consecutive rows.</li> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in</li> </ul>
	<ul> <li>a Click Process Report.</li> <li>b Click the Browse button.</li> <li>c Move to the \MassHunter\Di 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> </ul>	<ul> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in the Ribbon.</li> </ul>
	<ul> <li>a Click Process Report.</li> <li>b Click the Browse button.</li> <li>c Move to the \MassHunter\D: 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 first Compound Graph</li> </ul>	<ul> <li>this check box is marked, then related graphics are printed on consecutive rows.</li> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in the Ribbon.</li> </ul>
	<ul> <li>a Click Process Report.</li> <li>b Click the Browse button.</li> <li>c Move to the \MassHunter\D: 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 first Compound Graph</li> </ul>	<ul> <li>this check box is marked, then related graphics are printed on consecutive rows.</li> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in the Ribbon.</li> </ul>
	<ul> <li>a Click Process Report.</li> <li>b Click the Browse button.</li> <li>c Move to the \MassHunter\Di 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> </ul>	<ul> <li>this check box is marked, then related graphics are printed on consecutive rows.</li> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in the Ribbon.</li> </ul>

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

### 5 Graphics

Task 2. Display multiple graphics per row



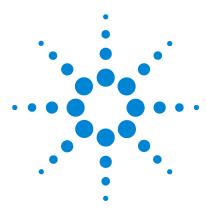


Six different graphics are printed in each row. Each is one sixth the width of the page and one sixth the height of the page.

Also, the graphics from two different data files are printed on the same line. You read the graphics from left to right on the page. For example, the graphics for the second data file are printed to the right of the graphics for the first data file.

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

<ul> <li>4 Save the changes to the template, iii_11_Custom_ISTD_ Summary.</li> <li>You have to clear the results first.</li> </ul>	b c d	Click Clear Results in the MassHunter Reporting tab in the Ribbon. Click File > Save As. In the Save As dialog box, type <i>iii_</i> 11_Custom_ISTD_Summary. Verify the folder selected in Save in is correct. Click Save.	•	The <b>Save as type</b> is <b>Excel Template</b> .
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Agilent MassHunter Workstation Software Reporting Familiarization Guide

# Exercise 6 Advanced topics

Task 1. Add a page break and a sheet break116Task 2. Use Test Mode120Task 3. Add a single repeating section125Task 4. Add a nested repeating section129Task 5. Change values on the Options worksheet133Task 6. Add a formula using the IF function136Task 7. Use the VLOOKUP function140

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

Each exercise is presented in a table with three columns:

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



Task 1. Add a page break and a sheet break

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

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

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

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

Task 1. Add a page break and a sheet break

Step		Detailed instructions			
1 Open the Quantitative Analysis template, \MassHunter\Report Templates\Quant\en-US\Letter\ ISTD\Results_NoGraphics\ Parts\iii_11_Custom_ ISTD_Summary.		Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, <i>i</i> ii_11_Custom_ISTD_Summary, where "iii" are your initials.	<ul> <li>If you do not have this template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the Familiarization Templates folder.</li> </ul>		
2	Add a sheet break to the Quantitation Results section. • Select Compound to label the worksheet.	<ul> <li>a Select the row containing the SampleID column in the Quantitation Results section.</li> <li>b Right-click the row and click Insert. A row is added above the table.</li> <li>c Click the first column in this new row.</li> <li>d Click Add Formatting &gt; Sheet Break in the MassHunter Reporting tab in the Ribbon.</li> <li>e Select Compound.</li> <li>f Click OK.</li> </ul>	<ul> <li>You can only select an item that is included between that row and the end of the template to use as the label for the worksheet.</li> <li>If the item is not part of the template, you can add it to the template and hide that column or cell.</li> <li>If you do not want to specify an item to use to label the new worksheet, click Cancel. The CMD:Sheet Break command is still added to the template.</li> </ul>		

Task 1. Add a page break and a sheet break

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

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

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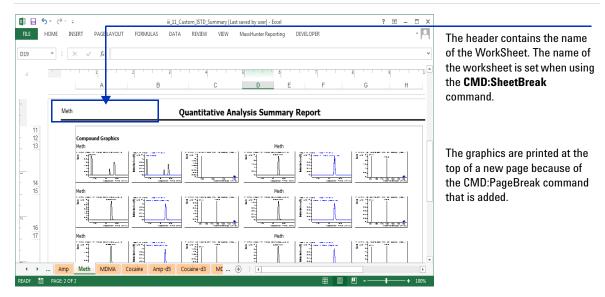
**Figure 79** Adding a Sheet Break and a Page Break

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

Task 1. Add a page break and a sheet break

Task 1. Add a pa	age break and a	sheet break	(continued)
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Step	Detailed instructions	Comments			
5 Test the changes to the template.	<ul> <li>a Click the MassHunter Reporting tab.</li> <li>b Click Process Report.</li> <li>c Click the Browse button.</li> <li>d Move to the \MassHunter\Data\ DrugsOfAbuse\QuantReports\ DrugsOfAbuseDemo folder.</li> <li>e Select report.results.xml.</li> <li>f Click Open.</li> <li>g Click OK.</li> <li>h Click the Meth worksheet. Each worksheet is labeled with the name of a different compound.</li> <li>i Click the View tab in the Ribbon.</li> <li>j Click the Page Layout button or the Page Break Preview button.</li> <li>k The compound graphics are printed starting at the top of the next page.</li> </ul>	<ul> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in the Ribbon.</li> </ul>			



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

Task 1. Add a page break and a sheet break

Step	Detailed instructions	Comments		
<ul> <li>6 Save the changes to the template, iii_12_Custom_ISTD_ Summary.</li> <li>You have to clear the results first.</li> </ul>	<ul> <li>a Click Clear Results in the MassHunter Reporting tab in the Ribbon.</li> <li>b Click File &gt; Save As.</li> <li>c In the Save As dialog box, type <i>iii_12_Custom_ISTD_Summary.</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.</li> </ul>		

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.

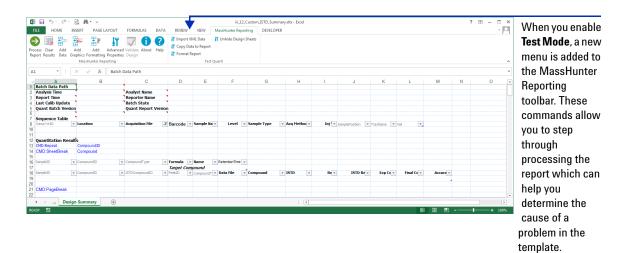
If you click **Unhide Design Sheets**, you can view the Design worksheets at the same time as the final report. The Design worksheets are hidden after the Format Report step.

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

Task 2. Use Test mode

Task 2. Use Test mode (	continued)
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S	Step		etailed instructions	C	Comments		
3	Change the TestMode enabled line from <b>False</b> to <b>True</b> .	a b c d e	Quant.config file and click Open. You can open this file with Notepad. Find the line " <testmode enabled="False"/&gt;".</testmode 				
4	Open the Quantitative Analysis template, \MassHunter\Report Templates\Quant\en-US\Letter\ ISTD\Results_NoGraphics\ Parts\iii_12_Custom_ ISTD_Summary.	Q pa iii	ollow the instructions in "Task 4. Open a cantitative Analysis Excel template" on age 40 to open the template, _12_Custom_ISTD_Summary, where ii are your initials.	•	If you do not have the iii_12_Custom_ISTD_Summary template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the Familiarization Templates folder.		





Task 2. Use Test Mode

### Task 2. Use Test mode (continued)

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

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	5	CMAMCal_L5.d	BarCode 123567 Calib-L5	L5	Calibration	APCIautotune.m	5	P1-C17							
	6	CMAMQC_L2.d	BarCode 123456 QC-L2	L2	QC	APCIautotune.m	5	P1-C9							
	7	CMAMQC_L4.d	BarCode 123456 QC-L4	L4	qc	APCIautotune.m	5	P1-C15							
	8	CMAMSam_01.d	BarCode 123456 Sample - 1		Sample	APCIautotune.m	5	P1-C22							
	9	CMAMSam_02.d	BarCode 123456 Sample -2		Sample	APCIautotune.m	5	P1-C8							
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Figure 82 After the Test Quant > Import XML Data step

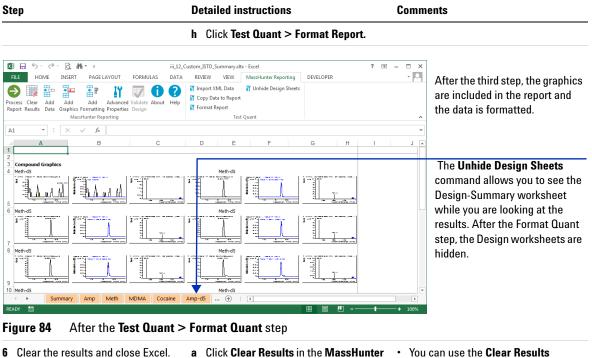
### Task 2. Use Test mode (continued)

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Process Clear Add Add Add Advanced Validate Abr MassHunter Reporting		ut Help I' Import XML Data I' L Copy Data to Report I' Format Report				Y Unhide Design Sheets				<ul> <li>After the second step, the data is placed onto the appropriate worksheet and it is</li> </ul>		
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233	0		3 Cocaine-d3					pectrum\PeakSpect				
34	0		4 MDMA					pectrum (PeakSpect				
235	0		5 MDMA-d5					pectrum (PeakSpect				
236 237	0		6 Meth					pectrum PeakSpect				
237	0		7 Meth-d5					pectrum (PeakSpect				
230	1		0 Amp 1 Amp-d5					pectrum\PeakSpect				
240	1		2 Cocaine					pectrum/PeakSpect				
241	1		3 Cocaine-d3					pectrum/PeakSpect				
242	1		4 MDMA					pectrum (PeakSpect				
243	1		5 MDMA-d5					pectrum PeakSpect				
244	1		6 Meth					pectrum (PeakSpect				
245	1		7 Meth-d5					pectrum PeakSpect				
246	2		0 Amp					pectrum (PeakSpect				
	Meth N	IDMA Cocaine		Cocaine-d3	MDMA-			Design-Summ		: •		

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

Task 2. Use Test Mode

#### Task 2. Use Test mode (continued)



Reporting tab in the Ribbon.

click Close.

**b** Click the **Microsoft Office button** and

command after any of the steps.

Agilent MassHunter Workstation Software Reporting Familiarization Guide

## Task 3. Add a single repeating section

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

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

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

S	tep	Detailed instructions	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.</i>	Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, iii_Custom_QuantReport_ ESTD_Summary, where "iii" are your initials.	<ul> <li>Make a copy of the QuantReport_ESTD_Summary_B_ 04_00 template and rename it to iii_Custom_QuantReport_ ESTD_Summary, where "iii" are your initials.</li> </ul>		
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>	<ul> <li>a Select the first column in row 25.</li> <li>b Click Add Data &gt; Target Compound Table in the MassHunter Reporting tab in the Ribbon. The Target Compound Information table is added at the end of the report.</li> <li>c Select rows 26 to 27. Click row 26 and drag to include row 27.</li> </ul>	<ul> <li>You can also fix the headers of this table to match the headers of the other tables in this template.</li> <li>Right-click the headers, and click the B in the shortcut menu to change the font.</li> </ul>		

Task 3. Add a single repeating section

Task 3. Add a single repeating section

Task 3 Ad	d a	single	reneating	section	(continued)	١
IUSK J. AU	uu	Sillyic	repeating	300000	Continucu	1

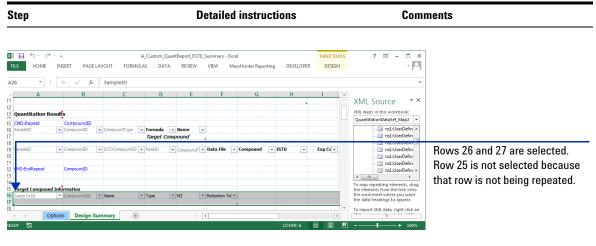
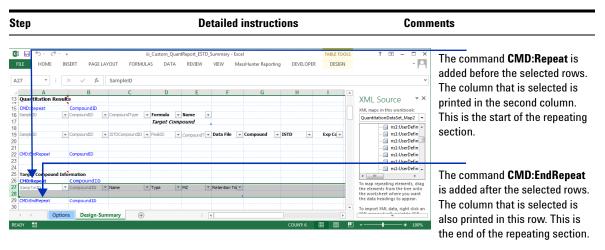


Figure 85 Adding a single repeating section

d	Click Add Formatting > Repeating Section in the MassHunter Reporting tab in the Ribbon.	Usually, you repeat using one of the ID columns. To have the compound information
е	In the Select Column dialog box, select	printed together, select the
	CompoundID.	CompoundID.
f	Click <b>OK</b> .	Two commands are added to the template. <b>CMD:Repeat</b> is added before row 26 and <b>CMD:EndRepeat</b> is added after row 27.

Task 3. Add a single repeating section



#### Task 3. Add a single repeating section (continued)

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

<b>3</b> Test the changes to the template.	a Click Process Report.	In the Advanced Properties dialog
	<b>b</b> Click the <b>Browse</b> button.	box, you can click Hide Header Row
	c Move to the \MassHunter\Data\	if you don't want to repeat the
	DrugsOfAbuse\QuantReports\	header row for each compound.
	DrugsOfAbuseDemo folder.	
	d Select report.results.xml.	
	e Click Open.	
	f Click OK.	
	g Scroll the report until you find the	
	Target Compound Information table.	
	All of the information for each	
	compound is grouped together. The	
	column headers are repeated between	
	each compound because that row is	
	part of the repeating section.	

Task 3. Add a single repeating section

Step	Detailed instructions	Comments
Image: Solution of the second seco	EW MassH DEVELO ADD-IN	The rows about each compound are grouped together.
A         D         CLID         E         F         G         L         M         N         C           C         Torget         F         Reference         Time         Tigget         Reference         Re	XML Source  XML maps in this workbook: QuantitationDataSet,Map2 Quantit	
30         Amp-ds         ISTD         93.4         2.077783333           31         Amp-ds         ISTD         93.4         2.077783333           32         Amp-ds         ISTD         93.4         2.077783333           33         Amp-ds         ISTD         93.4         2.077783333           34         Amp-ds         ISTD         93.4         2.077783333           34         Amp-ds         ISTD         93.4         2.077783333           35         Amp-ds         ISTD         93.4         2.077783333           36         Amp-ds         ISTD         93.4         2.077783333           37         Amp-ds         ISTD         93.4         2.077783333           36         Amp-ds         ISTD         93.4         2.077783333           4         Amp-ds         ISTD         93.4         2.07783434 <td>To map repeating elements, drag the elements from the tree onto the worksheet where you want the data headings to appear. To import XML data, right click an XML mapped cells point to XML and then click import.</td> <td></td>	To map repeating elements, drag the elements from the tree onto the worksheet where you want the data headings to appear. To import XML data, right click an XML mapped cells point to XML and then click import.	

## Task 3. Add a single repeating section (continued)

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

<ul> <li>4 Save the changes to the template, iii_1_Custom_QuantReport_ ESTD_Summary.xlt.</li> <li>You have to clear the results first.</li> </ul>		Reporting tab in the Ribbon. Click File > Save As. In the Save As dialog box, type <i>iii_</i> 1_Custom_QuantReport_ ESTD_Summary. Verify the folder selected in Save in is correct.	•	The <b>Save as type</b> is <b>Excel Template</b> .
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## Task 4. Add a nested repeating section

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

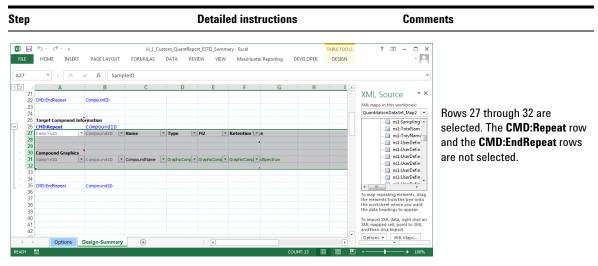
In this task, you group different tables together using a nested repeating section. A nested repeating section is simply a repeating section that is within another repeating section. When repeating sections are nested, the inner repeating section needs to end before the outer repeating section ends.

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

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

Step	Detailed instructions	Comments		
Open the Quantitative Analysis template, \MassHunter\Report Templates\Quant\Letter\ESTD\ Parts iii_1_Custom_QuantReport_ESTD _Summary.	Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, iii_1_Custom_QuantReport_ ESTD_Summary, where "iii" are your initials.	<ul> <li>If you do not have the iii_1_Custom_QuantReport_ESTD_ Summary template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the Familiarization Templates folder.</li> </ul>		
<ul> <li>Add a nested repeating section at 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 MassHunter Reporting tab in the Ribbon.</li> <li>e Select rows 27 to 32. Click row 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



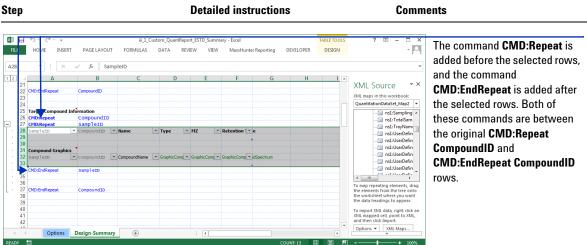
#### Task 4. Add a nested repeating section (continued)

Figure 88 Selecting both tables inside of the Repeating Section

- f Click Add Formatting > Repeating Section in the MassHunter Reporting tab in the Ribbon.
- g In the Select Column dialog box, select SampleID.
- h Click OK.

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

Task 4. Add a nested repeating section

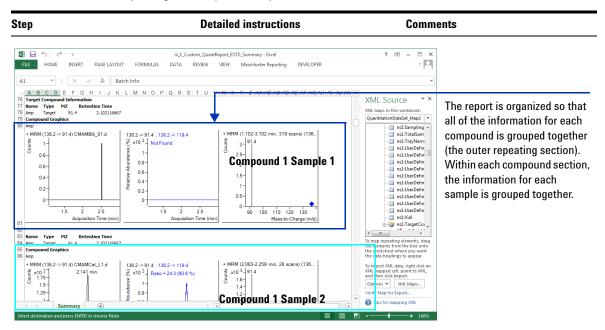


#### Task 4. Add a nested repeating section (continued)

aı	ure	<b>89</b> A	An inner re	epeating s	ection is add	ed which includ	des b	0	th tables
ADY	5					COUNT: 13	E		+ 100%
4	÷	Options	Design-Summary	+			Þ		
	42							-	Options - XML Maps
	41								XML mapped cell, point to XML, and then click Import.
	40								To import XML data, right click an
	39								the data headings to appear.
	38	ALL IUNOPEDL	CompoundID						the elements from the tree onto the worksheet where you want
	36 37 смс	):EndRepeat	CompoundID						To map repeating elements, drag
	35								۰ E
1		):EndRepeat	SampleID						ns1:UserDefin

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

Task 4. Add a nested repeating section



#### Task 4. Add a nested repeating section (continued)

Figure 90 The results of a repeating section using the CompoundID

	Save the changes to the template, iii_2_Custom_QuantReport_ESTD _Summary.xlt. • You have to clear the results first.	b c	Click Clear Results in the MassHunter Reporting tab in the Ribbon. Click File > Save As. In the Save As dialog box, type iii_2_Custom_QuantReport_EST D_Summary. Verify the folder selected in Save in is correct. Click Save.	•	The Save as type is Excel Template.
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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		
Open the Qualitative Analysis template \MassHunter\Report Templates\Qual\Letter\ iii_4_CustomAnalysisReport, where iii are your initials.	Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 30 to open the template, iii_4_CustomAnalysisReport, where "iii" are your initials.	<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 template.</li> </ul>	

Task 5. Change values on the Options worksheet

Task 5. Change values on the Options worksheet

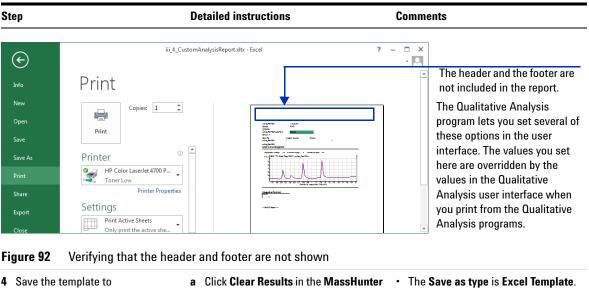
	Task 5.	Change valu	es on the Opti	ons worksheet	(continued)
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tep		D	etailed instructions	Comm	ents
🚺 🔒 🗲 e e e		iii_4_Custor	nAnalysisReport - Excel	? 📧 – 🗆 🗙	
FILE     HOME     INSERT       IncludeFo     *     ×	PAGE LAYOUT	FORMULAS DATA	A REVIEW VIEW MassHunter Reporting D	EVELOPER - M	Each cell in the Value column i explicitly named. You can see the name of the cell here.
Parameter	Туре	Value	Comment	<b></b>	the name of the cell here.
Use Options	Boolean	TRUE	Comment		
	Boolean	TRUE			
Include Header	Boolean	FALSE			
Include Footer	Boolean	FALSE	<b>v</b>		
Landscape	Boolean	FALSE			
Fit to	Integer	1	F ge(s) wide		
	Integer	0	Page(s) tall		Only change the Value column
Hide Empty Colum		0 TRUE	Page(s) tall		, 0
Note: The followi	Boolean	TRUE	Page(s) tall less of the Use Options value.		In this example, the Include Header and Include Footer
Note: The followi	Boolean	TRUE	less of the Use Options value.		In this example, the Include
Note: The followi Hide ID Columns Add Smart Page	Boolean	TRUE	les of the Use Options value.		In this example, the Include Header and Include Footer values are set to False. The
Note: The followi Hide ID Columns Add Smart Page Breaks and Table	Boolean ng options will Boolean	be observed regard	less of the Use Options value.		In this example, the Include Header and Include Footer
Note: The followi Hide ID Columns Add Smart Page Breaks and Table Headers	Boolean	TRUE	les of the Use Options value.		In this example, the Include Header and Include Footer values are set to False. The header and footer will not be
Note: The followi Hide ID Columns Add Smart Page Breaks and Table Headers Adjust columns to	Boolean ng options will Boolean Boolean	be observed regard	less of the Use Options value.		In this example, the Include Header and Include Footer values are set to False. The
Note: The followi Hide ID Columns Add Smart Page Breaks and Table Headers	Boolean ng options will Boolean	be observed regard	less of the Use Options value.		In this example, the Include Header and Include Footer values are set to False. The header and footer will not be
Note: The followi Hide ID Columns Add Smart Page Breaks and Table Headers Adjust columns to	Boolean ng options will Boolean Boolean	be observed regard	les of the Use Options value. Use inserting and merging cells to allow adjusting table column widths		In this example, the Include Header and Include Footer values are set to False. The header and footer will not be
Note: The followi Hide ID Columns Add Smart Page Breaks and Table Headers Adjust columns to fit data Protect Results	Boolean ng options will Boolean Boolean Boolean	TRUE  TRUE  TRUE  TRUE  TRUE  TRUE	less of the Use Options value.		In this example, the Include Header and Include Footer values are set to False. The header and footer will not be
Note: The followi Hide ID Columns Add Smart Page Breaks and Table Headers Adjust columns to fit data Protect Results	Boolean Boolean Boolean Boolean Boolean	be observed regard TRUE TRUE TRUE TRUE FALSE	les of the Use Options value. Use inserting and merging cells to allow adjusting table column widths I not an imported option		Header and Include Footer values are set to False. The header and footer will not be

## Figure 91 Change the values in the Options worksheet

<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 Move to the \MassHunter \Reports\Temp folder.</li> <li>d Double-click one of the folders that contains analysis results.</li> <li>e Select Report.xml.</li> </ul>	<ul> <li>The Process Report command is part of the MassHunter toolbar in the MassHunter Reporting tab in the Ribbon.</li> </ul>
	e Select Report.xml.	
	f Click Open.	
	g Click <b>OK</b> .	
	h Click the Microsoft Office button and	
	click Print > Print Preview.	

Task 5. Change values on the Options worksheet



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

Save the template toaClick Clear Results in the MassHunter• The Save asiii\_5\_CustomAnalysisReport,<br/>where iii are your initials.aClick File > Save As.• See the Ma<br/>Designer Tra• You have to clear the results<br/>first.bClick File > Save As.• In the Save As dialog box, type<br/>iii\_5\_CustomAnalysisReport.• The Save as<br/>• See the Ma<br/>Designer Tra• You have to clear the results<br/>first.cIn the Save As dialog box, type<br/>iii\_5\_CustomAnalysisReport.• In the Save in is<br/>correct.

#### e Click Save.

The **Save as type** is **Excel Template**. See the MassHunter Report Designer Training for more information on the different options. Task 6. Add a formula using the IF function

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

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

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

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

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

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

Task 6. Add a formula	using the	IF function
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S	tep	Detailed instructions	Comments
1	Open the Qualitative Analysis template \ <b>MassHunter\Report</b> <b>Templates\Qual\Letter\</b> <b>iii_5_CustomAnalysisReport</b> , where <b>iii</b> are your initials.	Follow the instructions in "Task 1. Open a Qualitative Analysis template" on page 30 to open the template, iii_5_CustomAnalysisReport, where "iii" are your initials.	<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>
2	<ul> <li>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 MassHunter Reporting tab in the Ribbon.</li> <li>d Click the Formulas tab.</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

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

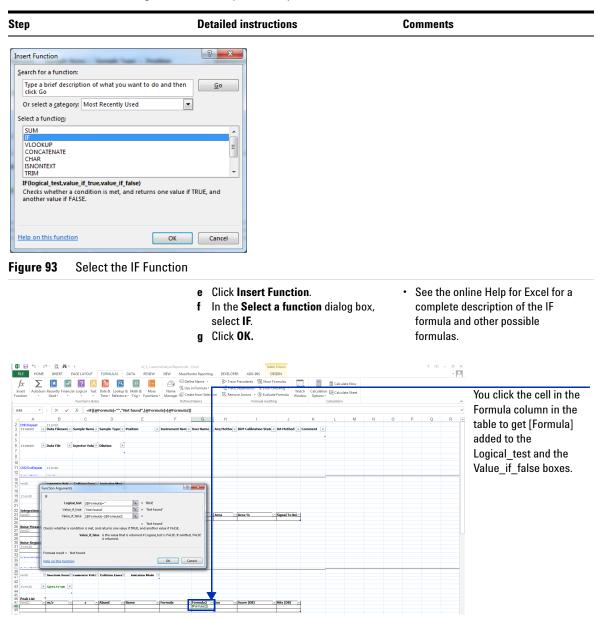


Figure 94 Enter the formula using the Function Arguments dialog box

Task 6. Add a formula using the IF function

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

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

Task 6. Add a formula using the IF function

Step Detailed instructions	Comments
Image: Image	
Image: Second	When the cell in the Formula column is empty, the Formula2 column contains Not Found.
A B C D E F G I J K L M N O P Q R S T Formula Barl     Y Z F       2 suffac PoskutoMSMS.d     1 ng suffac       3 Sample     P1+1       4 CTOP P1     Suffac PoskutoMSMS_demo.m       6 Default     P1+1       7 Data File     Injective Volume       9 suffac PoskutoMSMS.d     1       10 suffac PoskutoMSMS.d     1       11 difac PoskutoMSMS.d     1       11 difac PoskutoMSMS.d     1       11 difac PoskutoMSMS.d     1       12 suffac PoskutoMSMS.d     1       13 difac PoskutoMSMS.d     1       14 Fragmentor Voltage     0 Collition Exergy       15 Integration Peak List     1	You can hide the original column using the Advanced Properties dialog box. You select the <b>Formula</b> column and click the <b>Hidden</b> button. The formula is visible in the <b>Formula2</b> column.
19         PVFH           24         0           25         Framemetor Voltase           26         1           27         12           28         12           27         0.6           28         224           27         0.6           28         224           29         0.4           20         25           21         12.1           22         25.0           23         22.1           24         12.1.1           28         22.0           29         11.1           21         12.2.1.1           21         1.2.1.1           21         1.2.1.1           21         1.2.1.1           21         1.2.1.1           21         1.2.1.1           21         1.2.1.1           21         1.2.1.1           21         1.2.1.1           21         1.2.1.1           21         1.2.1.1           21         1.2.1.1           21         1.2.1.1           21         1.2.1.1           21.2.1.1         1.4	

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

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

4 Save the template to iii\_6\_CustomAnalysisReport, where iii are your initials.

- You have to clear the results first.
- a Click Clear Results in the MassHunter The Save as type is Excel Template. Reporting tab in the Ribbon.
- b Click File > Save As.
- c In the Save As dialog box, type
  - *iii* 6 CustomAnalysisReport.
- d Verify the folder selected in **Save in** is correct.
- e Click Save.

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\ iii_2_Custom_QuantReport_ESTD _Summary.	Follow the instructions in "Task 4. Open a Quantitative Analysis Excel template" on page 40 to open the template, iii_2_Custom_QuantReport_ ESTD_Summary, where "iii" are your initials.	<ul> <li>If you do not have the iii_2_Custom_QuantReport_ESTD_ Summary template, example templates are available on the Agilent Technologies MassHunter Reporting User Information DVD in the Familiarization Templates folder.     </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>	the Familiarization Templates

Step	Detailed instructions	Comments
	iii_2_Custom_QuantReport_ESTD_Summary.xltx - Excel FORMULAS DATA REVIEW VIEW MassHunter Reporting	? E – C × DEVELOPER · O
A2         i         X         Imp         Amp           Compounds Limits         C         D         D           Amp         5         -         -         -           Amp         5         -         -         -         -           Amp         5         -         -         -         -         -           Amp         5         -	E F G H I J K	The Compounds and L M N O P added to the worksheet
8 9 9 10 11 12 12 13 14 15 15 16 17 17 19 19 19 10 10 10 10 10 10 10 10 10 10 10 10 10	nmary (+) : ()	The name of the worksheet is changed to Limits.

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

Figure 96 Adding the new worksheet and renaming it Limits

 k Click Advanced Properties in the MassHunter Reporting tab in the Ribbon.
 I Click the Design Worksheet tab.

m Mark the Active worksheet is a design worksheet check box.
 n Mark the Exclude worksheet from final report check box.

o Click Close.

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

Advanced Properties

Tendate Design Worksheet [ od ] Table

Vorticities Tendate Design Worksheet [ od ] Table

P Active worksheet is design worksheet

E Exclude worksheet from final report

Core

Mark both check boxes in this

dialog box.

Figure 97Advanced Properties dialog box

Task 7. Use the VLOOKUP function

Step	Detailed instructions Comments	
3 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>	<ul> <li>See Task 3. Add a formula column to a table for more information on adding a formula column.</li> </ul>

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

OOKUP - :	× √ fx	=VLOOKUP(List2[	[#Headers	],[Compound]]-	VLOOKUP	mpound]]+[Limits]				· · ·	value that you want to
A	В	С	D	E	Table array	mpoundji+tennesi 🔤	- number				look up in the Limits
Batch Info				1	Col index num		= number				
Batch Data Path	1	•			Range lookup		= logical		-		worksheet. So, you cli
Analysis Time	•	Analyst Name		1	Range_tookap	HIL	= logical				the cell in the
Report Time	3	Reporter Name				2000 00 0	-	100			the cell in the
Last Calib Update		Batch State			Looks for a value in the leftmost column specify. By default, the table must be so		a value in the sam	ie row from a co	olumn you		Compound column the
Sequence Table	-				Lookup value	is the value to be found in t	he first column of	the table and o	an he a		Compound column the
				- Volui -	cookap_raide	value, a reference, or a text	string.	the table, and t			contains the results.
SampleID	✓ Data File	▼ Sample Name ▼	Position	Volui -							contains the results. L
					Formula result =						not click the column
Quantitation Resu	lts				romula result =		_				
CMD:Repeat	CompoundID				Help on this function			OK	Cancel		header.
		✓ CompoundType ✓	Formula	v Name v							noudon
			Target Co	mpound							
SampleID	CompoundID	▼ ISTDCompoundID ▼	PeakID	CompoundTy -			Exp Co 👻	Re -	ISTD Re -	R	
					d]]+[Li	nits])					
CMD:EndRepeat	CompoundID										
										•	·
Optio	ns Limits	Design-Summary	(+)		: 4					Þ	

Figure 98 Add the Lookup\_value to the Function Arguments dialog box

- I Click the Table\_array box in the Function Arguments dialog box.
- m Click the Limits worksheet tab.
- n Click and drag to select the area containing the compound names and the limits.
- · When you click the Limits worksheet tab, "Limits!" is added to the Table\_array box.

Step		Detailed instructions	Comments	
■ 日 ち・ぐ・ @ FLE HOME INSE	RT PAGE LAYOUT FORMULAS DATA	t_ESTD_Summary (version 1) slib [Recovered] - Excel TABLE REVIEW Function Arguments VLOOKUP	2 × P	
H20 I Batch Info Batch Data Path Analysis Time Report Time Last Calib Update Sequence Table IO SampleD V I		E Table_array Design.Summary/A285 Col_index_mum Range_lookup Looks for a value in the leftmost column of a table, and then specify. By default, it table must be softed in an ascending or	order. Ind in the first column of the table, and can be a	Select the area containing the compound names and limits. You do not
6 SampleID  C	CompoundID  CompoundID  CompoundType  Formula  Target Comp	ound .	OK         Cancel           v         Exp Cd v         Rd v         ISTD Rd v         R	include the column headers.
0 1 2 CMD:EndRepeat 3 4 ▶ Options DIT RECOVERED 1	CompoundID Limits Design-Summary 🕑	i (		

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

Figure 99 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 (continued)

tep	Detailed instructions	Comments
specify. By default, the table m	[Compound]       [S]       =       0         'Design-Summary'IA2:B5       [S]       =       (0,0)"Batch Data Path",0)"Analysis T         2       [S]       =       2         False       [S]       =       FALSE         =       -       -         est column of a table, and then returns a value in the same row from a column nust be sorted in an ascending order.       -         e-lookup is a logical value: to find the closest match in the first column (sorte ascending order) = TRUE or omitted; find an exact match = FALSE.	уоц
Formula result =		
Help on this function	OK Cance	

**Figure 100** The Function Arguments dialog box for the VLOOKUP function

<ul> <li>4 Add the second formula column to check if the Final Concentration is below the value in the Limits column.</li> <li>If the value is below the limit, print the message Below limit.</li> <li>Otherwise, print Pass.</li> </ul>	<ul> <li>a Click the Final Conc column in the same table.</li> <li>b Click Add Data &gt; Formula Column.</li> <li>c Rename the column Limit Check.</li> <li>d Click the cell containing the words Enter formula here.</li> <li>e Click the Formulas tab in the Ribbon.</li> <li>f Click Insert Function.</li> <li>g In the select a category box, select Logical.</li> <li>h Select IF in the Select a function list.</li> <li>i Click the cell containing the value in the Final Conc column.</li> <li>k Type &lt;</li> <li>I Click the cell containing the value in the Limits column.</li> <li>m Type Below limit in the Value_if_talse box.</li> <li>o Click OK.</li> </ul>	<ul> <li>See Task 6. Add a formula using the IF function for more information on adding a formula column using the IF function.</li> </ul>
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### Advanced topics 6 Task 7. Use the VLOOKUP function

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

Step		Detailed instructions		Comments
Function Argument	5	_	? <mark>x</mark>	The quotation marks are automatically added when you leave the field.
Value	cal_test [[ Final Conc]] < [Limits] _if_true	=         #N/A           =         "Below limit"           =         "Pass"		
Checks whether a		= e value if TRUE, and another value if e that is returned if Logical_test is FA d.		
Formula result = <u>Help on this functi</u>	<u>on</u>	ОК	Cancel	

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

5	Test the changes to the template.	а	Click <b>Process Report</b> .	
			Click the <b>Browse</b> button.	
		C	Move to the \MassHunter\Data\	
			DrugsOfAbuse\QuantReports\	
			DrugsOfAbuseDemo folder.	
		d	Select report.results.xml.	
		е	Click <b>Open</b> .	
		f	Click <b>OK</b> .	
		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 (continued)

Step	Detailed instructions	Comments

🕼 🖯 🖓 🖓	- <u>C</u> #6 - =			iii_2_Custom	QuantRepo	rt_ESTD_Summary	altx - Excel				? 🗉 – 🗆 🗙	The <b>Limits</b> column
FILE HOME	INSERT PAG	E LAYOUT	FORMULAS D	ATA REVIEW	VIEW	MassHunter Repo	orting DEVELC	PER			- [0]	contains the value from
D6 👻 :	$\times \checkmark f$	Batc	h State								*	the Limits tab that was
ABCD	EFGHI			RSTUN				Fo	rmula Bar		AR AS AT AU AV AW AX 🔺	
Target Compou				<u> </u>			CADALAIA			O AF AQ		next to this Compound
Data File	Compound	Limits	s ISTD	Exp Conc	Resp	ISTD Resp	Resp Ratio	Final Conc	Limit Check	Accuracy		next to this compound
CMAMBIk_01.d	Cocaine	6	Cocaine-d3		20	15	1.3126	11.82	Pass			name.
CMAMCal_L1.d	Cocaine	6	Cocaine-d3	2.50	5189	20245	0.2563	2.31	Below limit	92.35		name.
CMAMCal_L2.d	Cocaine	6	Cocaine-d3	5.00	9716	20506	0.4738	4.27	Below limit	85.36		
CMAMCal_L3.d	Cocaine	6	Cocaine-d3	12.50	25187 50649	19625 18068	1.2834	11.56	Pass	92.49		
CMAMCal_L4.d CMAMCal_L5.d	Cocaine Cocaine	6	Cocaine-d3 Cocaine-d3	25.00	50649 199967	18068 14401	2.8033	25.25	Pass Pass	101.00 100.06		
CMAMOC L2.d	Cocaine	6	Cocaine-d3	5.00	9746	19445	0,4755	4.28	Below limit	85.66		
CMAMOC L4.d	Cocaine	6	Cocaine-d3	25.00	48582	17834	2,7241	24.54	Pass	98.15		
CMAMSam 02.d	Cocaine	6	Cocaine-d3		9735	20051	0.4855	4.37	Belevelmit			
CMAMSam_03.d	Cocaine	6	Cocaine-d3		24841	20472	1.2134	10.93	Pass			The Limit Check column
Target Compou	nd MDMA											
Data File	Compound	Limits		Exp Conc	Resp	ISTD Resp	Resp Ratio	Final Conc	Limit Check	Accuracy		contains the word <b>Below</b>
CMAMBIk_01.d	MDMA	#N/A	IDMA-d5		7	28	0.2635	1.93	#N/A			
CMAMCal_L1.d CMAMCal_L2.d	MDMA MDMA	#N/A #N/A	IDMA-d5	2.50	3794 7433	12175 11691	0.3117	2.28	#N/A #N/A	91.30 93.12		Limit if the Final
CMAMCal_L2.0	MDMA MDMA	#N/A #N/Δ	IDMA-d5	12.50	17023	11091	1.5393	11.27	#N/A #N/A	93.12		
CMAMCal_L4.d	MDMA	#N/A	IDMA-d5	25.00	33212	9780	3,3959	24.87	#N/A	99.48		Concentration is below t
CMAMCal L5.d	MDMA	#N/A	IDMA-d5	125.00	110142	6444	17.0911	125.17	#N/A	100.13		
CMAMQC_L2.d	MDMA	#N/A	IDMA-d5	5.00	7253	10938	0.6632	4.86	#N/A	97.13		Limit It contains the wor
CMAMQC_L4.d	MDMA	#N/A	1DMA-d5	25.00	31464	10004	3.1451	23.03	#N/A	92.13		Emili. It contains the wor
CMAMSam_01.d	MDMA	#N/A	IDMA-d5		476	620	0.7665	5.61	#N/A			Pass if the Final
CMAMSam_02.d	MDMA	#N/A	IDMA-d5		7651	10821	0.7070	5.18	: #N/A			
CMAMSam_03.d	MDMA	#81/A	IDMA-d5		16710	11355	1.4716	10.78	#N/A		*	Concentration is not less
<	mmary (+						4				Þ	001100111011011011000
EADY 🛗									III (II	1 🛄 -	+ 100%	than the Limit.

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

6	Save the changes to the template, iii_3_Custom_QuantReport_ESTD _Summary.xlt. • You have to clear the results first.		Reporting tab in the Ribbon. Click File > Save As. In the Save As dialog box, type iii_3_Custom_QuantReport_ESTD_Summary. Verify the folder selected in Save in is correct.	•	The Save as type is Excel Template.
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## In This Book

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

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July 2013

G3335-90159

