Notices

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Software Revision
This guide is valid for the B.07.xx or later revision of the Agilent MassHunter Workstation Software - Quantitative Analysis program, until superseded.

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

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Safety Notices

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

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A WARNING notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in personal injury or death. Do not proceed beyond a WARNING notice until the indicated conditions are fully understood and met.
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The Quantitative Analysis Report Builder Familiarization Guide presents step-by-step exercises to help you learn to use the Report Builder program. You can do these exercises with the demo batches DrugsofAbuse and LC-QTOF Pesticide, shipped with the system in the Data folder of your installation disk, or with data you acquire.
Access the Report Builder

The MassHunter Quantitative Analysis Report Builder software is installed with MassHunter Quantitative Analysis B.08.00.

To access the Report Builder, go to Start > Agilent MassHunter > Report Builder. To create a shortcut icon on your desktop, right-click Report Builder in the Start menu and select Send to > Desktop.

Report Builder menu


- Use the Edit section to Delete an element.
- Use the Font, Alignment, and Colors sections to set the font styles, results alignment, and the fore color and back color in the report template.
- Use the Insert section to insert Page, Textbox, Image, List, Table, and Scriptbox elements into a report template.
- Use the Preview section to Setup the Quantitative Analysis batch file that can then be used to Preview the report output.
Access Report Builder PDF Templates

Report Builder PDF Templates are located at: D:\MassHunter\Report Templates\Quant\PDF-ReportBuilder.

In this directory there are PDF templates for `Quant` analysis and `Unknowns` analysis. Each of these templates can be opened and edited in the Report Builder.

Example report outputs are provided on the MassHunter Quantitative Analysis Shipping DVD at \Supplemental\MassHunter\Report Templates\Quant\Index.

Before You Begin

Either back up the PDF templates before you modify them, or immediately save the PDF template as a new template. Modified or damaged PDF templates can only be restored by re-installing the MassHunter Quantitative Analysis software.
1 Introduction
Before You Begin
Modify a Report Template

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In this section you will modify a report template by completing a series of tasks, such as replacing the logo, modifying tables, filtering results, adjusting graphic sizes, and adding an expression.
1. Open the Report Builder.

2. Select File > Open.

3. Navigate to D:\MassHunter\Report Templates\Quant\PDF-ReportBuilder\Quant, and open Gen_Samples_ISTD.template.xml.

4. The Agilent logo is in the upper right corner of the report template. This is the header section of the report page.

   Select the logo graphic. The filename AgilentLogo.tif appears in the right panel.

5. If the logo you want to use is in the same file location as the report template, enter the file name in the File field, and press Enter.

   If the logo you want to use is in a different location than the report template, enter the full path of the file in the File field, and press Enter.

6. Save the template.
Replace a Column in the Report

You can replace a column in a table through either the Columns window or the Textbox Properties window.

Replace a column using the Columns window

1. Navigate to D:\MassHunter\Report Templates\Quant\PDF-ReportBuilder\Quant, and open Gen_Samples_ISTD.template.xml.
2. Right-click the ResponseRatio column header, and select Select > Table (Results).
3. In the Columns field in the Properties pane, click the ellipsis.
2 Modify a Report Template
Replace a column using the Columns window

4 In the Columns window, select ResponseRatio, and click Remove.

5 Select TargetPeak from the Select columns from: list, select SignalToNoiseRatio in the Available columns pane, and click Add.

6 Click Move Up or Move Down to move the column to the desired location.

7 Click OK. The ResponseRatio column is replaced by the SignalToNoiseRatio column.
Replace a column using the Textbox Properties window

1. Navigate to D:\MassHunter\Report Templates\Quant\PDF-ReportBuilder\Quant, and open Gen_Samples_ISTD.template.xml.

2. Right-click the ResponseRatio column header, and select Textbox Properties.

3. Select SignalToNoiseRatio from the Field Caption > Field list, and click OK.
2 Modify a Report Template
Replace a column using the Textbox Properties window

4 Right-click the ResponseRatio value, and select Textbox Properties.

5 Select SignalToNoiseRatio from the Field Value > Field list, and click OK.

6 The ResponseRatio column is replaced by the SignalToNoiseRatio column. Save the template.
Remove a Column From the Report

1. Navigate to D:\MassHunter\Report Templates\Quant\PDF-ReportBuilder\Quant, and open Gen_Samples_ISTD.template.xml.

2. Select the table that contains the **QualifierResponseRatio** column (Results).

3. In the **Column Count** field in the Properties pane, change the column count from 9 to **8**.

   ![Image showing the Column Count field]

   The last column in the table, **QualifierResponseRatio**, is removed.

4. Save the template.

   **To remove a column that is not the last column in the table:**

   1. Right-click the column to remove, and select **Move Right**.

      Repeat this step until the column is the last column in the table.

   2. In the **Column Count** field in the Properties pane, reduce the column count by 1 to remove the last column.

   3. Save the template.
Modify a Report Template
Adjust the Width of a Column

Adjust the Width of a Column

1. Navigate to D:\MassHunter\Report Templates\Quant\PDF-ReportBuilder\Quant, and open Gen_Samples_ISTD.template.xml.

2. Select a table.

3. In the Relative Column Widths field in the Properties pane, change the values to adjust the widths of the columns in the table.

4. Save the template.
Filter Results Using Special Conditions

1. Navigate to D:\MassHunter\Report Templates\Quant\PDF-ReportBuilder\Quant, and open Gen_Sample_AboveLOQ.template.xml. This report filters results lower than the LOQ. Use this procedure to modify the data binding to filter results lower than the LOD.

2. Select the Results table in the Properties pane, and click the ellipsis in the Data Binding field.
2 Modify a Report Template
Filter Results Using Special Conditions

3 In the **Data Binding** window, select **Target Peak**, and then select **AND <CalculatedConcentration> >= <TargetCompound:LimitOfQuantitation>**.

4 Click **Edit**.

5 Select **LimitOfDetection** from the **Field name** list, and click **OK**.

6 Click **OK**.

7 Save the template.
Adjust the Size of a Graphic

1. Navigate to D:\MassHunter\Report Templates\Quant\PDF-ReportBuilder\Quant, and open Gen_Samples_ISTD.template.xml.

2. Select the graphic to resize.

3. In the Height and Width Percentage fields in the Properties pane, change the values to adjust the size of the graphic.

4. Save the template.
2 Modify a Report Template
Add a New Column to an Existing Report

Add a New Column to an Existing Report

1. Navigate to D:\MassHunter\Report Templates\Quant\PDF-ReportBuilder\Quant, and open Gen_Samples_ESTD.template.xml.

2. Select the Results table from the Properties pane, and change the Column Count value from 8 to 9.

A new empty column is added to the end of the table.
3 Add a textbox to the empty column header and value. Separately select the empty cells in the table, and click **Textbox**.

4 Right-click the column header textbox and select **Textbox Properties**.
2 Modify a Report Template
Add a New Column to an Existing Report

5 Select **Field caption**, select **TargetPeak** from the **Binding name** list, and then select **SignalToNoiseRatio** from the **Field** list.

6 Click **OK**.

7 Right-click the column value textbox and select **Textbox Properties**.
8. Select **Field value**, select **TargetPeak** from the **Binding name** list, and then select **SignalToNoiseRatio** from the **Field** list.

9. Select **True** for the **Bold** field in the **Properties** pane for the field caption and field value.

10. Save the template.
Modify a Report Template

Edit an Expression

1. Navigate to D:\MassHunter\Report Templates\Quant\PDF-ReportBuilder\Quant, and open Gen_Samples_ISTD.template.xml.

2. Select the expression in the FinalConc column in Table 2, and click the ellipsis for the Expression field in the Properties pane.

3. Modify the expression as needed in the ExpressionWindow window, and click OK.

4. Save the template.
Preview the Report

After changes have been made to the report template, you can preview the report by setting up the Report Builder with your dataset.

1. Navigate to D:\MassHunter\Report Templates\Quant\PDF-ReportBuilder\Quant, and open Gen_Samples_ISTD.template.xml.

2. Click **Preview**.

3. In the **Setup Preview** window, click **Browse**, then navigate to and select your batch file.

4. Select the **Instrument type** to match your dataset.
5 Click Preview. A PDF report is generated using the batch file selected.

Navigate the report page by page. Below is an example of page 4 using the DrugofAbuse dataset.

![Quantitative Analysis Sample Based Report](image)