

Agilent MassHunter Workstation Software

Quantitative Analysis

**Report Builder
Familiarization Guide**



Agilent Technologies

Notices

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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for the B.07.xx or later revision of the Agilent MassHunter Workstation Software - Quantitative Analysis program, until superseded.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_l-cms@agilent.com.

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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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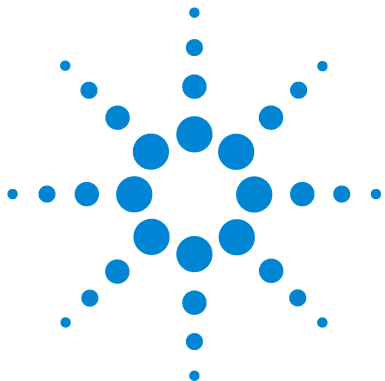
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The Quantitative Analysis Report Builder Familiarization Guide presents step-by-step exercises to help you learn to use the Report Builder program. You can do these exercises with the demo batches DrugsofAbuse and LC-QTOF Pesticide, shipped with the system in the **Data** folder of your installation disk, or with data you acquire.



Access the Report Builder

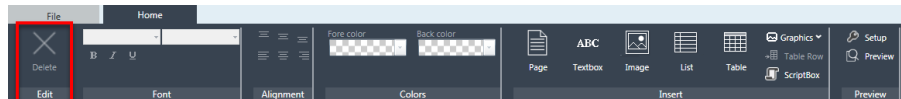
The MassHunter Quantitative Analysis Report Builder software is installed with MassHunter Quantitative Analysis B.08.00.

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**.

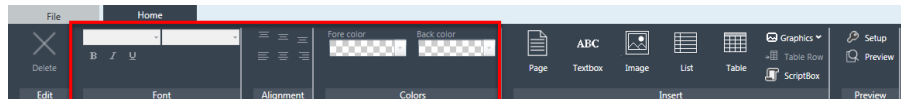
Report Builder menu

The Report Builder menu contains six sections: **Edit**, **Font**, **Alignment**, **Colors**, **Insert**, and **Preview**.

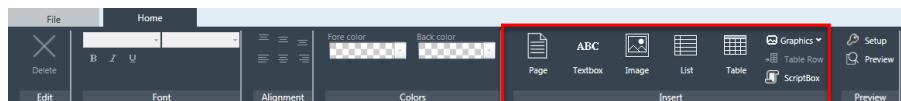
- Use the **Edit** section to **Delete** an element.



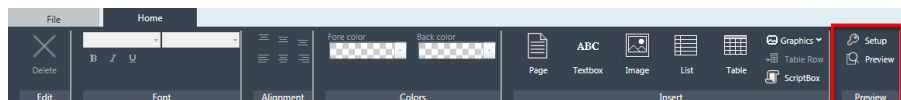
- Use the **Font**, **Alignment**, and **Colors** sections to set the font styles, results alignment, and the fore color and back color in the report template.



- Use the **Insert** section to insert **Page**, **Textbox**, **Image**, **List**, **Table**, and **Scriptbox** elements into a report template.



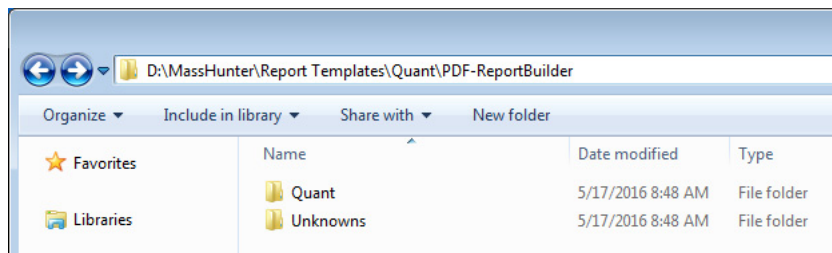
- Use the **Preview** section to **Setup** the Quantitative Analysis batch file that can then be used to **Preview** the report output.



Access Report Builder PDF Templates

Report Builder PDF Templates are located at:

D:\MassHunter\Report Templates\Quant\PDF-ReportBuilder.



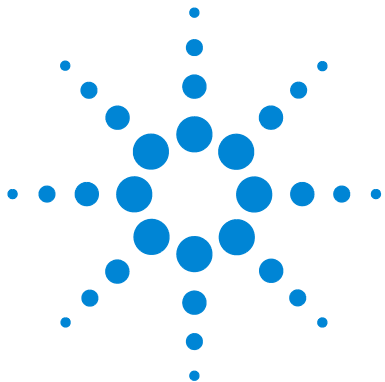
In this directory there are PDF templates for **Quant** analysis and **Unknowns** analysis. Each of these templates can be opened and edited in the Report Builder.

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



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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.



2 Modify a Report Template

Replace the Agilent Logo with Your Own

Replace the Agilent Logo with Your Own

- 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**.

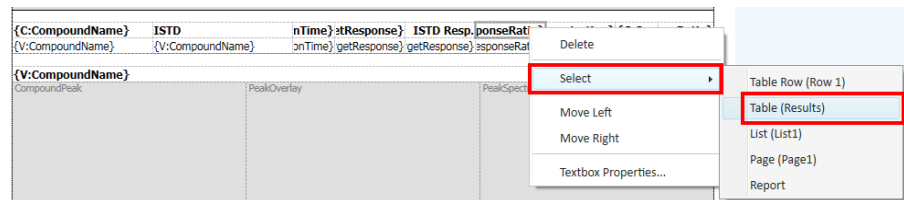
- 6 Save the template.

Replace a Column in the Report

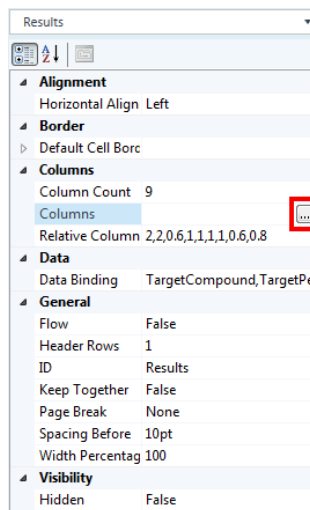
You can replace a column in a table through either the **Columns** window or the **Textbox Properties** window.

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)**.



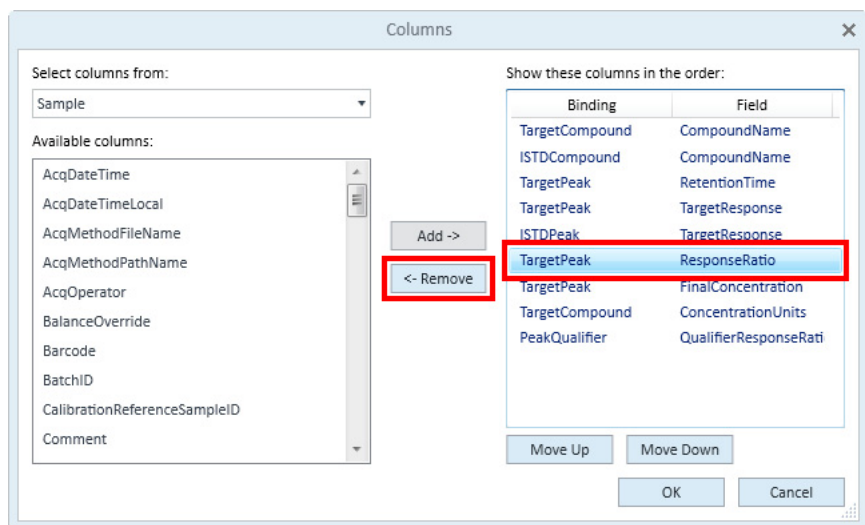
- 3 In the **Columns** field in the **Properties** pane, click the ellipsis.



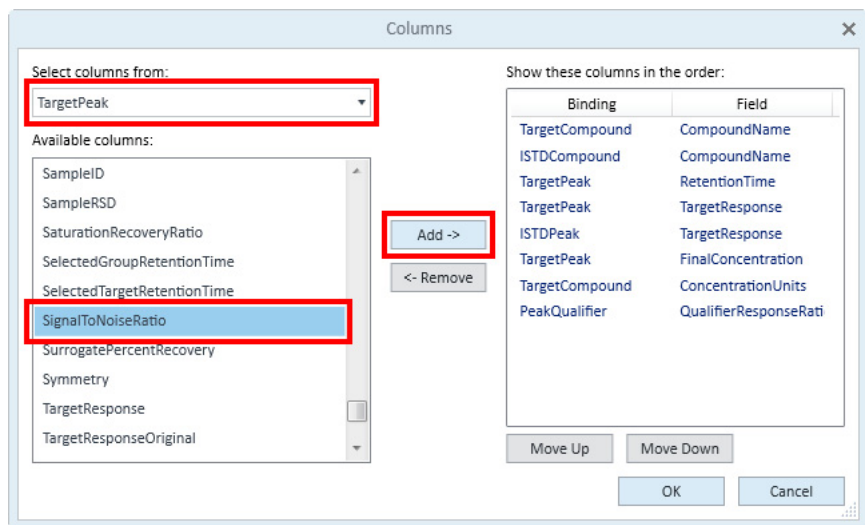
2 Modify a Report Template

Replace a column using the Columns window

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



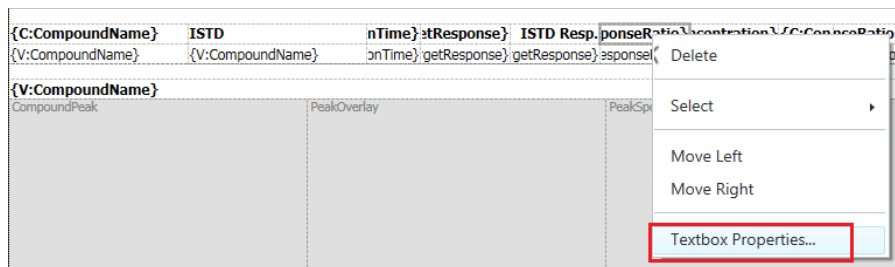
- 5 Select **TargetPeak** from the **Select columns from:** list, select **SignalToNoiseRatio** in the **Available columns** pane, and click **Add**.



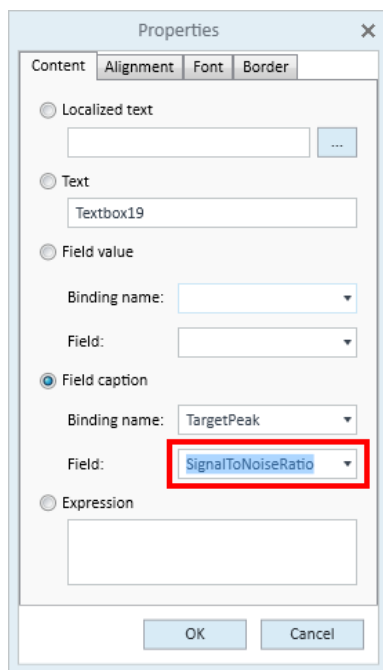
- 6 Click **Move Up** or **Move Down** to move the column to the desired location.
- 7 Click **OK**. The **ResponseRatio** column is replaced by the **SignalToNoiseRatio** column.

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**.



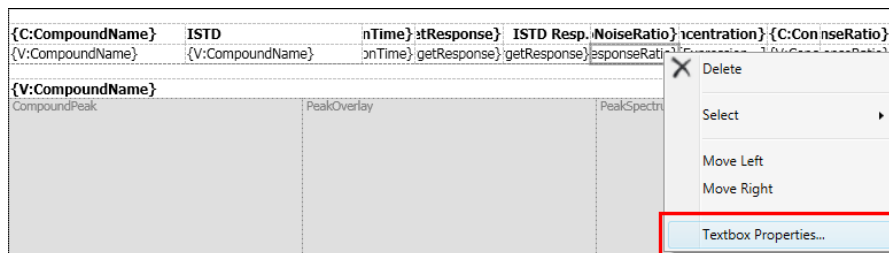
- 3 Select **SignalToNoiseRatio** from the **Field Caption > Field** list, and click **OK**.



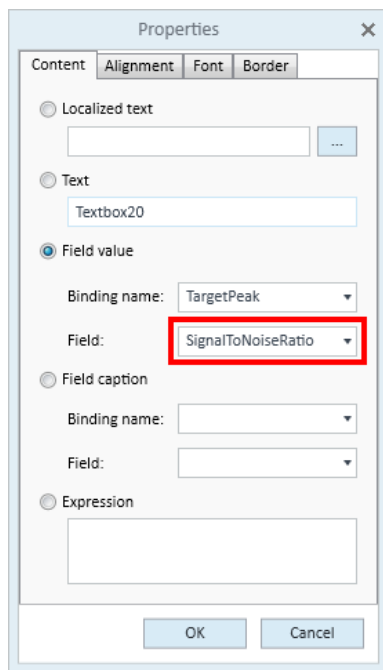
2 Modify a Report Template

Replace a column using the Textbox Properties window

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



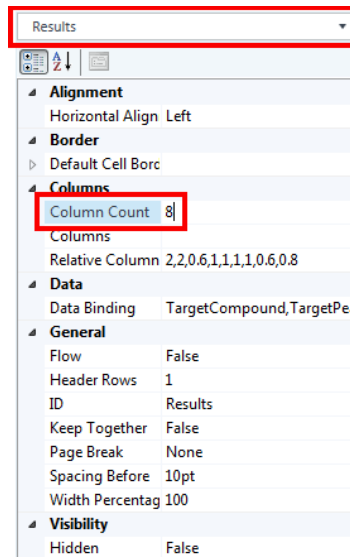
- 5 Select **SignalToNoiseRatio** from the **Field Value > Field** list, and click **OK**



- 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**.



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.

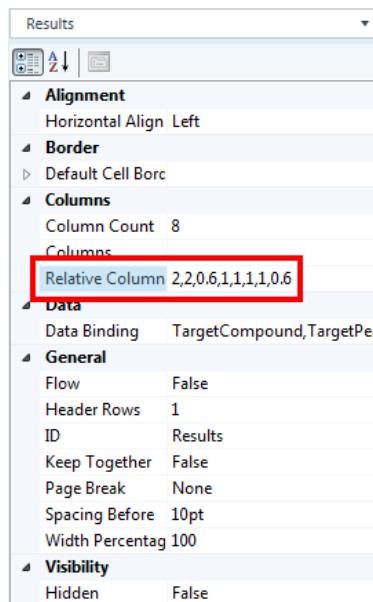
- 2 In the **Column Count** field in the **Properties** pane, reduce the column count by 1 to remove the last column.
- 3 Save the template.

2 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.



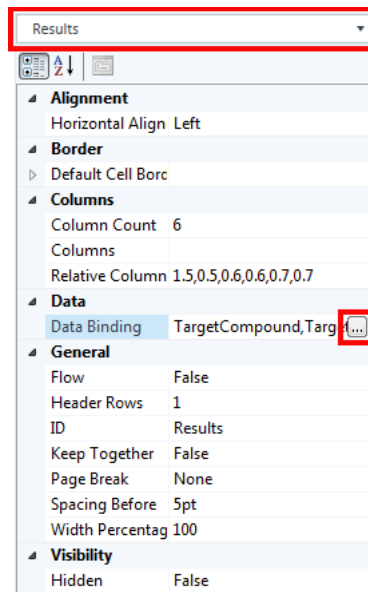
- 4 Save the template.

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**.

The screenshot shows the 'Data Binding' dialog box. On the left, under 'Data bindings', 'TargetPeak' is selected. The 'Binding name' is 'TargetPeak'. The 'Data name' is 'Peak'. The 'Filters' section contains the following conditions: '<BatchID> = <TargetCompound:BatchID>', 'AND <SampleID> = <TargetCompound:SampleID>', 'AND <CompoundID> = <TargetCompound:CompoundID>', 'AND <PeakID> = <TargetCompound:PrimaryHitPeakID>', and 'AND <CalculatedConcentration> >= <TargetCompound:LimitOfQuantitation>'. The last filter is highlighted. The 'Edit...' button next to it is also highlighted. The 'Orders' section is empty. The 'Expression' field is empty. The 'Left outer join' checkbox is unchecked. Buttons for 'Add', 'Delete', 'Move Up', 'Move Down', 'New...', 'Edit...', and 'Delete' are visible.

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

The screenshot shows the 'Data Binding Filter' dialog box. The 'Field' is 'CalculatedConcentration'. The 'Operator' is '>='. The 'Concatenation type' is 'AND'. The 'Value' section has 'Fixed value' and 'Bound value' fields. The 'Binding name' is 'TargetCompound'. The 'Field name' dropdown is set to 'LimitOfDetection'. Buttons for 'OK' and 'Cancel' are visible.

- 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.

The screenshot displays the Report Builder interface. On the left, the template editor shows a large rectangular area labeled "Sample Chromatogram" which is highlighted with a red border. Below it is a table with columns for compound name, ISTD response, and ISTD response ratio. On the right, the Properties pane is open to the "General" tab. The "Height" field is set to 180pt and the "Width" field is set to 100%. Both fields are highlighted with red boxes. Other properties like "ID", "Name", "BatchID", "SampleID", "Misc", "MS", and "Signal" are also visible in the pane.

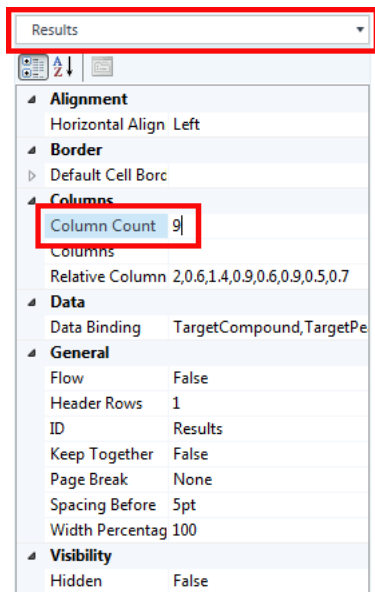
- 4 Save the template.

2 Modify a Report Template

Add a New Column to an Existing Report

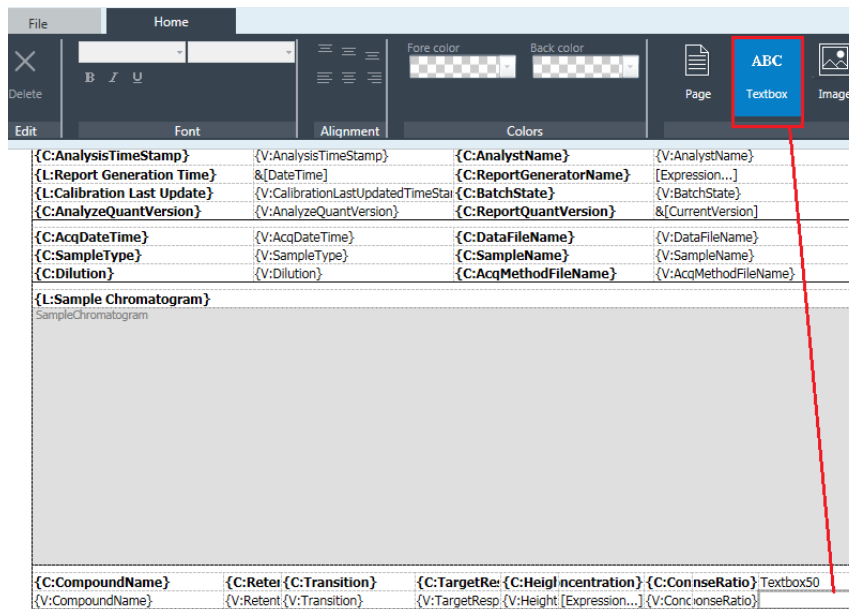
Add a New Column to an Existing Report

- 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**.

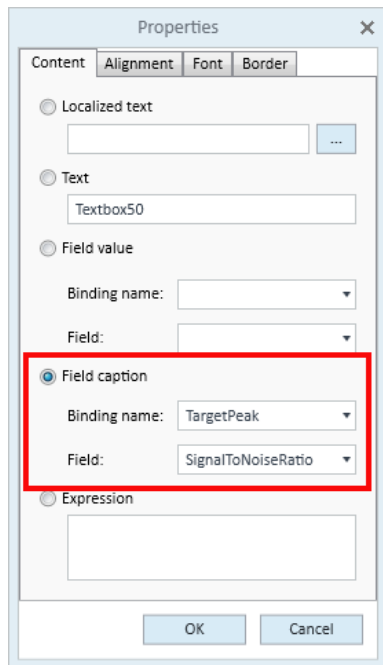


- 4 Right-click the column header textbox and select **Textbox Properties**.

2 Modify a Report Template

Add a New Column to an Existing Report

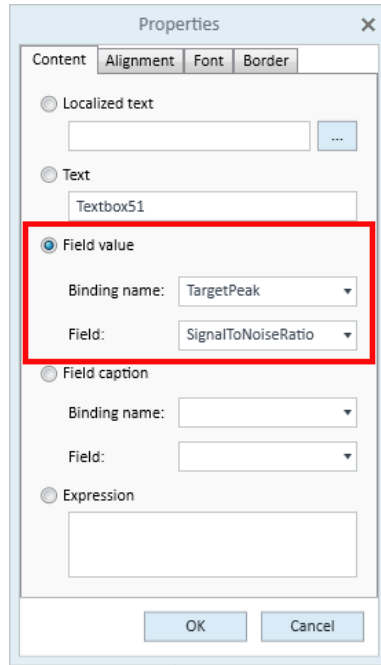
- 5 Select **Field caption**, select **TargetPeak** from the **Binding name** list, and then select **SignalToNoiseRatio** from the **Field** list.



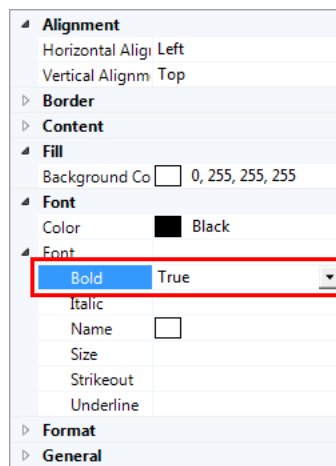
The screenshot shows a 'Properties' dialog box with four tabs: 'Content', 'Alignment', 'Font', and 'Border'. The 'Content' tab is active. It contains several radio button options: 'Localized text', 'Text', 'Field value', 'Field caption', and 'Expression'. The 'Field caption' option is selected and highlighted with a red rectangular box. Below this option, there are two dropdown menus: 'Binding name' is set to 'TargetPeak' and 'Field' is set to 'SignalToNoiseRatio'. At the bottom of the dialog are 'OK' and 'Cancel' buttons.

- 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.



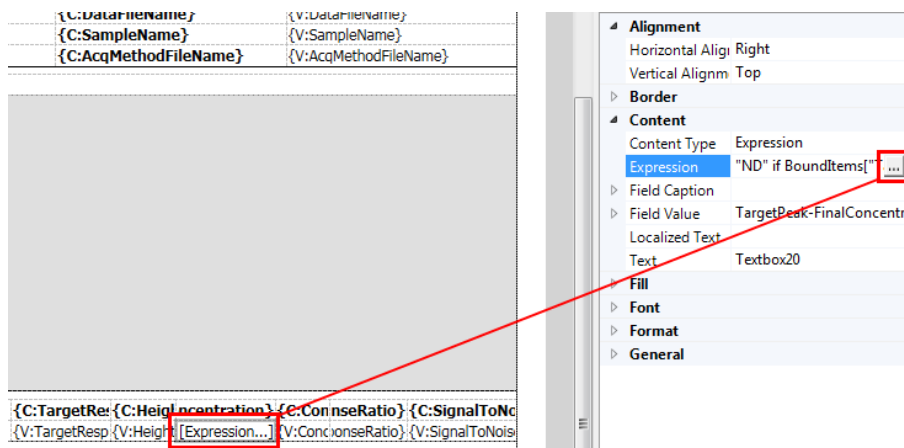
- 9 Select **True** for the **Bold** field in the **Properties** pane for the field caption and field value.



- 10 Save the template.

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.

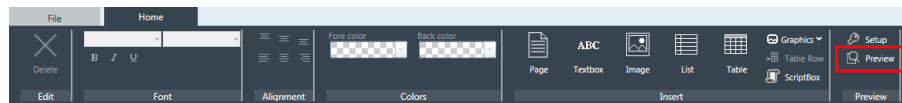


- 3 Modify the expression as needed in the **ExpressionWindow** window, and click **OK**.
- 4 Save the template.

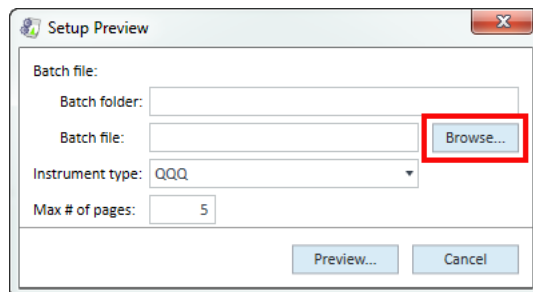
Preview the Report

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

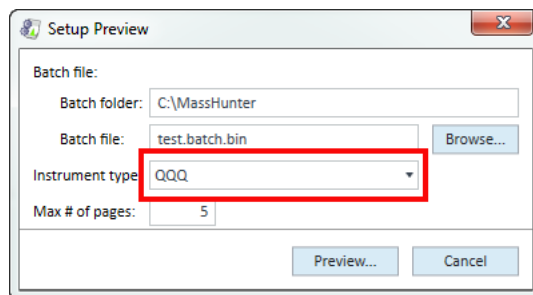
- 1 Navigate to **D:\MassHunter\Report Templates\Quant\PDF-ReportBuilder\Quant**, and open **Gen_Samples_ISTD.template.xml**.
- 2 Click **Preview**.



- 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.

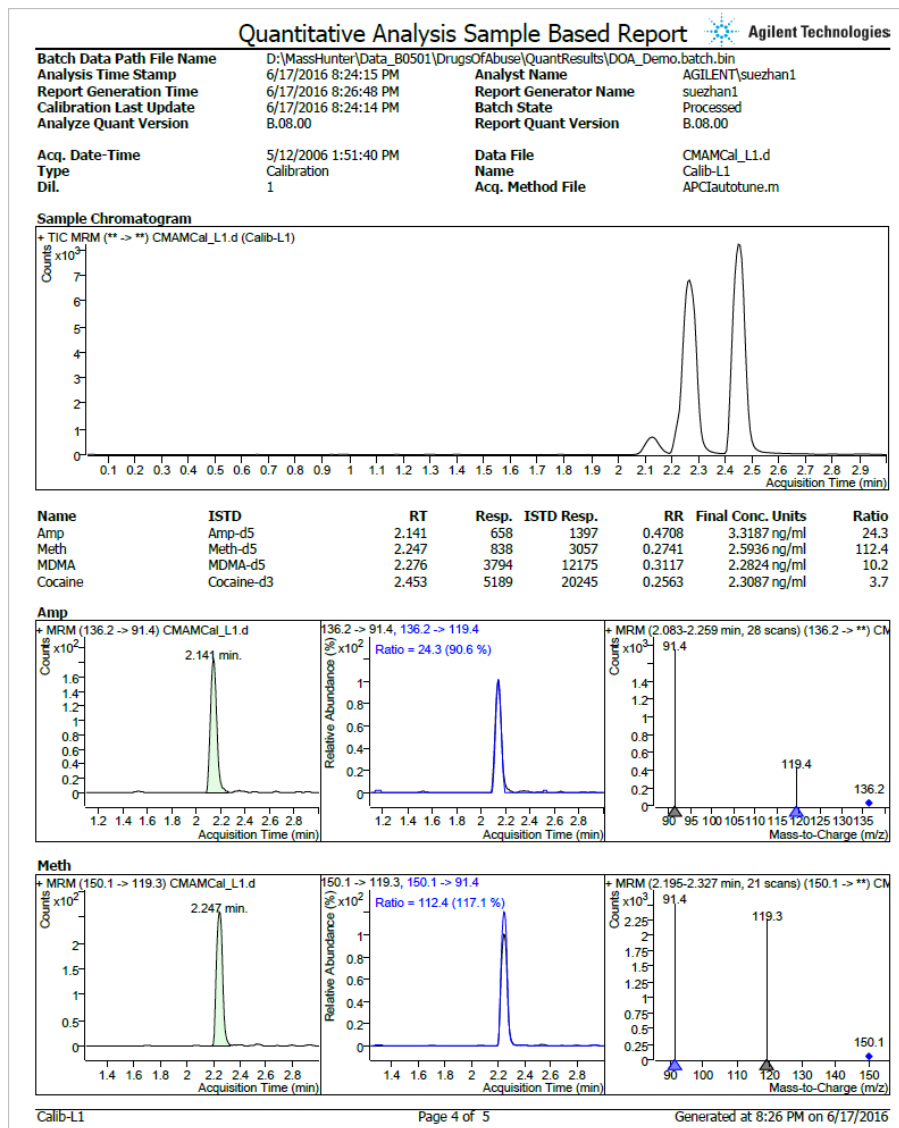


2 Modify a Report Template

Preview the Report

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.





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