Agilent

Agilent MassHunter Workstation Software

Report Builder Familiarization Guide

Notices

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1 Introduction

Access the Report Builder 5

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Before You Begin 7

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

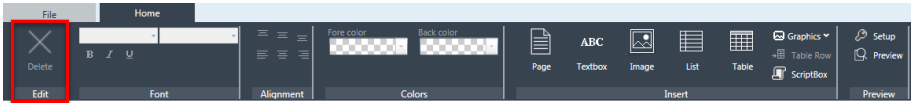
The MassHunter Quantitative Analysis Report Builder software is installed with MassHunter Quantitative Analysis.

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**.

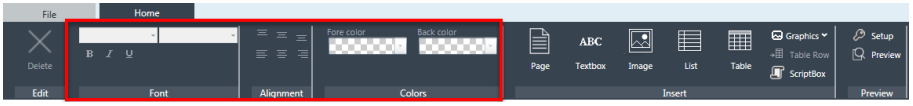
Report Builder menu

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

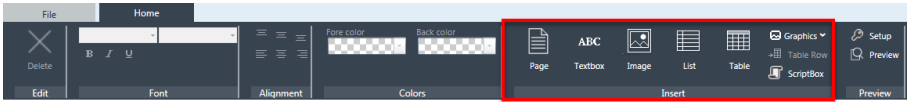
- Use the **Edit** section to **Delete** an element.



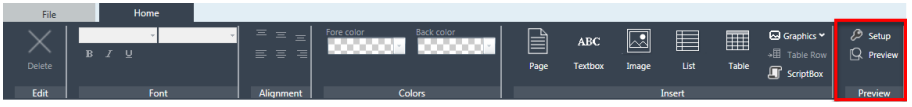
- Use the **Font, Alignment**, and **Colors** sections to set the font styles, results alignment, and the fore color and back color in the report template.



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

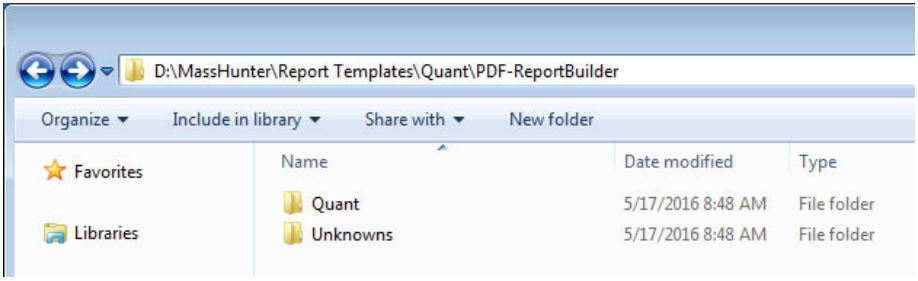


- Use the **Preview** section to **Setup** the Quantitative Analysis batch file that can then be used to **Preview** the report output.



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.

2 Report Template Workflows

Quantitative Analysis - Calibration Report Template 9

Unknowns Analysis - Area Percent Report Template 50

In this section, you will create example report templates from scratch to give you a better understanding of how to use the MassHunter Quantitative Analysis Report Builder.

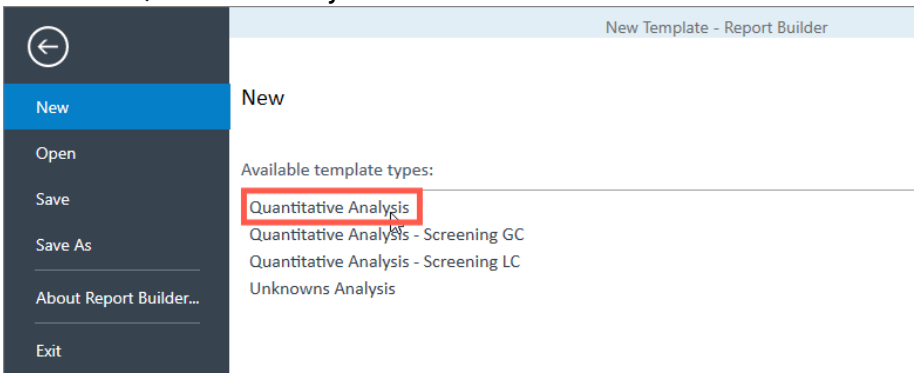
Quantitative Analysis - Calibration Report Template

For this example, you will create a Calibration Report by completing the following procedures.

1. **Create a new Quantitative Analysis report template** on page 9
2. **Edit the Batch information table** on page 14
3. **Add a Calibration Curve table with a graph** on page 17
4. **Add a Calibration Results table** on page 30
5. **Add a report title** on page 46
6. **Preview the report template** on page 48

Create a new Quantitative Analysis report template

To create a new Quantitative Analysis report template, select **File > New**, and then select **Quantitative Analysis**.



Each template type links to a different dataset. A dataset is an in-memory relational database that stores all of the information on and the relationships between samples, compounds, qualifiers, and calibration levels.

In a Quantitative Analysis dataset, a one-to-many (1:n) relationship exists between the following tables:

- Each **Batch** (sample) has one or more **TargetCompounds**.

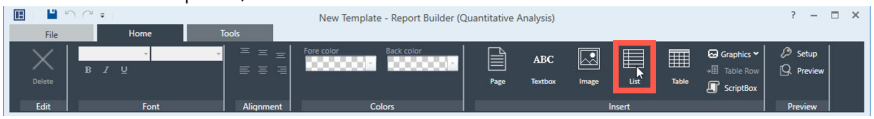
- Each **TargetCompound** (method) has one or more **TargetQualifiers** (method).
- Each **TargetCompound** (method) has one or more **Peaks** (result).
- Each **Qualifier** (method) has one or more **QualifierPeaks** (result).
- Each **TargetCompound** has one **Calibration** with many levels.

As a general rule, Target tables hold the method, and Peak tables hold the results:

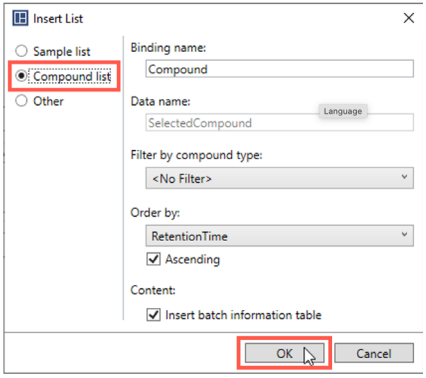
- **TargetCompound table** - contains the method information for compounds
- **TargetQualifier table** - contains the method information for their qualifiers
- **Peak table** - contains the result information for compounds
- **PeakQualifier table** - contains the result information for their qualifiers

Insert a list

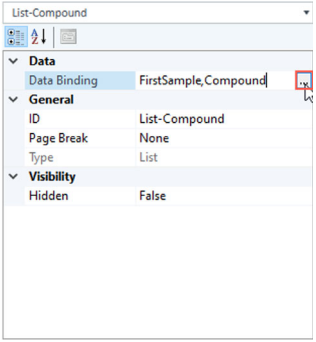
1 From the Insert pane, click **List**.



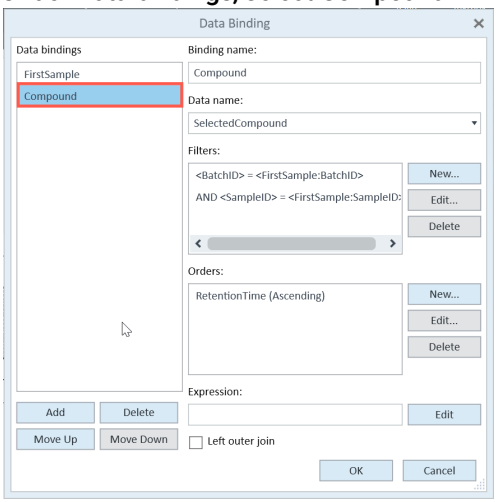
2 Select **Compound list**, and click **OK**.



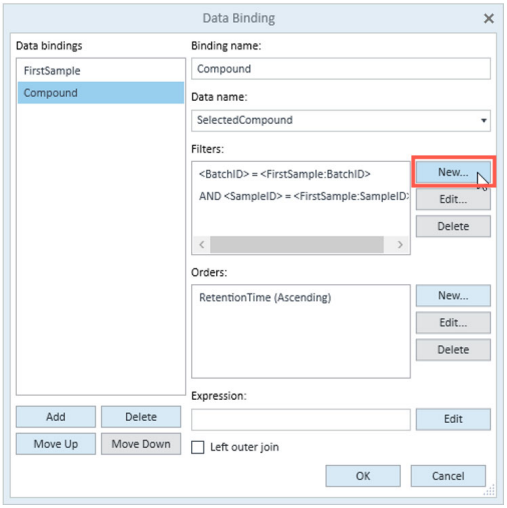
3 Edit the **Data Binding** filters. Click the **Data Binding** field in the Properties pane, then click the ellipsis.



a Under **Data bindings,** select **Compound**.



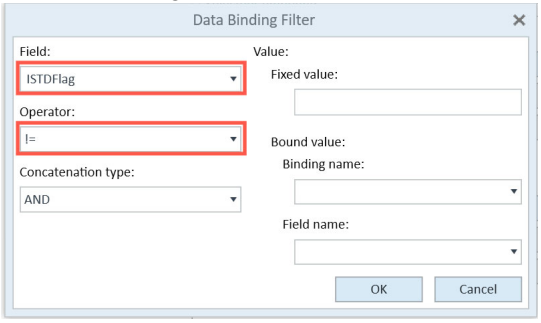
b Under **Filters**, click **New**.



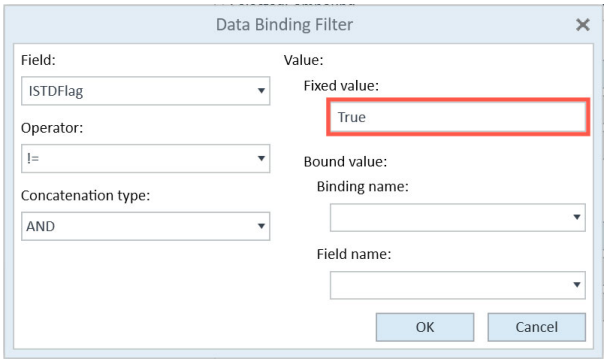
NOTE

An ID is a unique identifier for a table row in a Dataset. IDs such as BatchID, SampleID, CompoundID, etc. have system-assigned numbers. The combination of IDs can rapidly locate and link to the unique table row in a Quantitative Analysis dataset.

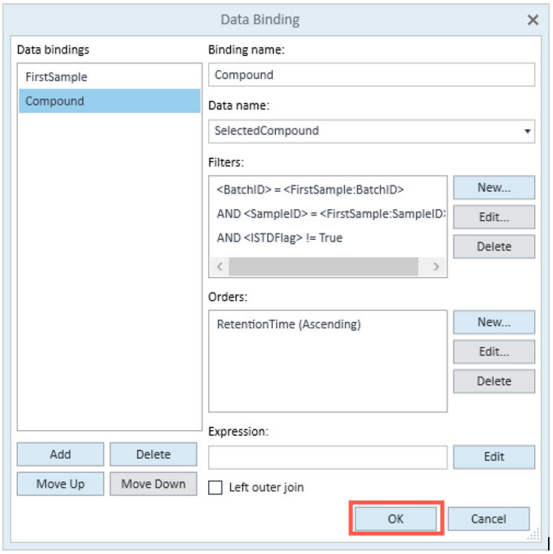
c Select **ISTDFlag** from the **Field** list, and select **!=** from the **Operator** list.



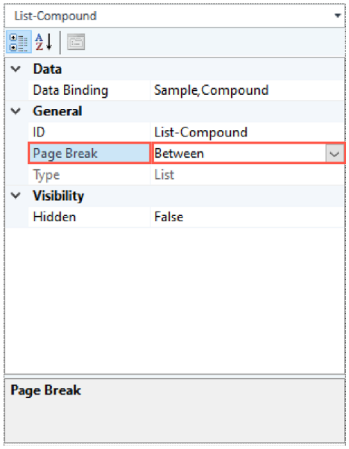
d Enter **True** in the **Fixed value** field, and click **OK**.



e Click **OK** to close the **Data Binding** window.

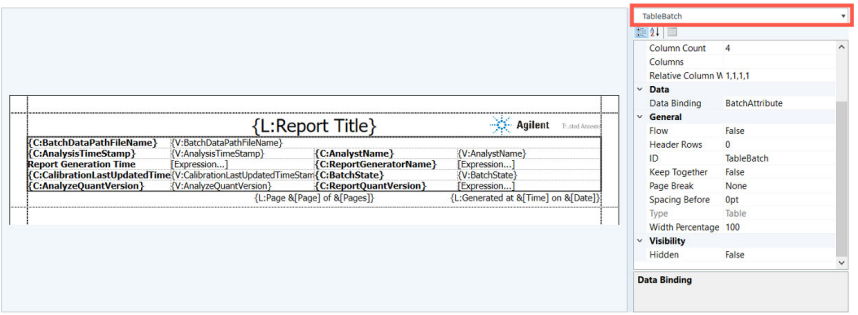


4 In the Properties pane, under General, click **Page Break**, then select **Between** from the list.



Edit the Batch information table

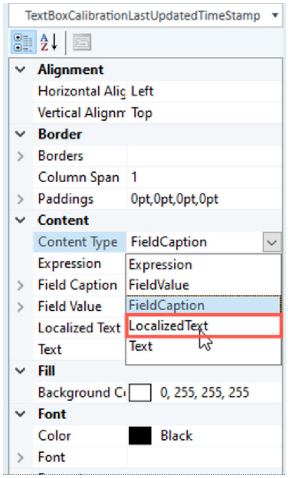
1 Select **TableBatch** from the drop-down menu at the top of the Properties pane. This highlights the table filled with batch information in your report. Each cell contains a caption, value, or expression.



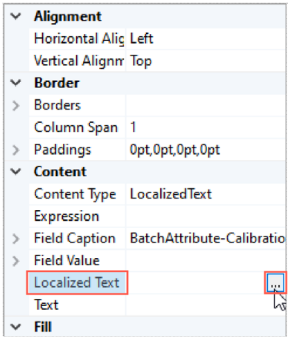
A table contains a header row, rows, and cells. Table cells can include the following:

- (**C**) - Caption (same term that is displayed in the Quantitative Analysis software)
- (**L**) - Localized text
- (**V**) - Value (same number that is displayed in the Quantitative Analysis software)
- (**E**) - Expressions (can be used to format numbers and data as desired)

2 The caption **{C:CalibrationLastUpdatedTimeStamp}** is too long to fit in its cell. Select it, click **Content Type** in the Properties pane, and select **LocalizedText** from the drop-down menu.

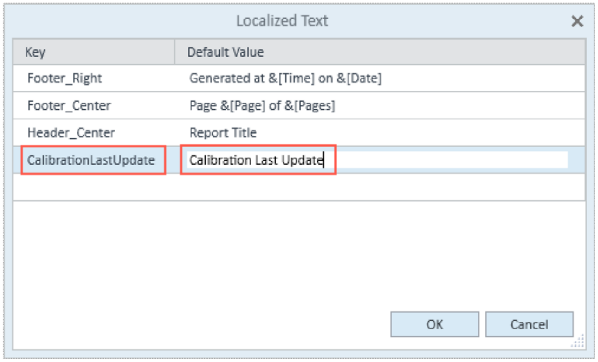


3 Click **Localized Text**, then click the ellipsis.



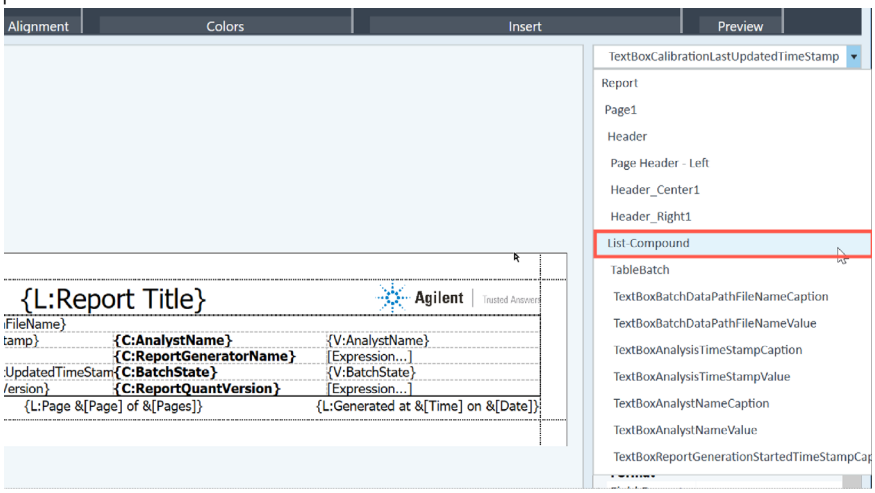
4 On the bottom row, enter **CalibrationLastUpdate** in the **Key** column, and **Calibration Last Update** in the **Default Value** column.

5 Click **OK**. The caption has been updated in the table.

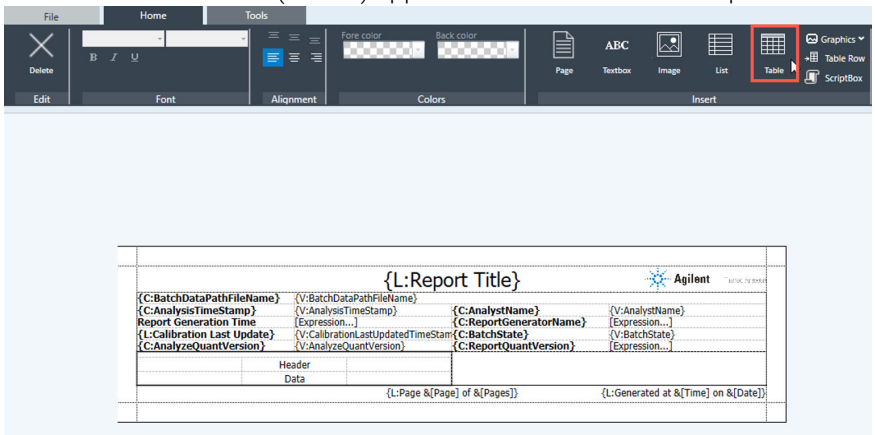


Add a Calibration Curve table with a graph

1 Select **List-Compound** from the drop-down menu at the top of the Properties pane.



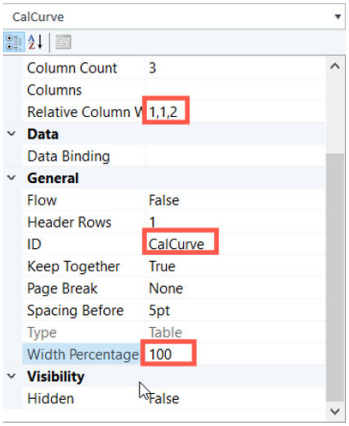
2 Click **Table**. A new table (Table1) appears at the bottom of the report.



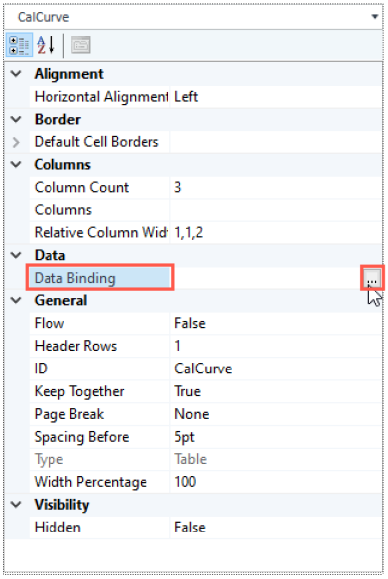
In the properties pane, make the following changes:

- Change the **Relative Column Width** to 1,1,2 to resize the columns in relation to the table width
- Enter CalCurve in the **ID** field to update the table name

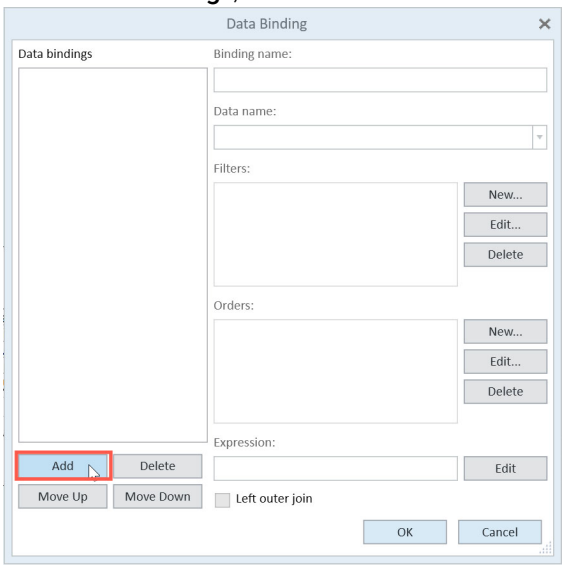
- Enter 100 in the **Width Percentage** field to resize the table width



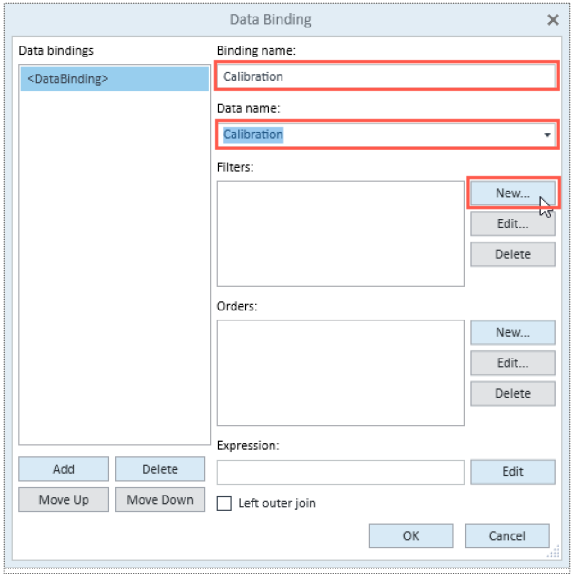
3 To add binding data to the table, click **Data Binding** in the Properties pane, then click the ellipsis.



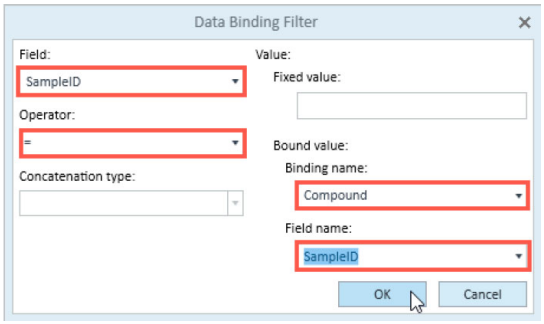
4 Under **Data Bindings**, click **Add**.



5 Enter **Calibration** for the **Binding name** and select **Calibration** from the **Data name** list. In the **Filters** section, click **New**.

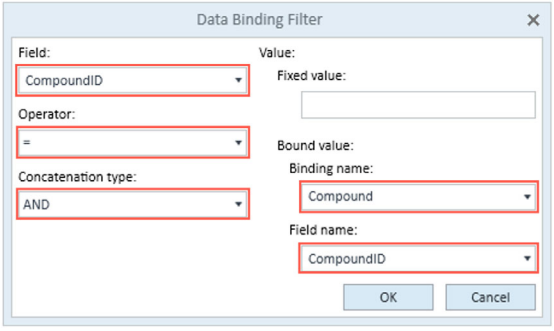


6 Select **SampleID** from the **Field** list and **=** from the **Operator** list. Select **Compound** from the **Binding name** list, and select **SampleID** from the **Field Name** list. Click **OK**.

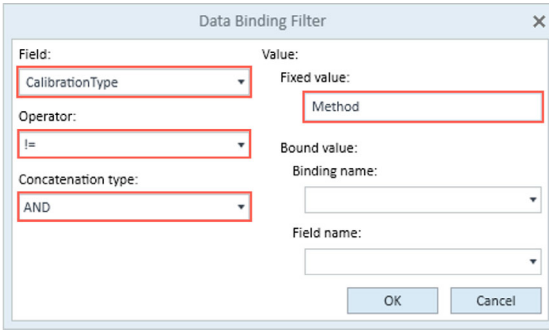


7 Add a data binding filter for each of the following configurations:

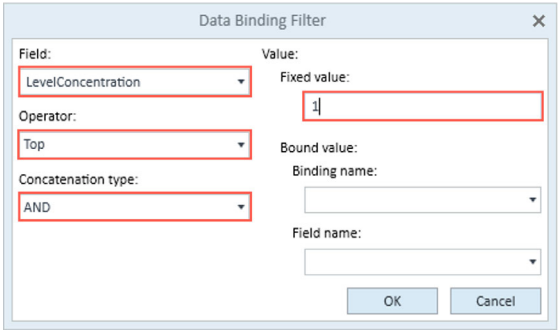
a Select **CompoundID** from the **Field** list, select **=** from the **Operator** list, select **AND** from the **Concatenation type** list, select **Compound** from the **Binding name** list, and select **CompoundID** from the **Field name** list.



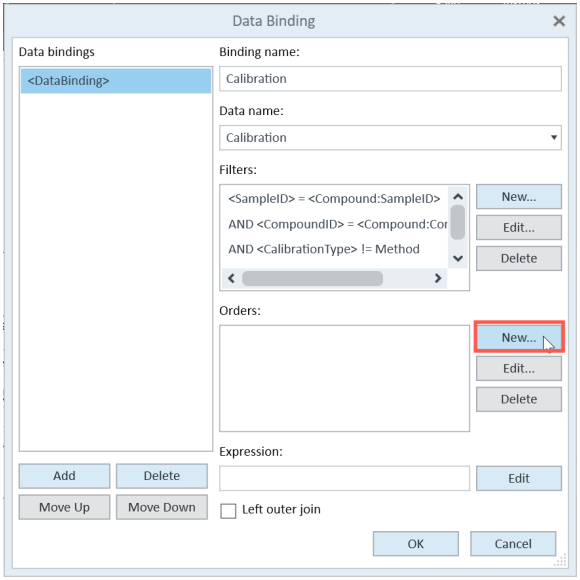
b Select **CalibrationType** from the **Field** list, select **!=** from the **Operator** list, select **AND** from the **Concatenation type** list, and select **Method** from the **Fixed value** list.



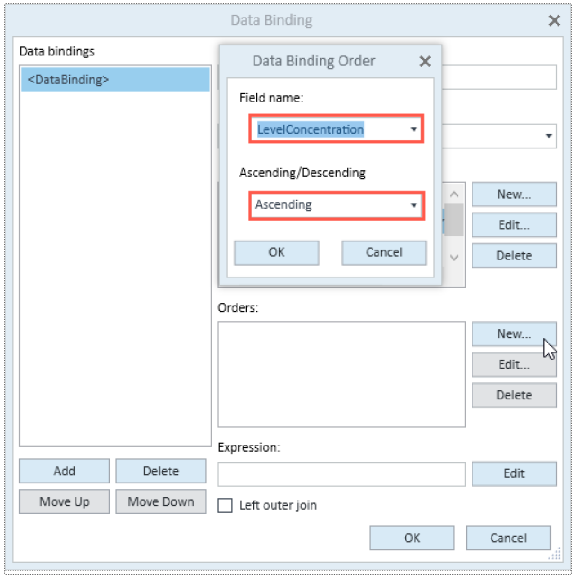
c Select **LevelConcentration** from the **Field** list, select **Top** from the **Operator** list, select **AND** from the **Concatenation type** list, and enter **1** for the **Fixed value**.



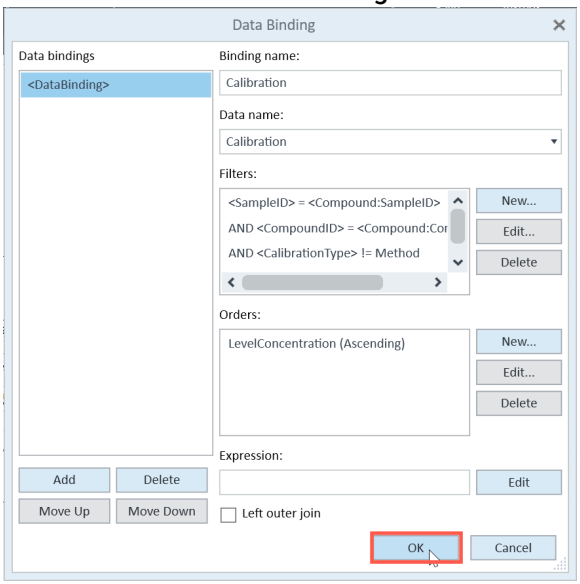
8 In the **Orders** section, click **New**.



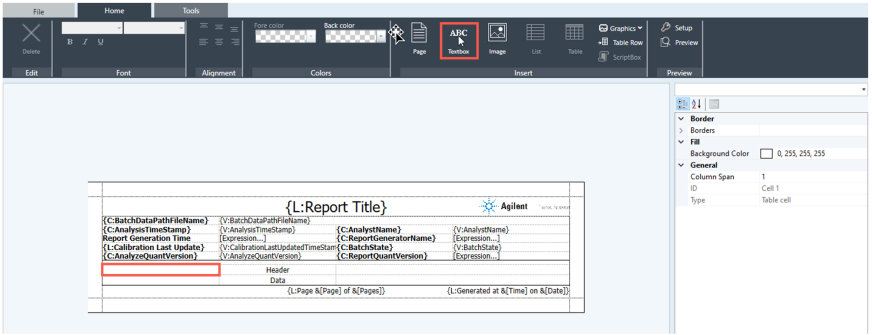
9 Select **LevelConcentration** from the **Field name** list, and select **Ascending** from the **Ascending/Descending** list. Click **OK**.



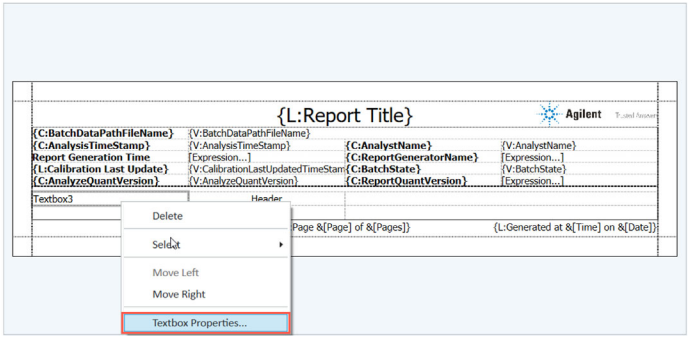
10 Click **OK** to close the **Data Binding** window.



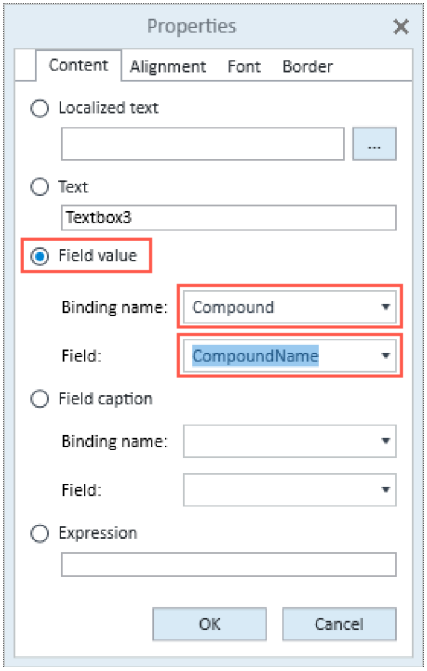
11 Select the empty cell to the left of the **Header**, and click **Textbox**.



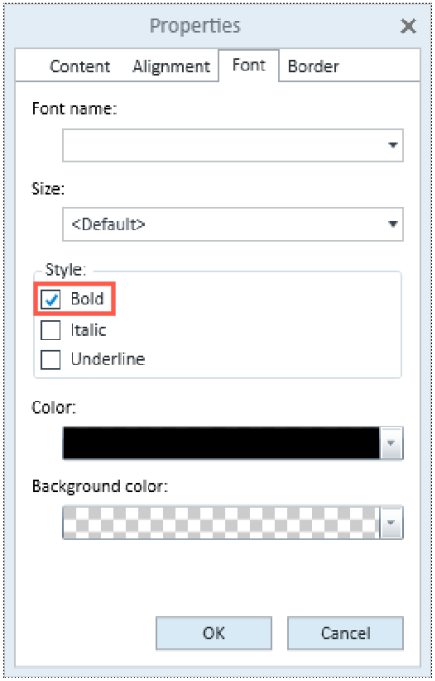
12 Right-click the cell and select **Textbox Properties**.



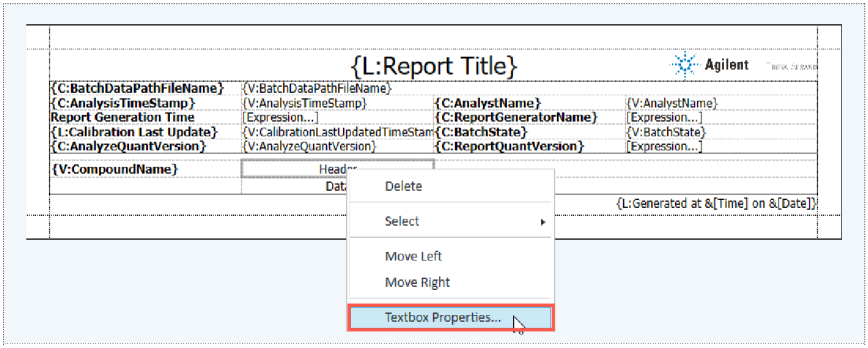
13 Select **Field value**, select **Compound** from the **Binding name** list, and then select **CompoundName** from the **Field** list.



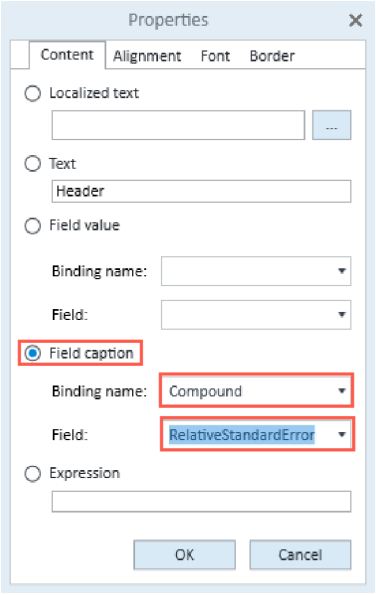
14 On the **Font** tab, select **Bold**, and click **OK**.



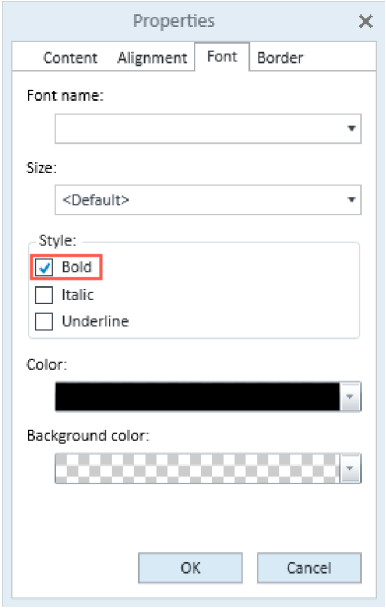
15 Right-click the **Header** cell and select **Textbox Properties**.



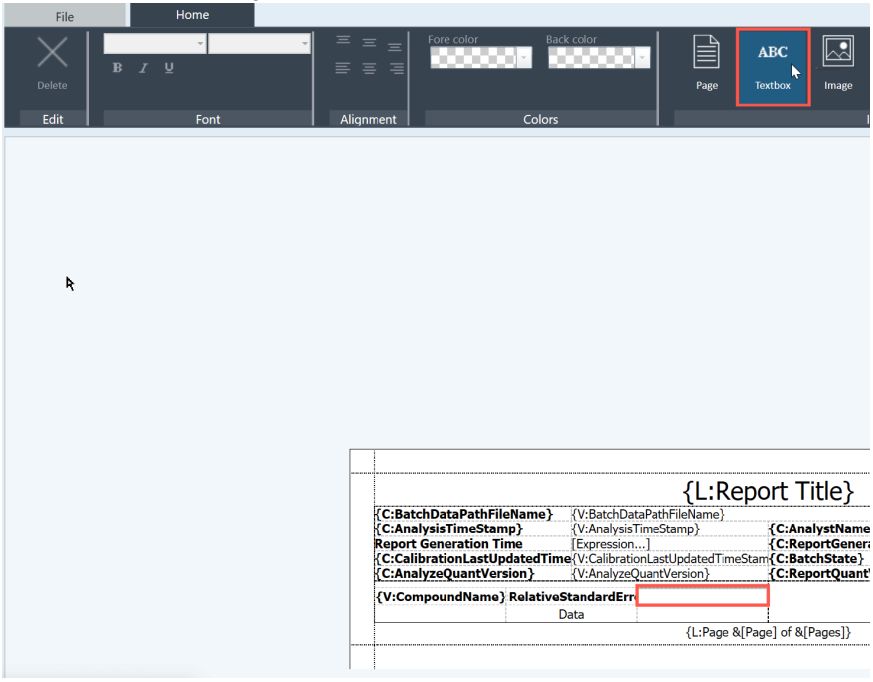
16 Select **Field Caption**, select **Compound** from the **Binding name** list, and select **RelativeStandandError** from the **Field** list.



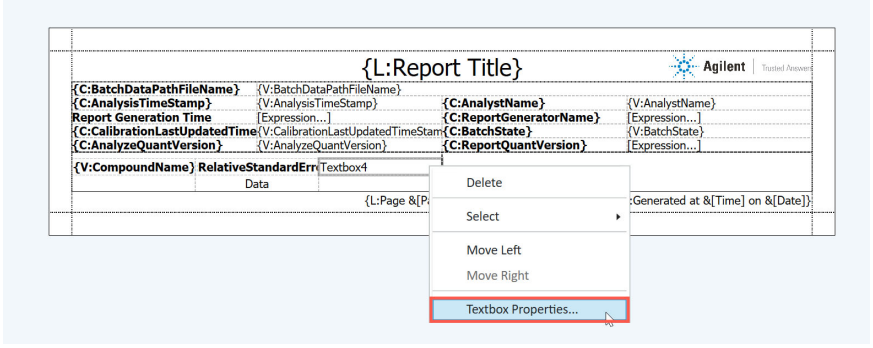
17 On the **Font** tab, select **Bold**, and click **OK**.



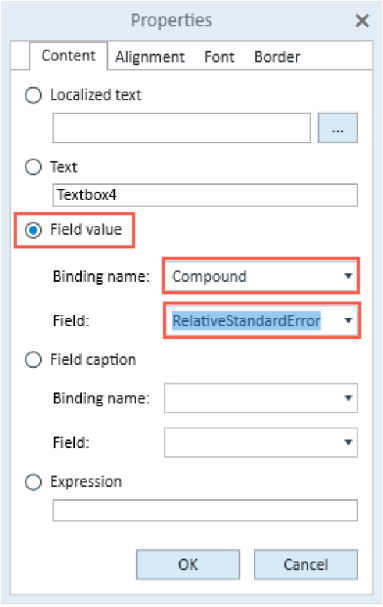
18 Select the cell to the right of **{C:RelativeStandardError}** and click **Textbox**.



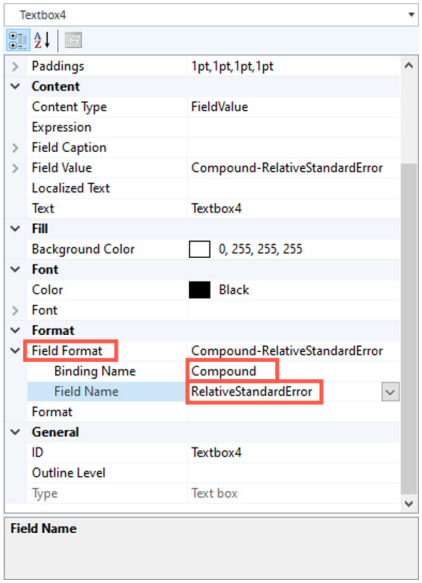
19 Right-click the cell and click **Textbox Properties**.



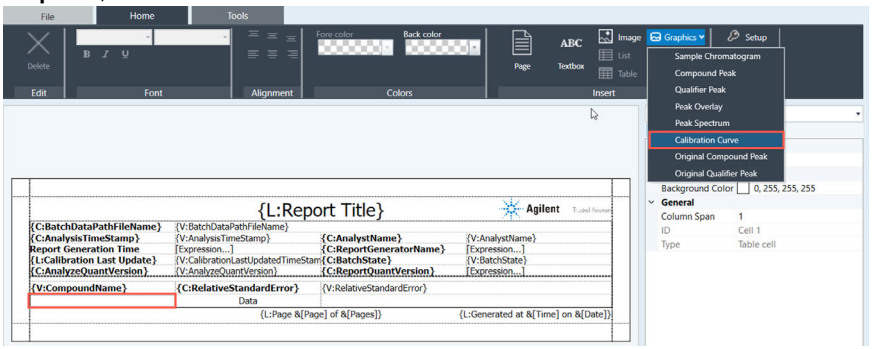
20 Select **Field Value**, select **Compound** from the **Binding name** list, and **RelativeStandardError** from the **Field** list. Click **OK**.



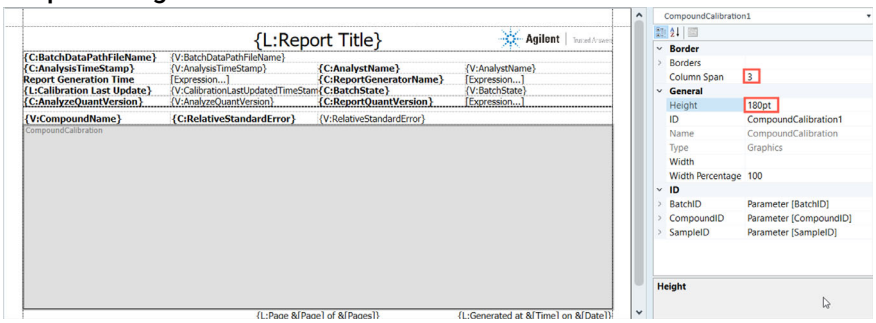
21 To use the same format in the current cell as is found in the Quantitative Analysis software, double-click **Field Format** in the **Properties** pane, and select **Compound** from the **Binding Name** list, and **RelativeStandardError** from the **Field Name** list.



22 To add a graphic, select the empty cell below **{V:CompoundName}**, click **Graphics**, and select **Calibration Curve**.



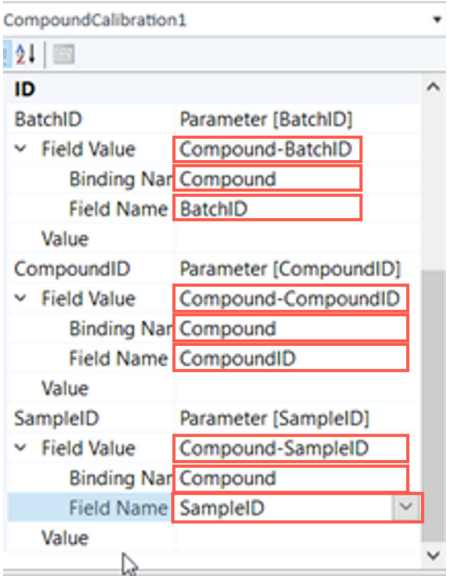
23 To resize the graphic, in the Properties pane, enter **3** for **Column Span** and **180pt** for **Height**.



ID fields like BatchID, SampleID, and CompoundID have system-assigned numbers which help to rapidly locate and link to unique table rows in a Quantitative Analysis dataset. To edit the ID fields, expand the ID section in the Properties pane. Enter the values for each ID:

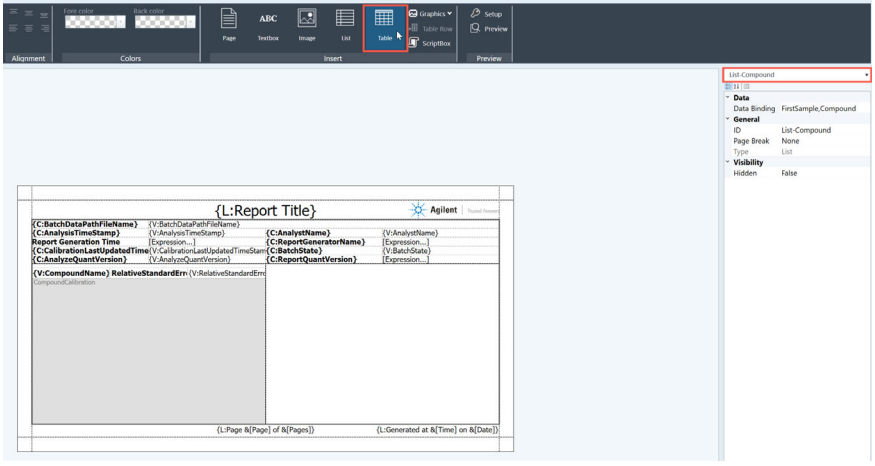
- BatchID
  - **Field Value**: Compound-BatchID
  - **Binding Name**: Compound
  - **Field Name**: BatchID
- CompoundID
  - **Field Value**: Compound-CompoundID
  - **Binding Name**: Compound
  - **Field Name**: CompoundID
- SampleID
  - **Field Value**: Compound-SampleID

- **Binding Name**: Compound
- **Field Name**: SampleID

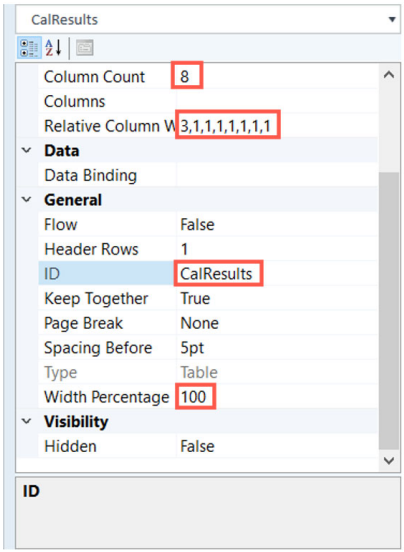


Add a Calibration Results table

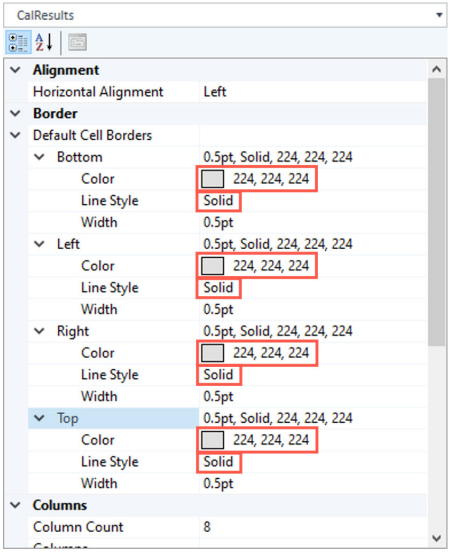
1 Select **List-Compound** from the list at the top of the Properties pane, and click **Table**.



2 In the Properties pane, adjust the number of columns by changing the **Column Count** to **8**, and adjust the widths of the columns by changing **Relative Column Widths** to **3,1,1,1,1,1,1,1**. Enter **CalResults** for **ID,** and **100** for **Width Percentage**.

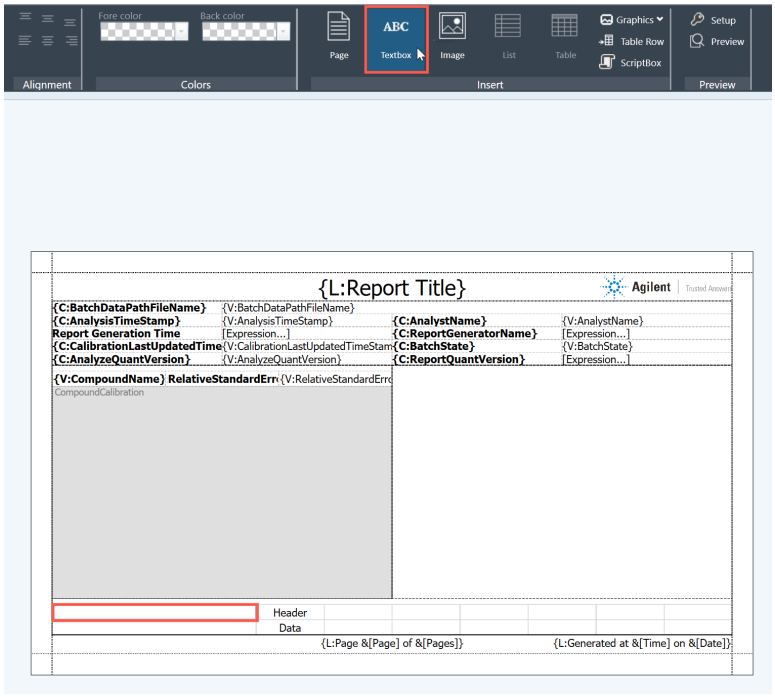


3 To add a border to the table, select **Solid** from the **Line Style** list and select a **Color** for each of the cell borders.

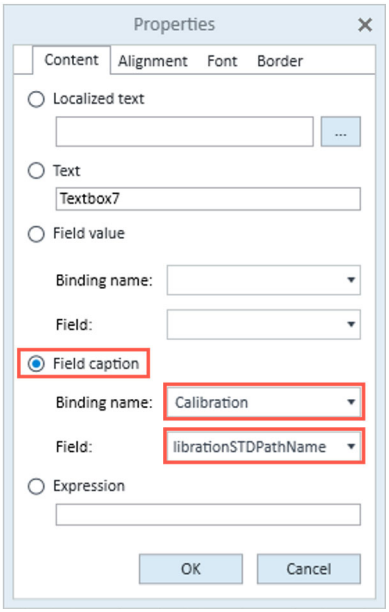


4 Repeat steps 3-10 from the section **Add a Calibration Curve table with a graph** on page 17 to add binding data to the table.

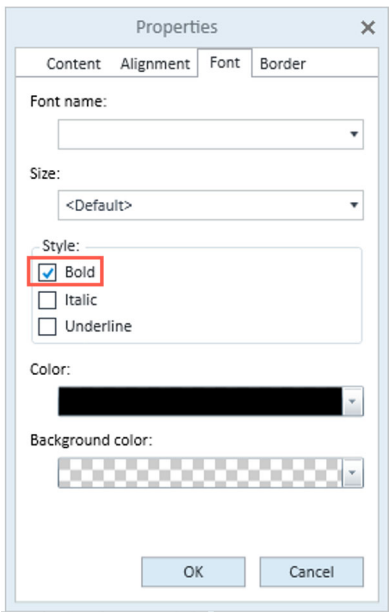
5 Select the first cell in the first row of the table, and click **Textbox**.



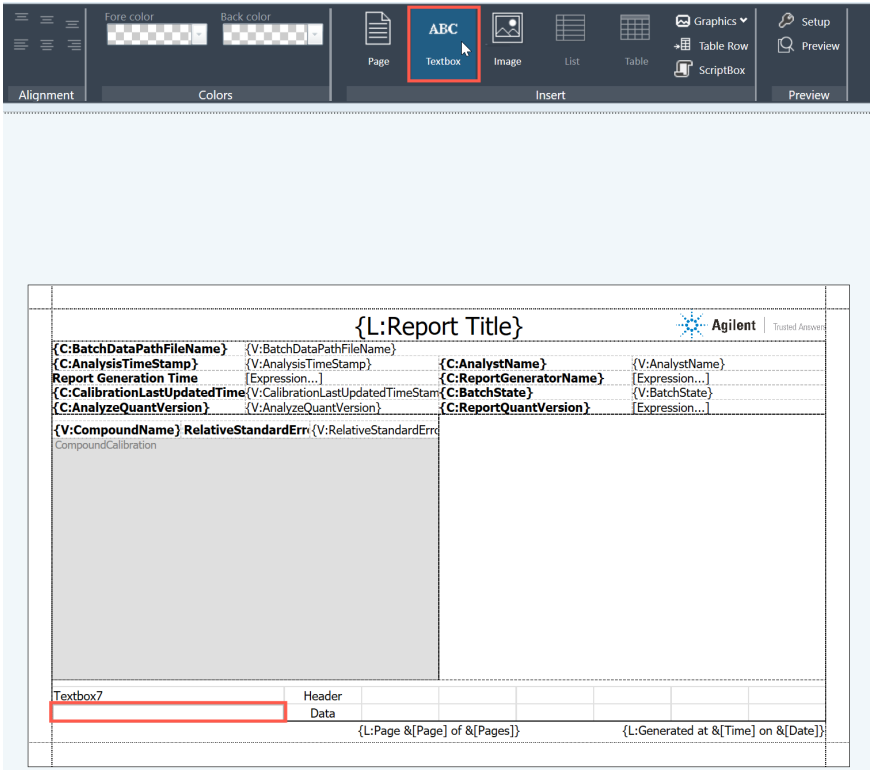
6 Right-click the cell and select **Textbox Properties**. Select **Field Caption,** select **Calibration** from the **Binding name** list, and **CalibrationSTDPathName** from the **Field** list.



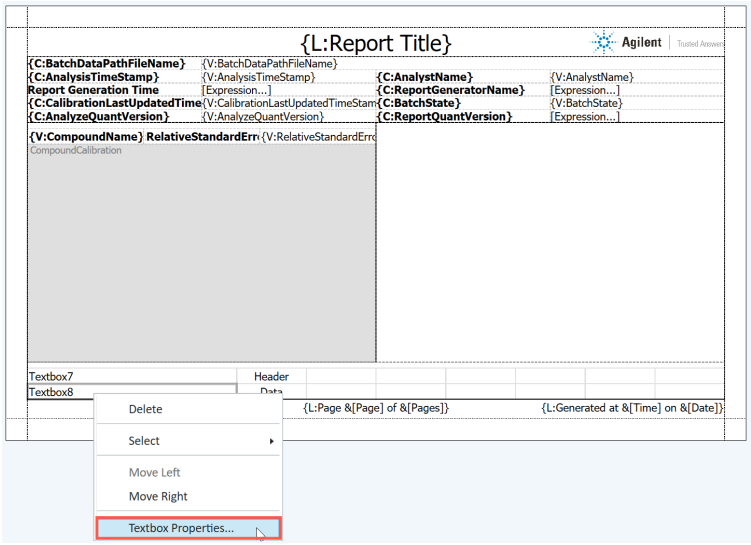
7 On the **Font** tab, select **Bold**. Click **OK**.



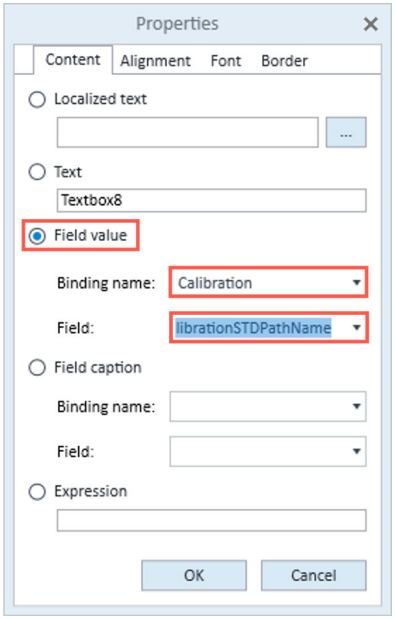
8 Select the first cell in the second row of the table, and click **Textbox**.



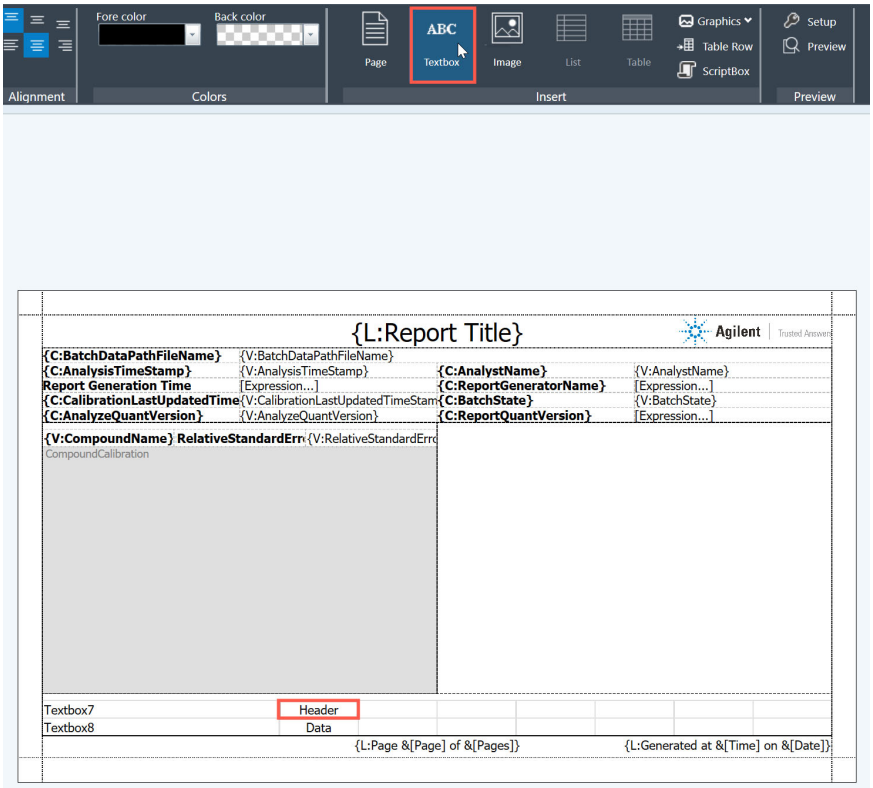
9 Right-click the cell and select **Textbox Properties**.



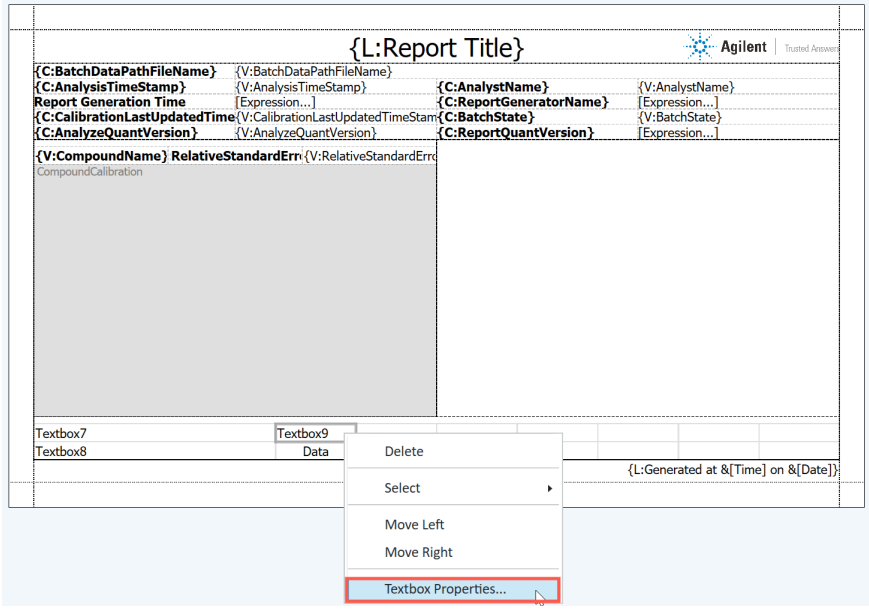
10 Select **Field Value**, select **Calibration** from the **Binding name** list, and select **CalibrationSTDPathName** from the **Field** list. Click **OK**.



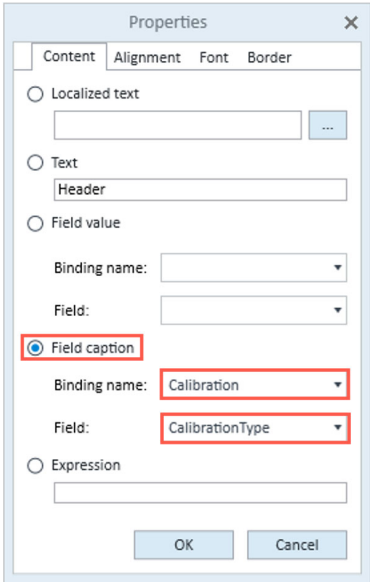
11 Select the cell labeled **Header**, and click **Textbox**.



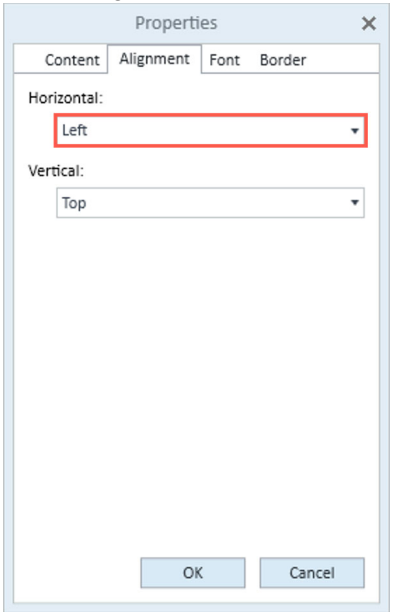
12 Right-click the textbox, and select **Textbox Properties**.



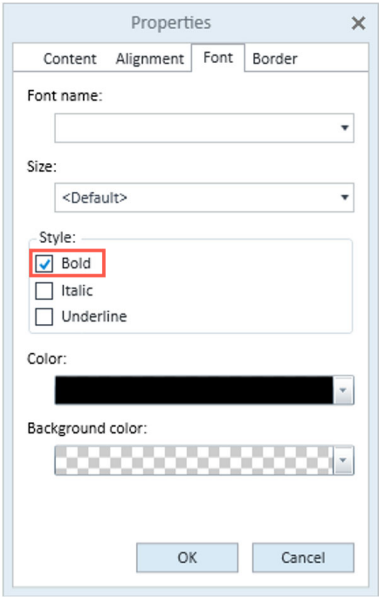
13 Select **Field Caption**, select **Calibration** from the **Binding name** list, and **CalibrationType** from the **Field** list.



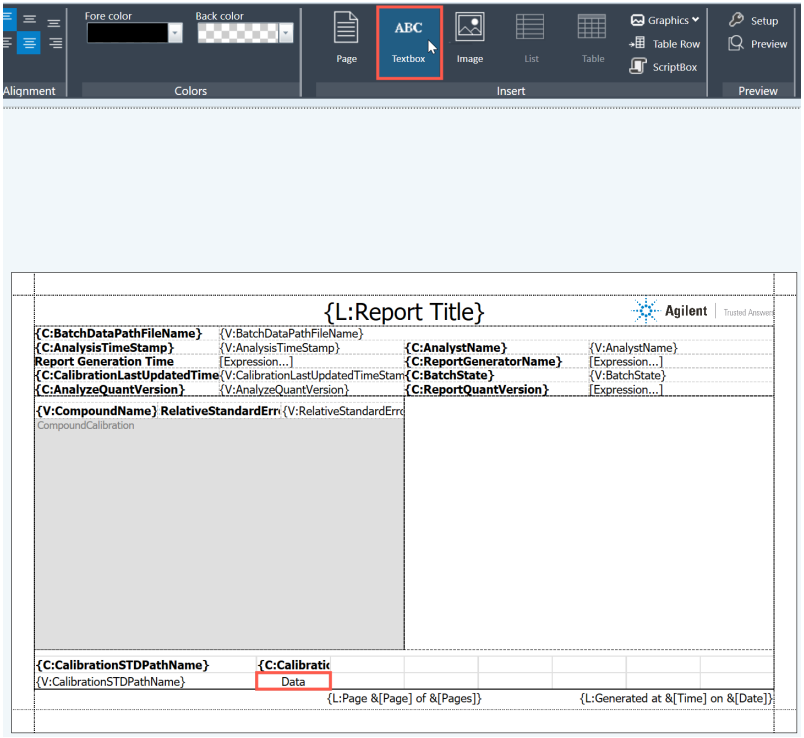
14 On the **Alignment** tab, select **Left** from the **Horizontal** list.



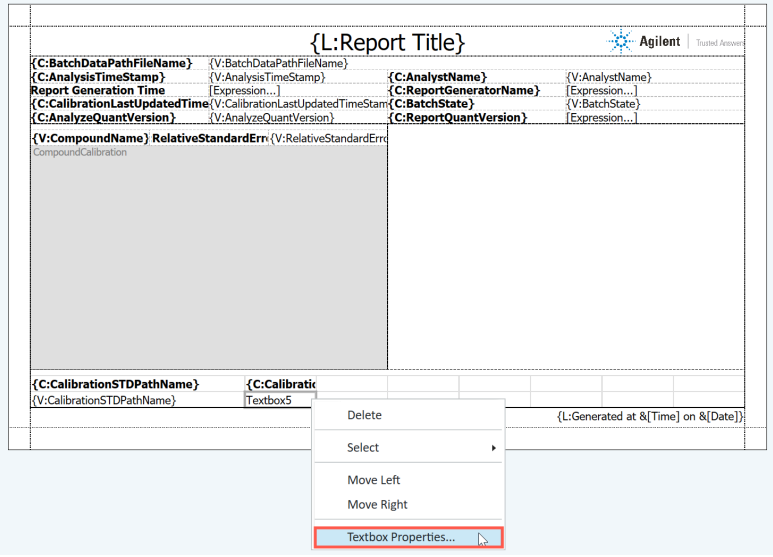
15 On the **Font** tab, select **Bold**. Click **OK**.



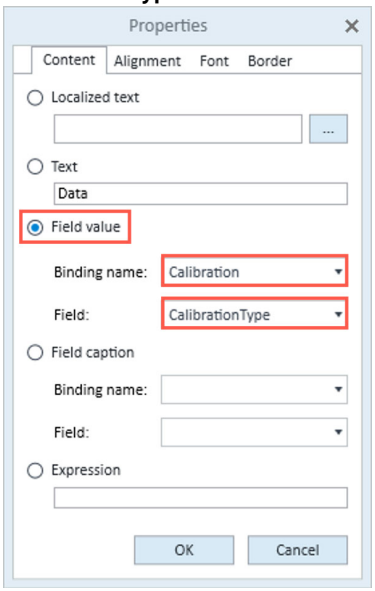
16 Select the cell labeled **Data**, and click **Textbox**.



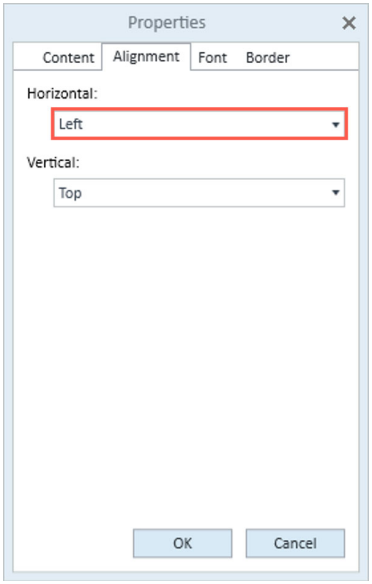
17 Right-click the cell, and select **Textbox Properties**.



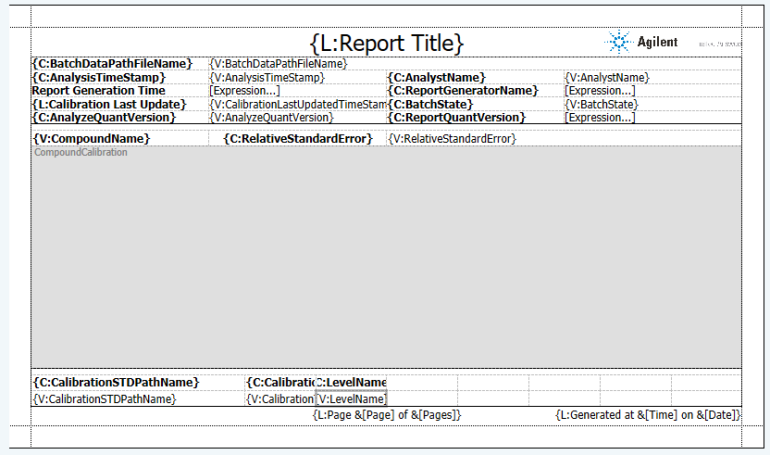
18 Select **Field Value**, select **Calibration** from the **Binding name** list, and select **CalibrationType** from the **Field** list.



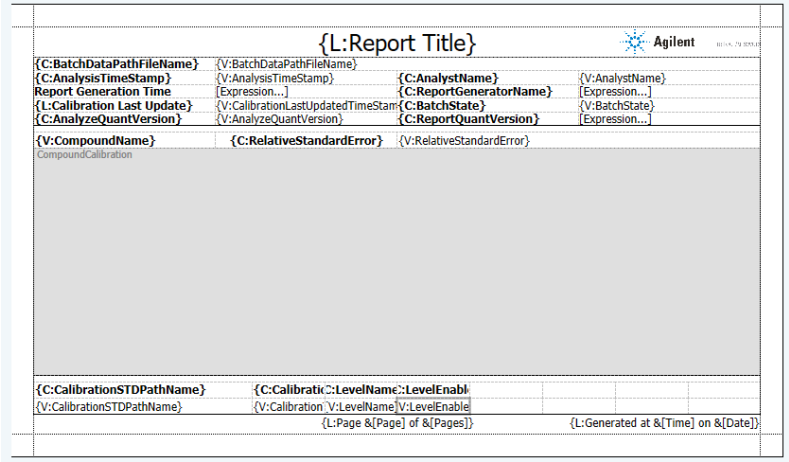
19 On the **Alignment** tab, select **Left** from the **Horizontal** list. Click **OK**.



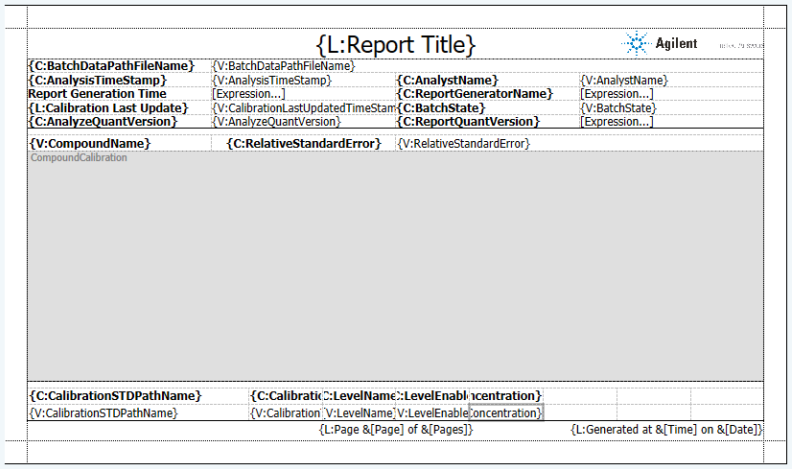
20 For the cells in the third column, use the instructions in the previous steps to select **Calibration** and **LevelName** for the **Field Caption** of the cell in the first row, and **Calibration** and **LevelName** for the **Field Value** of the cell below it. Bold the text of the cell in the first row, and change the horizontal alignment of both cells to **Center**. Click **OK**.



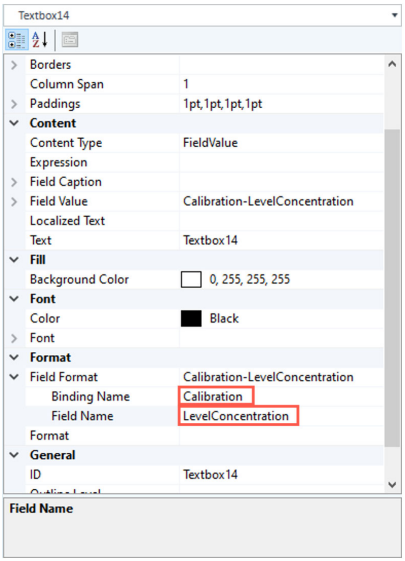
21 For the cells in the fourth column, select **Calibration** and **LevelEnable** for the **Field Caption** of the cell in the first row, and **Calibration** and **LevelEnable** for the **Field Value** of the cell below it. Bold the text of the cell in the first row, and set the horizontal alignment of both cells to **Center**. Click **OK**.



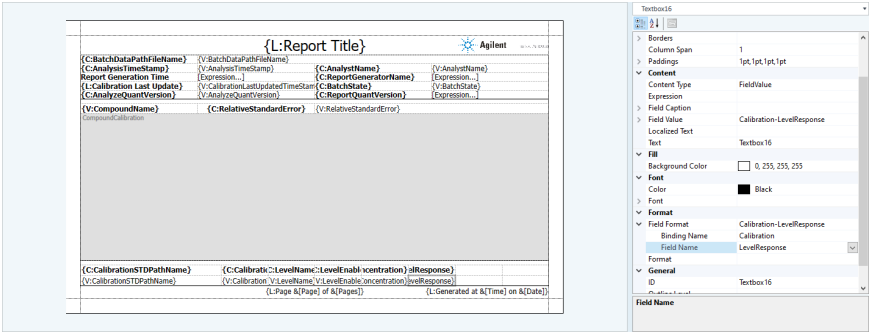
22 For the cells in the fifth column, select **Calibration** and **LevelConcentration** for the **Field Caption** of the cell in the first row, and **Calibration** and **LevelConcentration** for the **Field Value** of the cell below it. Bold the text of the cell in the first row, and set the horizontal alignment of both cells to **Right**. Click **OK**.



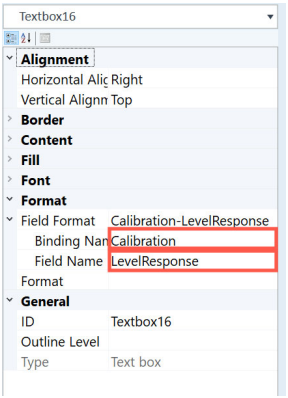
23 To use the same format in the {V:LevelConcentration} cell as is found in the Quantitative Analysis software, double-click **Field Format** in the properties pane, and select **Calibration** from the **Binding Name** list, and select **LevelConcentration** from the **Field Name** list.



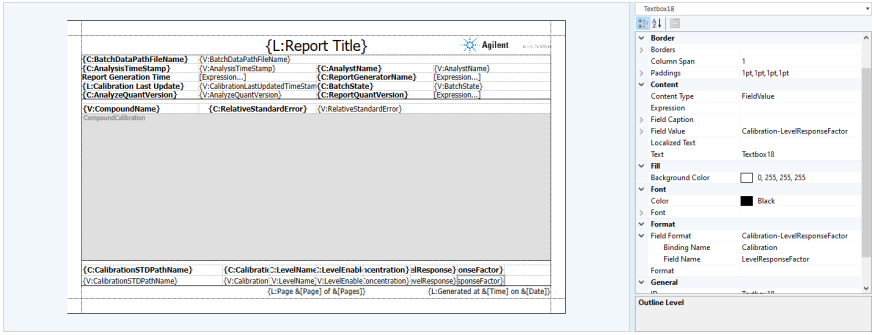
24 For the cells in the sixth column, select **Calibration** and **LevelResponse** for the **Field Caption** of the cell in the first row, and **Calibration** and **LevelResponse** for the **Field Value** of the cell below it. Bold the text of the cell in the first row, and set the horizontal alignment of both cells to **Right**.



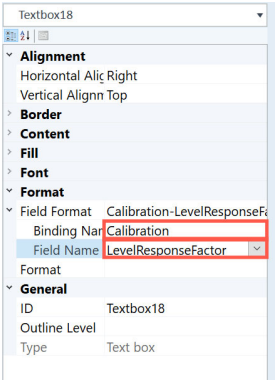
25 Select the **{V:LevelResponse}** cell, double-click **Field Format** in the Properties pane, and select **Calibration** from the **Binding Name** list and **LevelResponse** from the **Field Name** list.



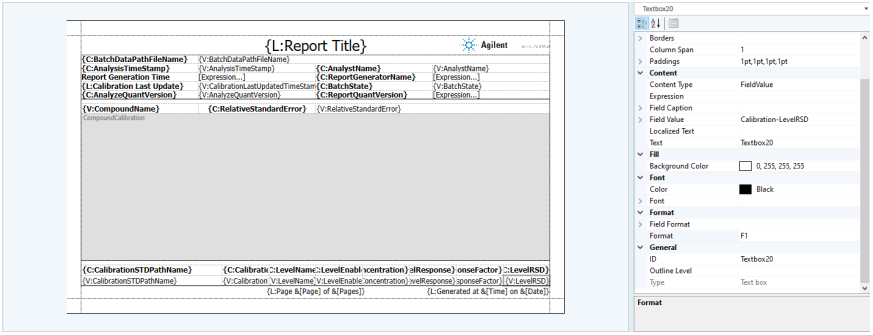
26 For the cells in the seventh column, select **Calibration** and **LevelResponseFactor** for the **Field Caption** of the cell in the first row, and **Calibration** and **LevelResponseFactor** for the **Field Value** of the cell below it. Bold the text of the cell in the first row, and set the horizontal alignment of both cells to **Right**.



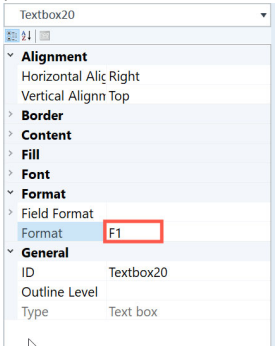
27 Select the **{V:LevelResponseFactor}** cell, double-click **Field Format** in the Properties pane, and select **Calibration** from the **Binding Name** list and **LevelResponseFactor** from the **Field Name** list.



28 For the cells in the eighth column, select **Calibration** and **LevelRSD** for the **Field Caption** of the cell in the first row, and **Calibration** and **LevelRSD** for the **Field Value** of the cell below it. Bold the text of the cell in the first row, and set the horizontal alignment of both cells to **Right**.

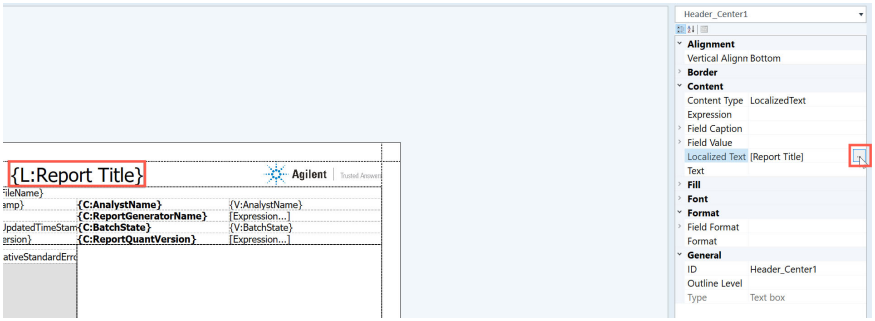


29 Select the **{V:LevelRSD}** cell, and enter **F1** in the **Format** field in the Properties pane.

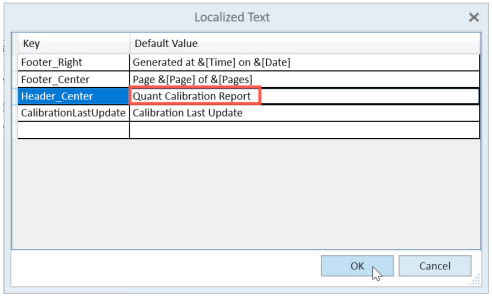


Add a report title

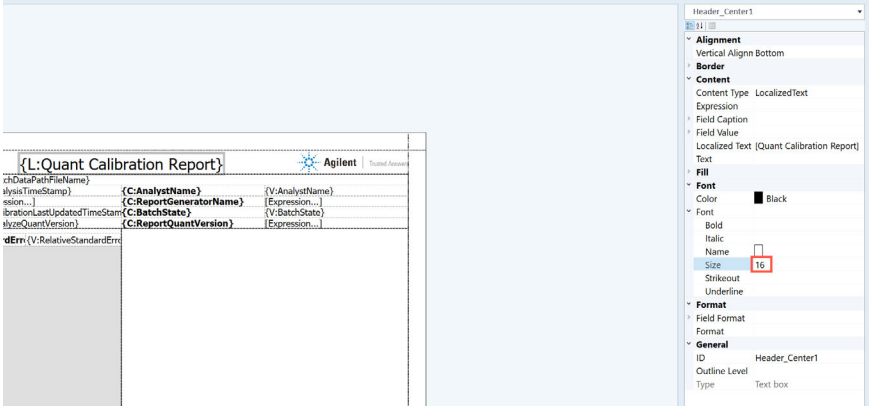
1 Select the **{L:Report Title}** cell in the page header. Click **Localized Text** in the Properties pane, then click the ellipsis.



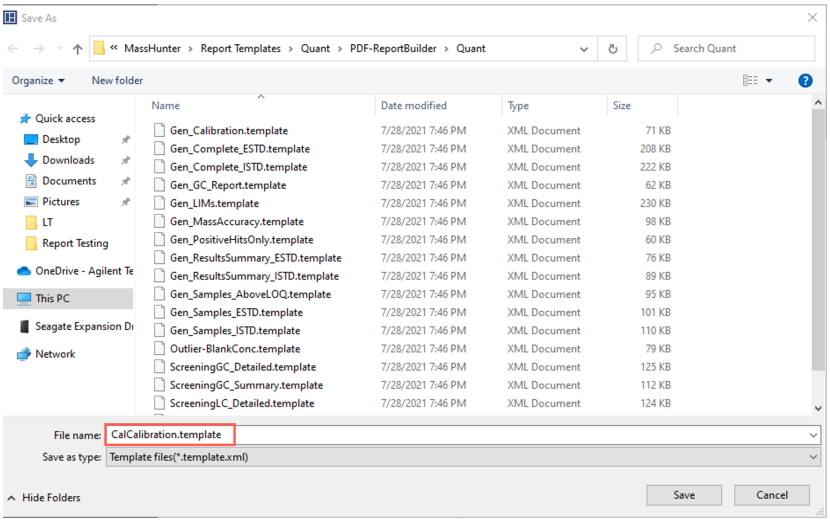
2 Enter **Quant Calibration Report** in the **Default Value** column for **Header Center**. Click **OK**.



3 In the Properties pane, change the font size to **16**.

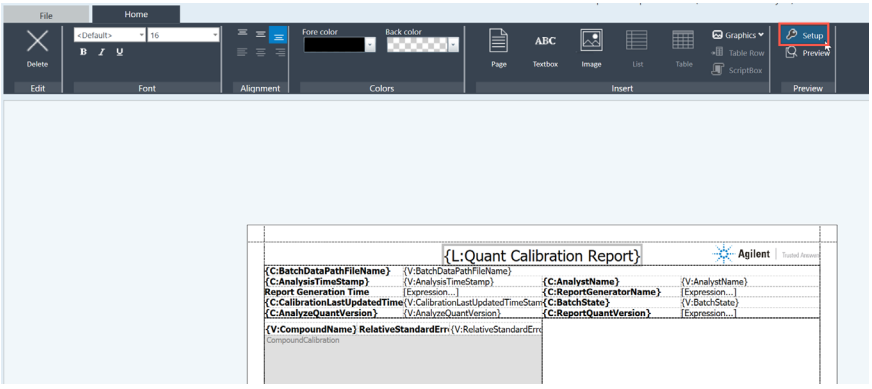


4 Click **File > Save As**, and save the template as **CalCalibration.template.xml**.

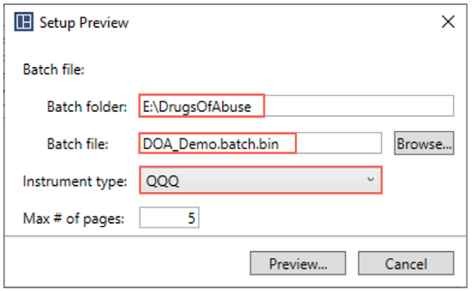


Preview the report template

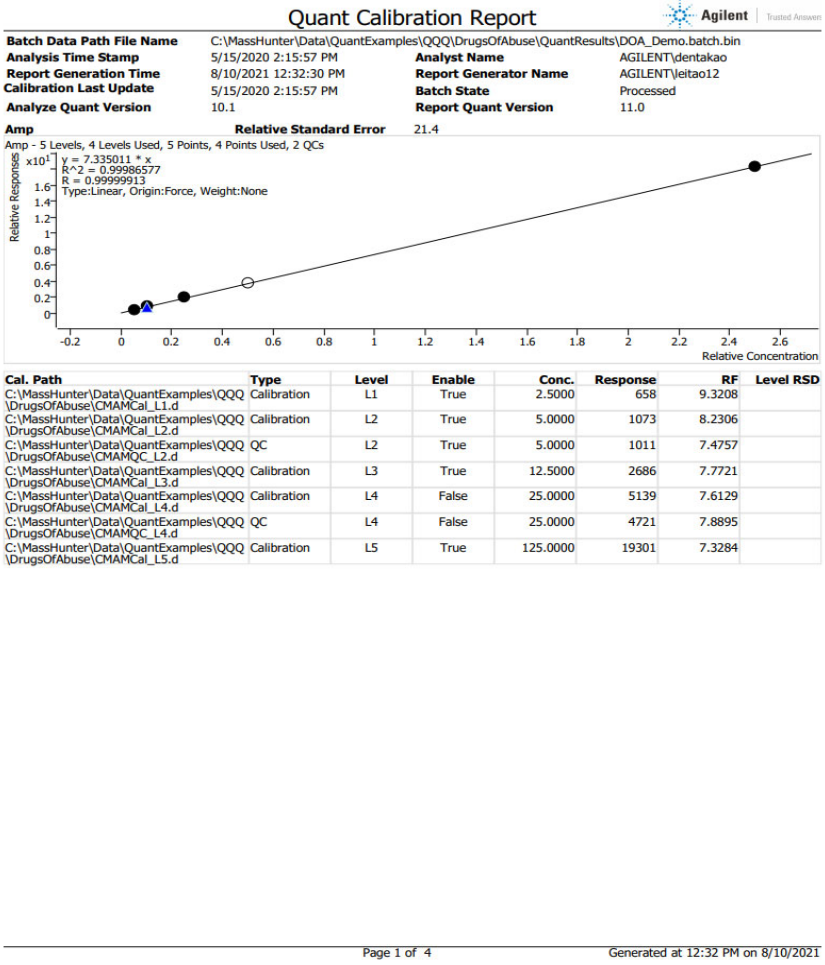
1 Click **Setup**.



2 Click **browse** in the Setup Preview window, navigate to the **DrugsOfAbuse** folder, and select **DOA_Demo.batch.bin**. Select **QQQ** for **Instrument type**.



3 Click **Preview**. A PDF report is generated using the selected batch file.



Quant Calibration Report

Agilent | Trusted Answers

Batch Data Path File Name	C:\MassHunter\Data\QuantExamples\QQQ\DrugsOfAbuse\QuantResults\DOA_Demo.batch.bin		
Analysis Time Stamp	5/15/2020 2:15:57 PM	**Analyst Name**	AGILENT\dentakao
Report Generation Time	8/10/2021 12:32:30 PM	**Report Generator Name**	AGILENT\leitao12
Calibration Last Update	5/15/2020 2:15:57 PM	**Batch State**	Processed
Analyze Quant Version	10.1	**Report Quant Version**	11.0

Amp **Relative Standard Error** 21.4

Amp - 5 Levels, 4 Levels Used, 5 Points, 4 Points Used, 2 QCs

Cal. Path	Type	Level	Enable	Conc.	Response	RF	Level RSD
C:\MassHunter\Data\QuantExamples\QQQ \DrugsOfAbuse\CMAMCal_L1.d	Calibration	L1	True	2.5000	658	9.3208	
C:\MassHunter\Data\QuantExamples\QQQ \DrugsOfAbuse\CMAMCal_L2.d	Calibration	L2	True	5.0000	1073	8.2306	
C:\MassHunter\Data\QuantExamples\QQQ \DrugsOfAbuse\CMAMQC_L2.d	QC	L2	True	5.0000	1011	7.4757	
C:\MassHunter\Data\QuantExamples\QQQ \DrugsOfAbuse\CMAMCal_L3.d	Calibration	L3	True	12.5000	2686	7.7721	
C:\MassHunter\Data\QuantExamples\QQQ \DrugsOfAbuse\CMAMCal_L4.d	Calibration	L4	False	25.0000	5139	7.6129	
C:\MassHunter\Data\QuantExamples\QQQ \DrugsOfAbuse\CMAMQC_L4.d	QC	L4	False	25.0000	4721	7.8895	
C:\MassHunter\Data\QuantExamples\QQQ \DrugsOfAbuse\CMAMCal_L5.d	Calibration	L5	True	125.0000	19301	7.3284	

Page 1 of 4 Generated at 12:32 PM on 8/10/2021

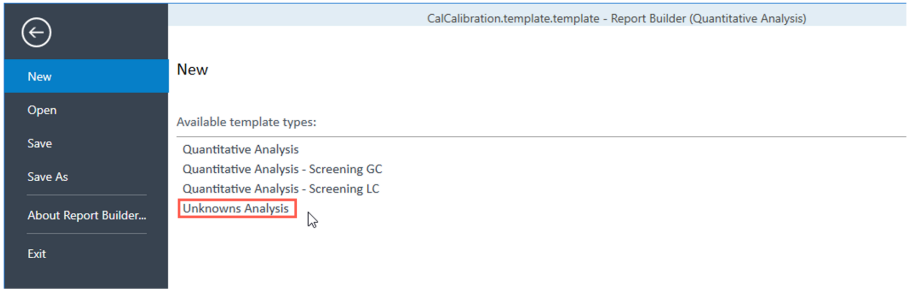
Unknowns Analysis - Area Percent Report Template

For this example, you will create a Calibration Report by completing the following procedures.

1. **Create a new Unknowns Analysis report template** on page 50
2. **Insert a list** on page 51
3. **Add a Sample Information table with a graph** on page 53
4. **Add a Compound Results table** on page 61
5. **Add a report title** on page 91
6. **Generate a report** on page 93

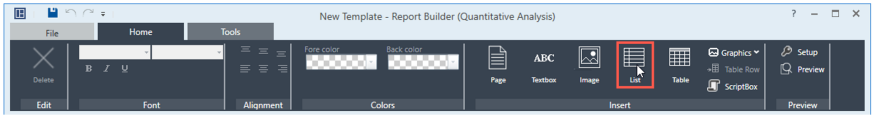
Create a new Unknowns Analysis report template

To create a new Unknowns Analysis report template, select **File > New**, and select **Unknowns Analysis**.

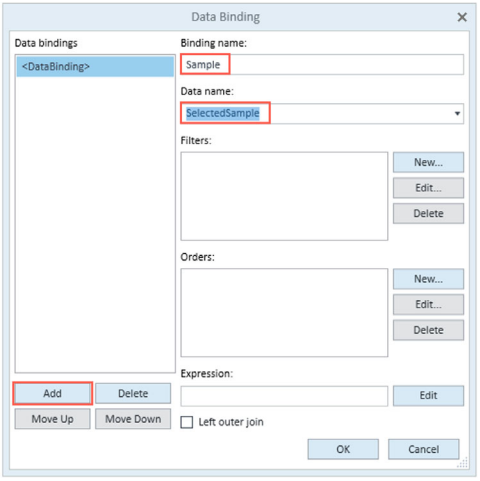


Insert a list

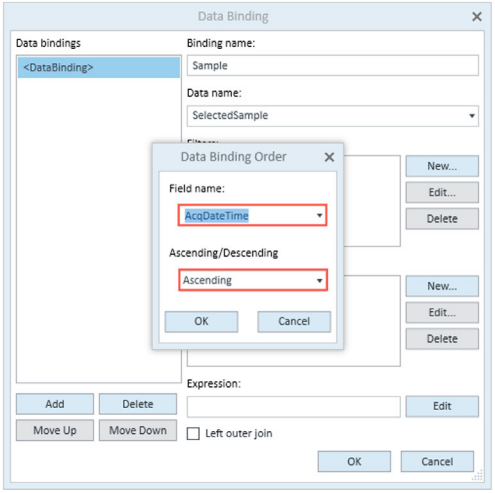
1 Click **List**.



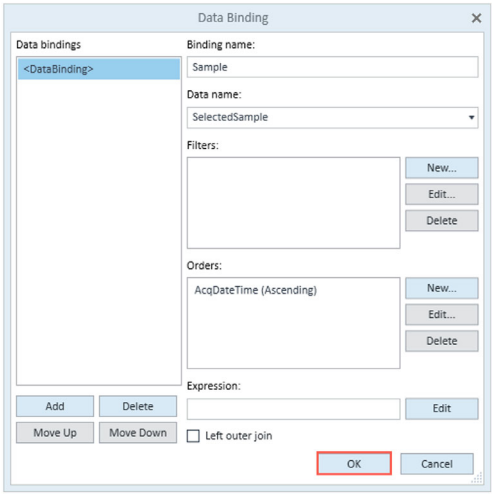
2 Under **Data bindings**, click **Add**. Enter **Sample** in the **Binding name** field, and select **SelectedSample** from the **Data name** list.



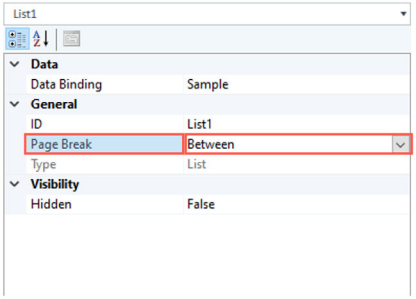
3 In the **Orders** section, click **New**. Select **AcqDateTime** from the **Field name** list, and select **Ascending** under the **Ascending/Descending** list. Click **OK**.



4 Click **OK** to close the **Data Binding** window.

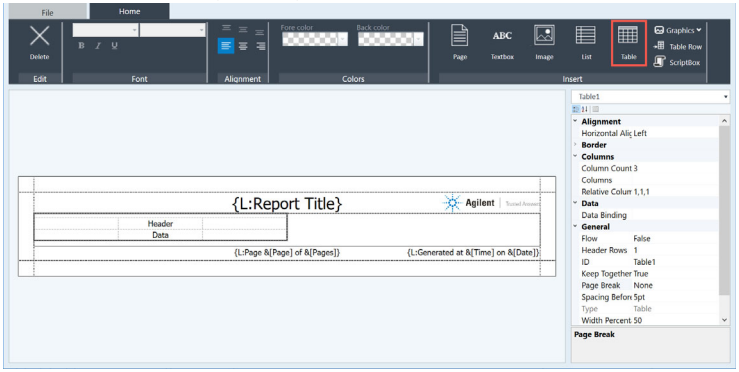


5 Select **Page Break** in the Properties pane, and select **Between** from the list.



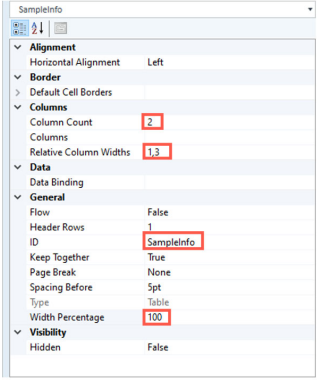
Add a Sample Information table with a graph

1 Select **List1** from the drop-down menu at the top of the Properties pane. Click **Table**. A new table (Table1) appears in the report.

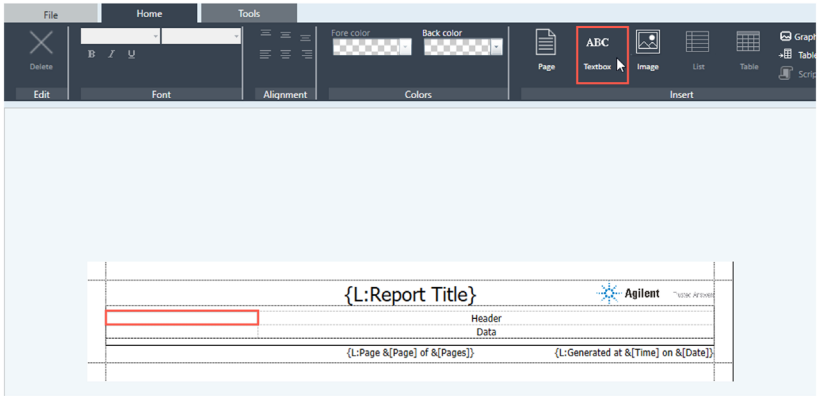


2 In the Properties pane, make the following changes:

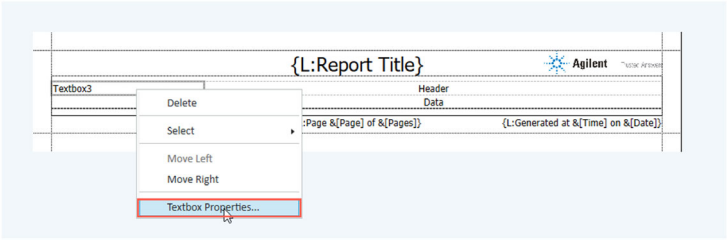
- Change the **Column Count** to 2
- Change the **Relative Column Widths** to 1,3 to resize the columns in relation to the table width
- Enter **SampleInfo** in the **ID** field to update the table name
- Enter 100 in the **Width Percentage** field to resize the table width.



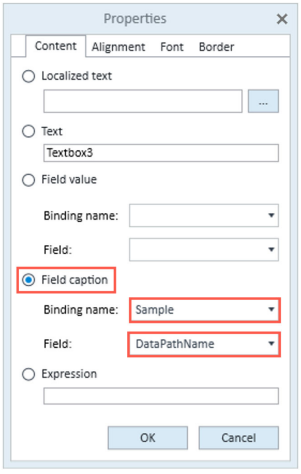
3 To edit a table cell, select the empty cell to the left of the **Header** cell, and click **Textbox**.



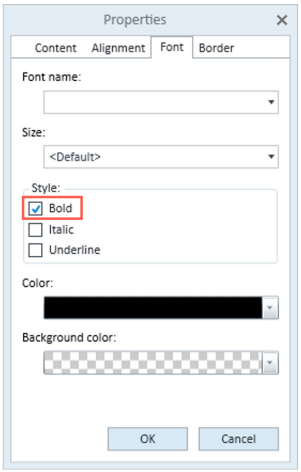
4 Right-click the cell and select **Textbox Properties**.



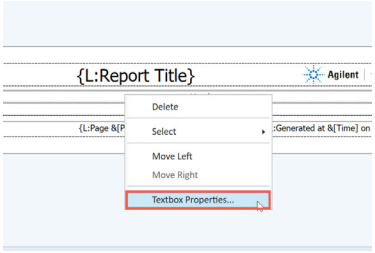
5 Select **Field caption**, then select **Sample** from the **Binding name** list, and select **DataPathName** from the **Field** list.



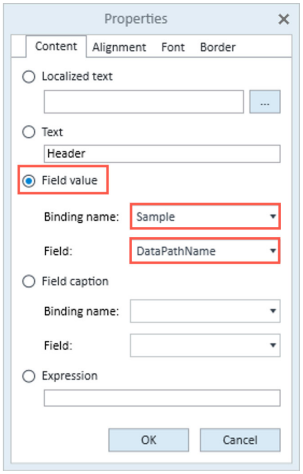
6 On the **Font** tab, select **Bold**. Click **OK**.



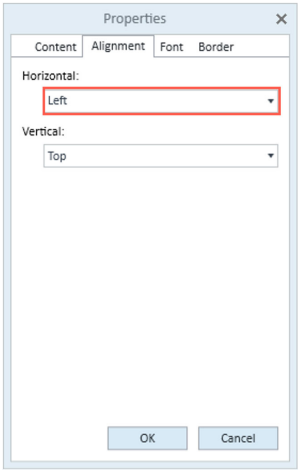
7 Right-click the **Header** cell, and select **Textbox Properties**.



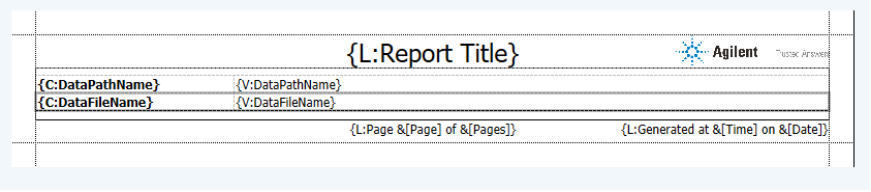
8 Select **Field Value**, select **Sample** from the **Binding name** list, and **DataPathName** from the **Field** list.



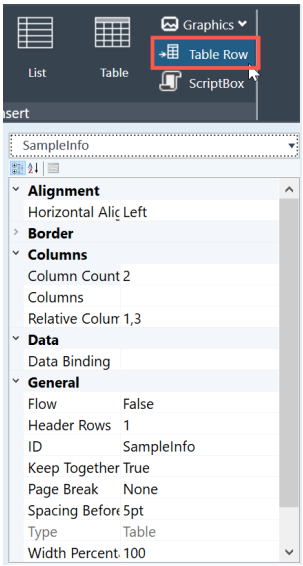
9 On the **Alignment** tab, select **Left** from the **Horizontal** list. Click **OK**.



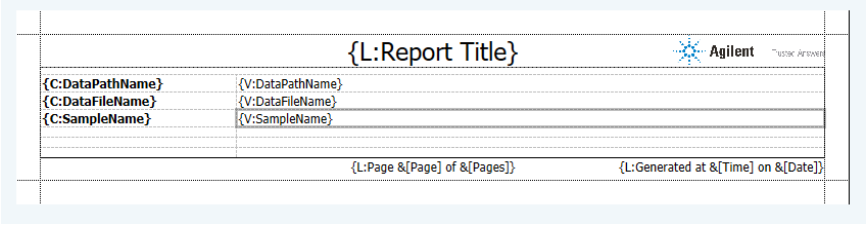
10 For the cells in the second row, use the instructions in the previous steps to select **Sample** and **DataFileName** for the **Field Caption** of the cell in the first column, and **Sample** and **DataFileName** for the **Field Value** of the cell in the second column. Bold the text of the cell in the first column, and set the horizontal alignment of both cells to **Left**. Click **OK**.



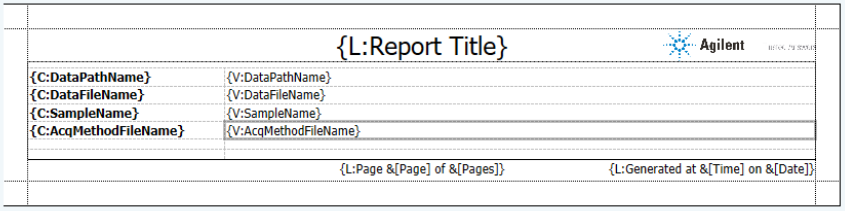
11 To add rows to the table, select **SampleInfo** from the list at the top of the Properties pane, and click **Table Row**. Click **Table Row** 3 more times to add a total of 4 rows.



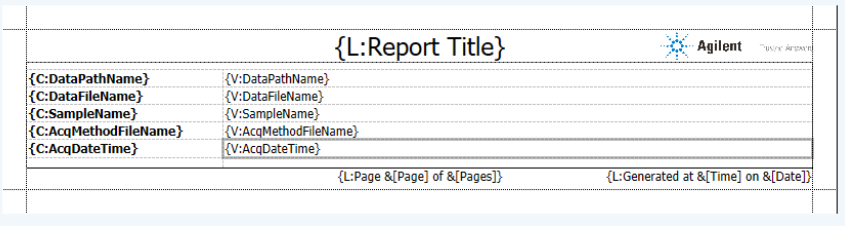
12 For the cells in the third row, select **Sample** and **SampleName** for the **Field Caption** of the cell in the first column, and **Sample** and **SampleName** for the **Field Value** of the cell in the second column. Bold the text of the cell in the first column, and set the horizontal alignment of both cells to **Left**.



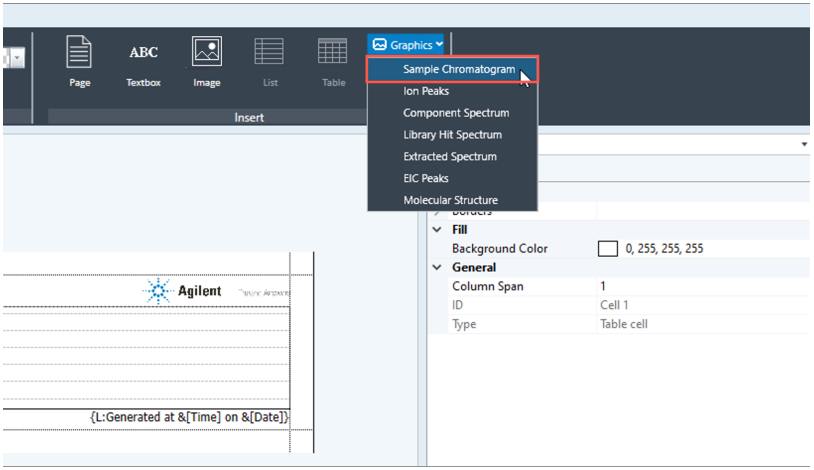
13 For the cells in the fourth row, select **Sample** and **AcqMethodFileName** for the **Field Caption** of the cell in the first column, and **Sample** and **AcqMethodFileName** for the **Field Value** of the cell in the second column. Bold the text of the cell in the first column, and set the horizontal alignment of both cells to **Left**.



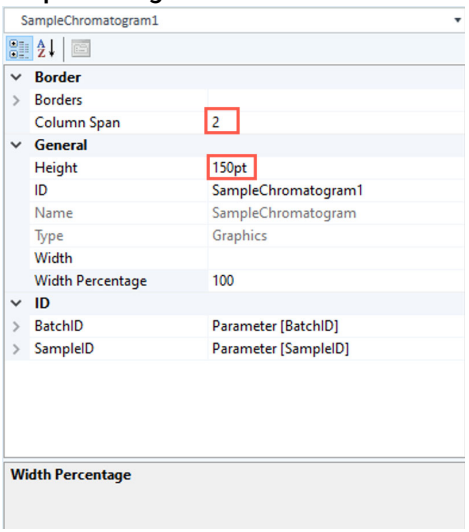
14 For the cells in the fifth row, select **Sample** and **AcqDateTime** for the **Field Caption** of the cell in the first column, and **Sample** and **AcqDateTime** for the **Field Value** of the cell in the second column. Bold the text of the cell in the first column, and set the horizontal alignment of both cells to **Left**.



15 To add a graphic, select the empty cell below **{C:AcqDateTime}**, click **Graphics**, and select **Sample Chromatogram**.



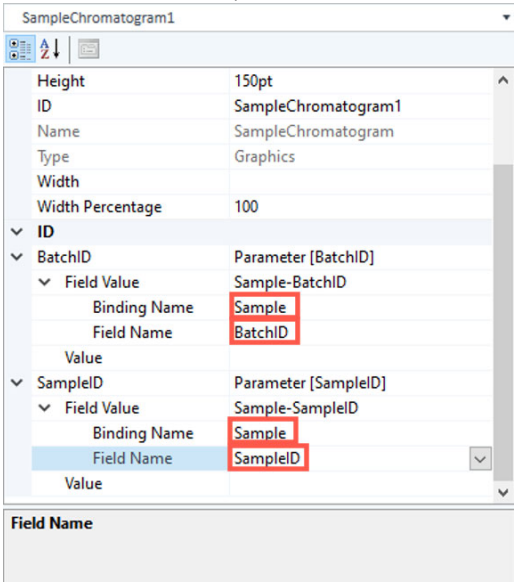
16 To resize the graphic, in the Properties pane, enter **2** for **Column Span** and **150pt** for **Height**.



17 ID fields like BatchID and SampleID have system-assigned numbers which help to rapidly locate and link to unique table rows in a Quantitative Analysis dataset. To edit the ID fields, expand the ID section in the Properties pane. Enter the values for each ID:

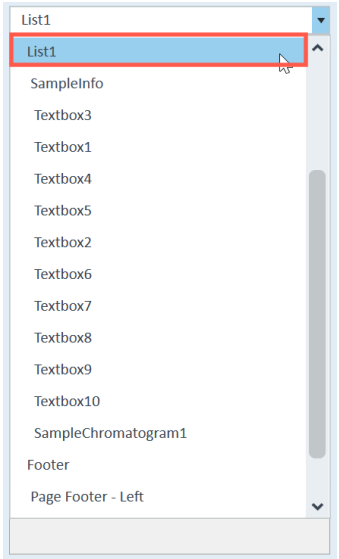
- BatchID
  - **Field Value**: Sample-BatchID
  - **Binding Name**: Sample
  - **Field Name**: BatchID
- SampleID
  - **Field Value**: Sample-SampleID
  - **Binding Name**: Sample

- **Field Name**: SampleID

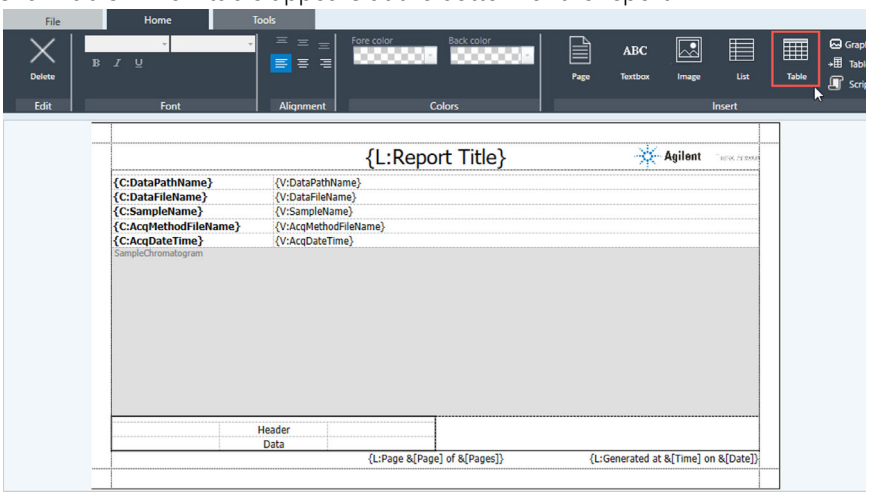


Add a Compound Results table

1 Select **List1** from the list at the top of the Properties pane.



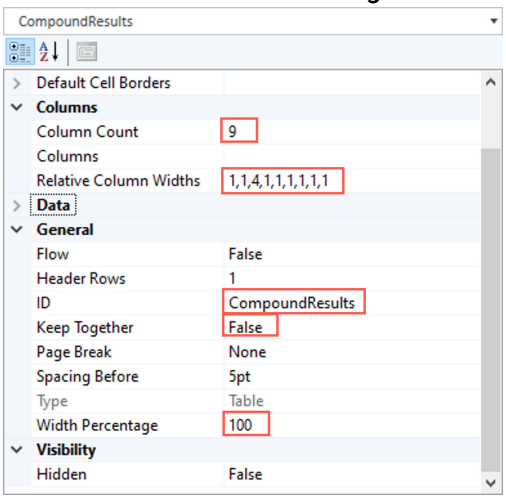
2 Click **Table**. A new table appears at the bottom of the report.



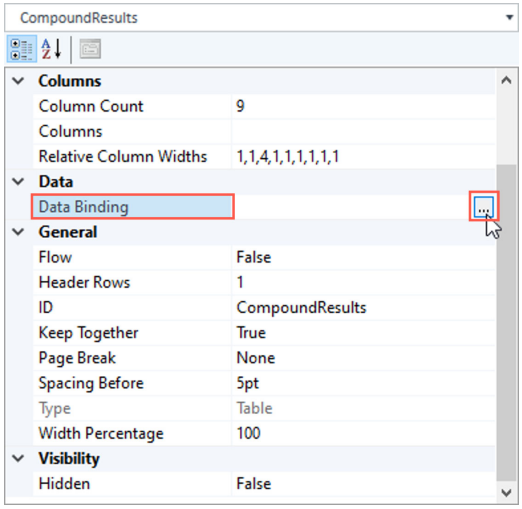
3 In the properties pane,

- change the **Column Count** to 9
- change the **Relative Column Width** to 1,1,4,1,1,1,1,1,1 to resize the columns in relation to the table width

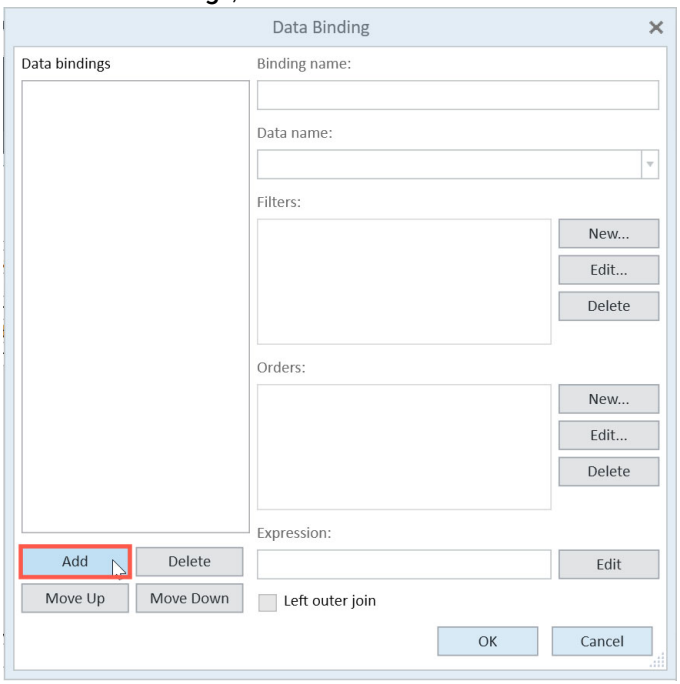
- enter CompoundResults in the **ID** field to update the table name
- select False for **Keep Together**
- enter 100 in the **Width Percentage** field to resize the table width



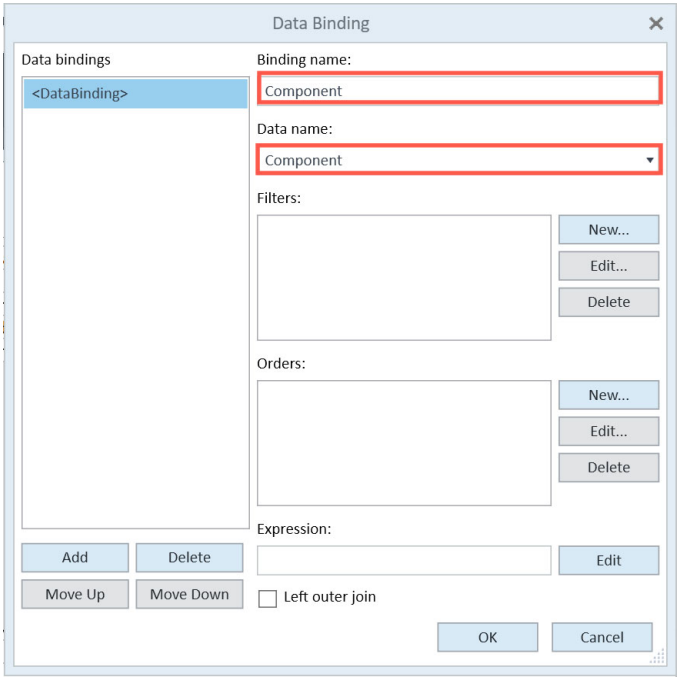
4 To add binding data to the table, click **Data Binding** in the Properties pane, then click the ellipsis.



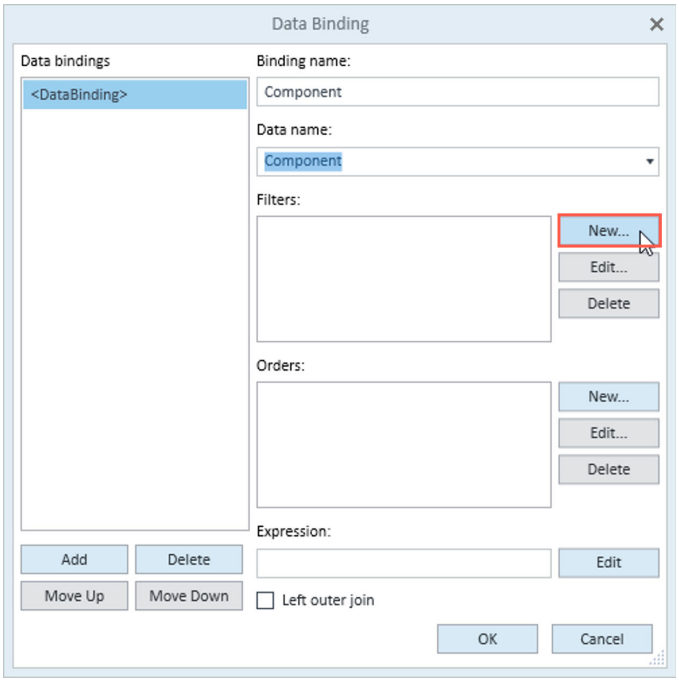
5 Under **Data Bindings**, click **Add**.



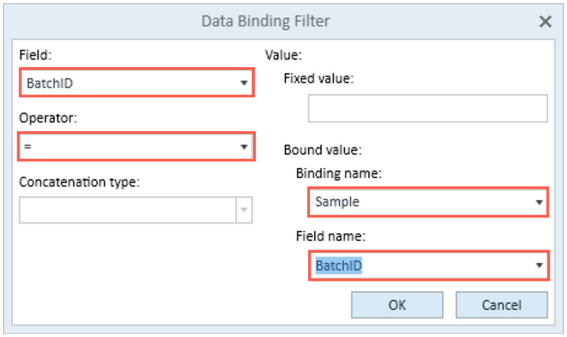
6 Enter **Component** for the **Binding name** and select **Component** from the **Data name** list.



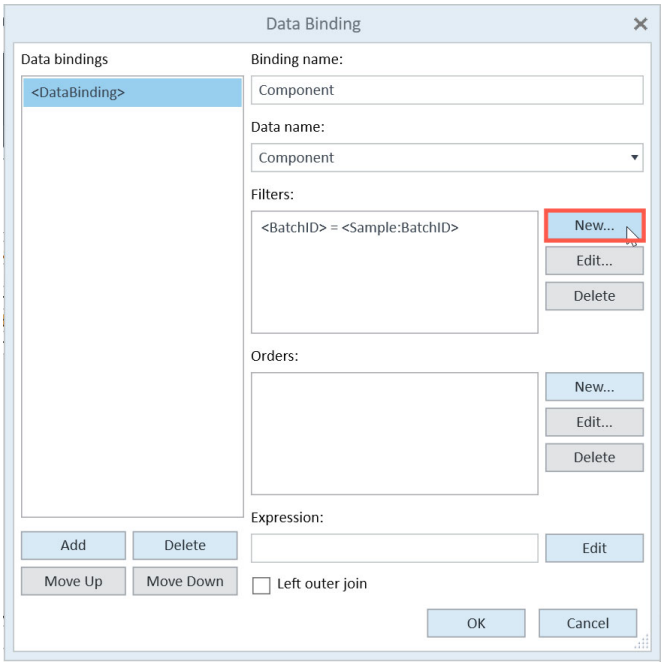
7 In the **Filters** section, click **New**.



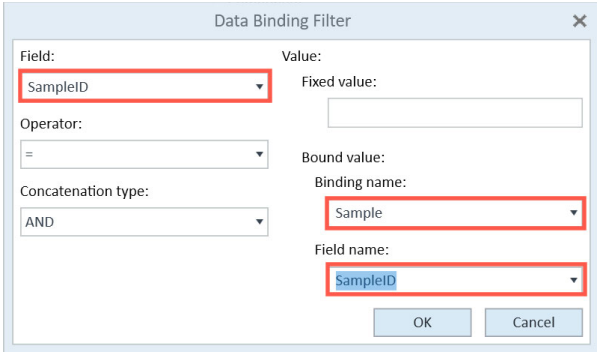
8 Select **BatchID** from the **Field** list, and **=** from the **Operator** list. Select **Sample** from the **Binding name** list, and select **BatchID** from the **Field name** list. Click **OK**.



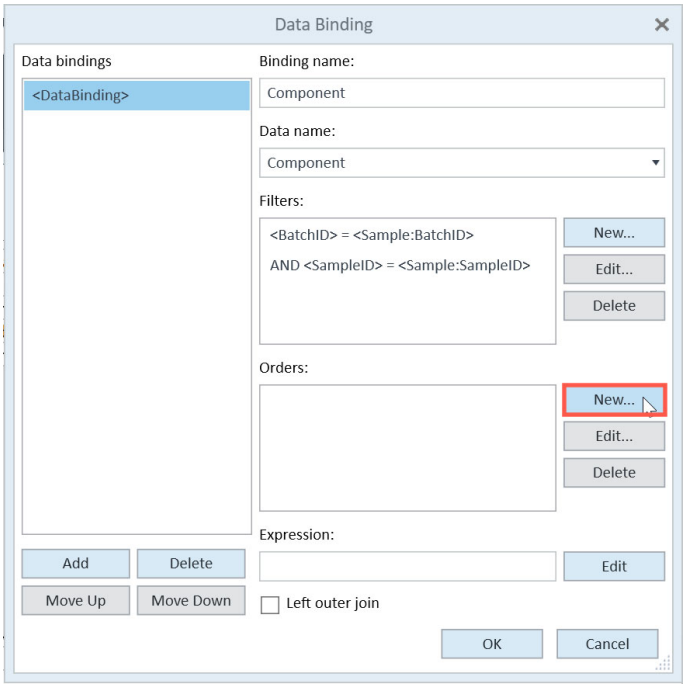
9 In the **filters** section, click **New**.



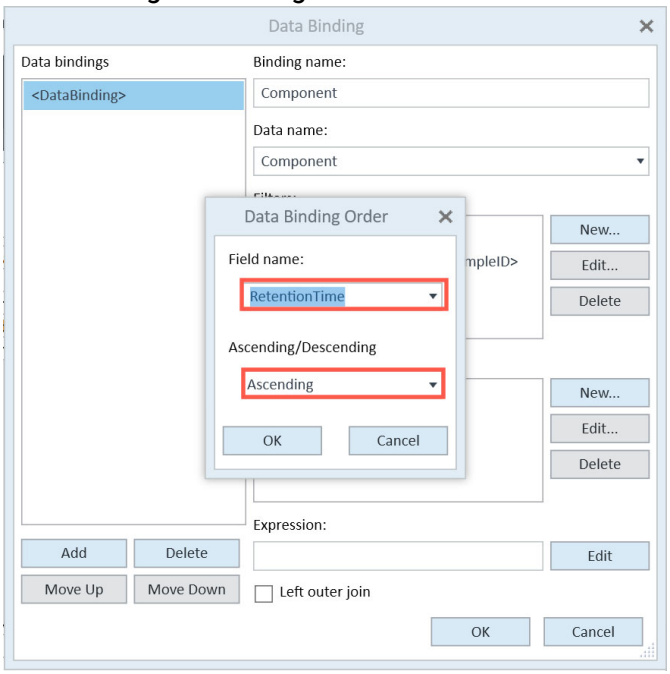
10 Select **SampleID** from the **Field** list, **Sample** from the **Binding Name list**, and **SampleID** from the **Field Name** list.



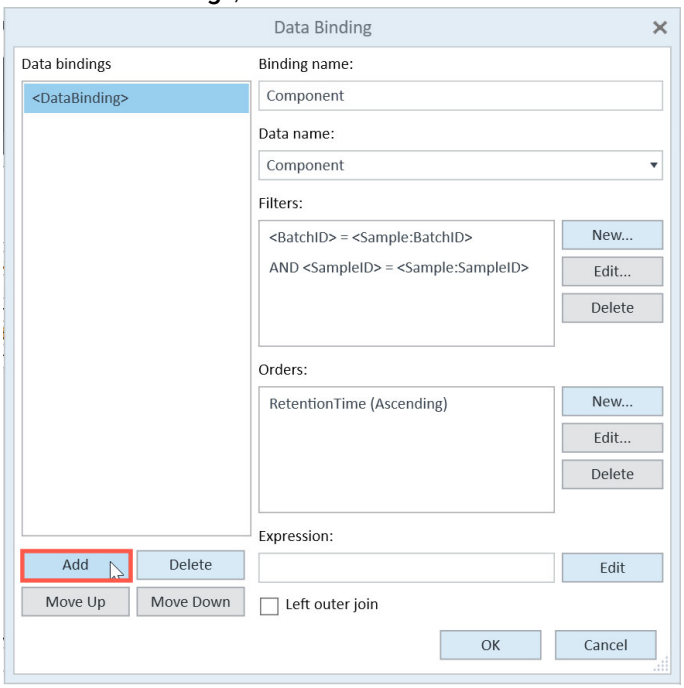
11 In the **Orders** section, click **New**.



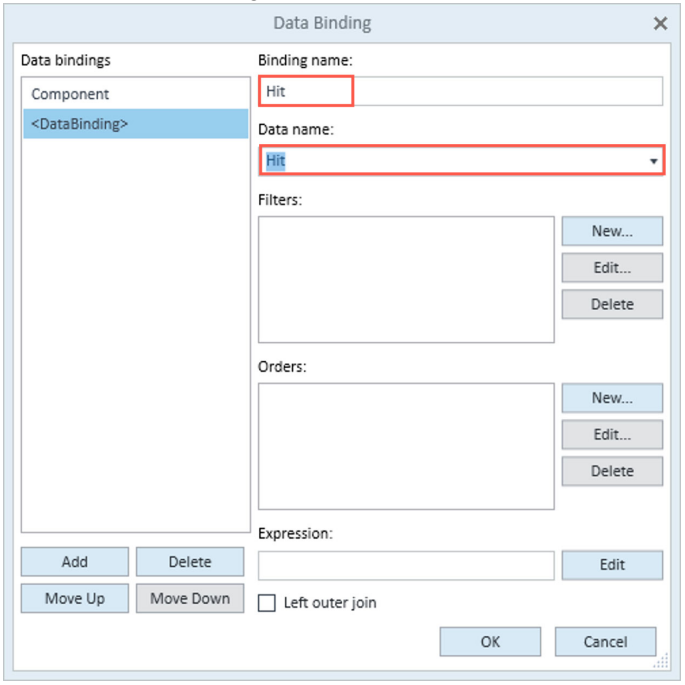
12 Select **RetentionTime** from the **Field name** list, and select **Ascending** from the **Ascending/Descending** list. Click **OK**.



13 Under **Data Bindings**, click **Add**.

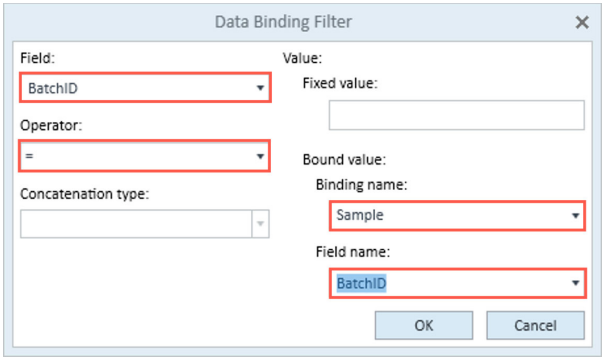


14 Enter **Hit** in the **Binding name** field, and select **Hit** from the **Data name** list.

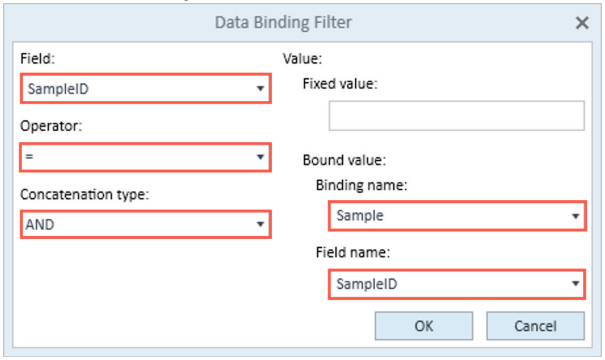


15 Add a data binding filter for each of the following configurations:

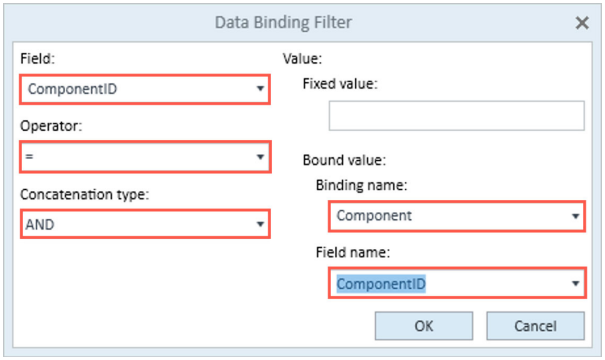
a Select **BatchID** from the **Field** list,
select **=** from the **Operator** list,
select **Sample** from the **Binding name** list,
and select **BatchID** from the **Field name** list.



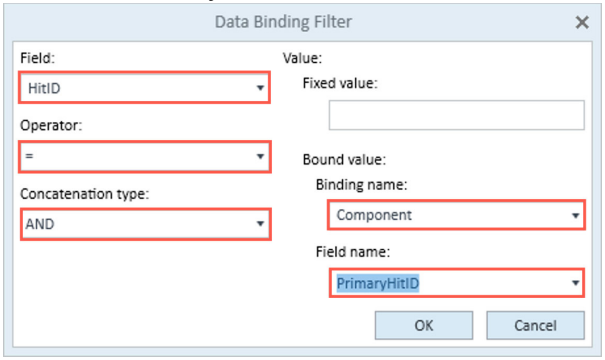
b Select **SampleID** from the **Field** list,
select **=** from the **Operator** list,
select **AND** from the **Concatenation type** list,
select **Sample** from the **Binding name** list,
and select **SampleID** from the **Field name** list.



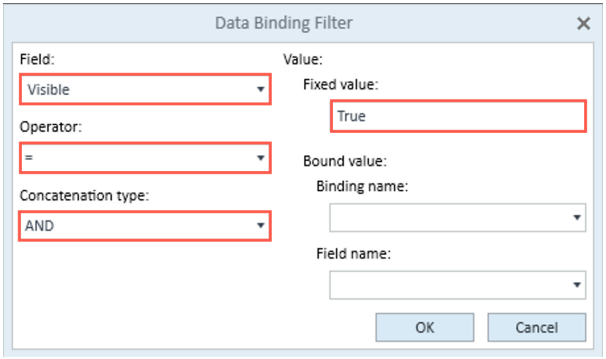
c Select **ComponentID** from the **Field** list,
select **=** from the **Operator** list,
select **AND** from the **Concatenation type** list,
select **Component** from the **Binding name** list,
and select **ComponentID** from the **Field name** list.



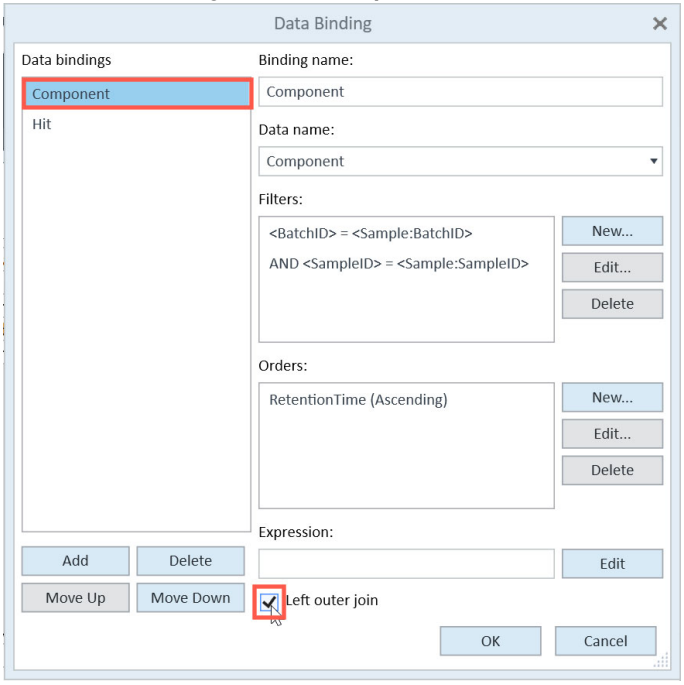
d Select **HitID** from the **Field** list,
select **=** from the **Operator** list,
select **AND** from the **Concatenation type** list,
select **Component** from the **Binding name** list,
and select **PrimaryHitID** from the **Field name** list.



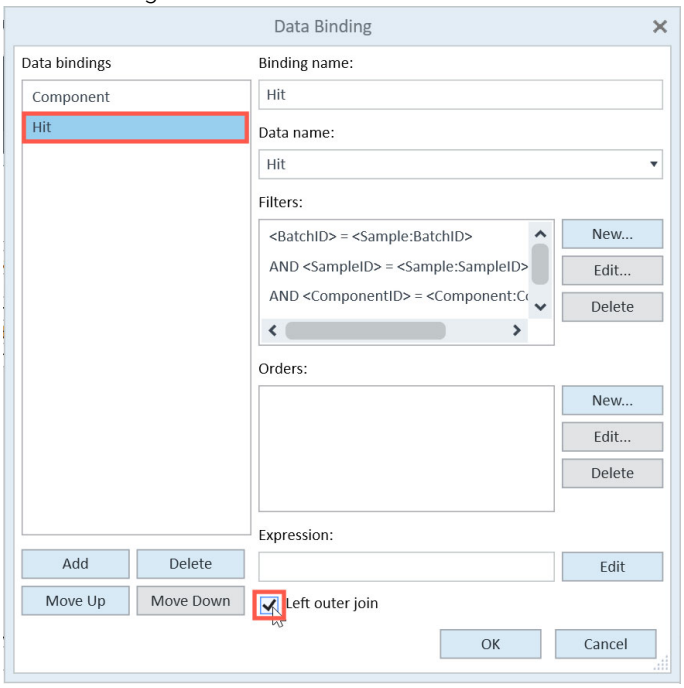
e Select **Visible** from the **Field** list,
select **=** from the **Operator** list,
select **AND** from the **Concatenation type** list,
and enter **True** in the **Fixed value** field.



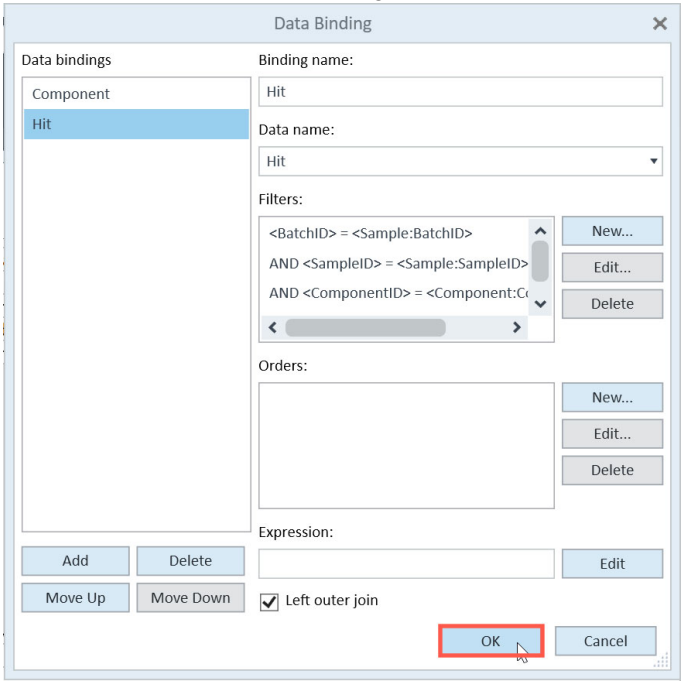
16 Under **Data Bindings**, select **Component**, and select **Left outer join**.



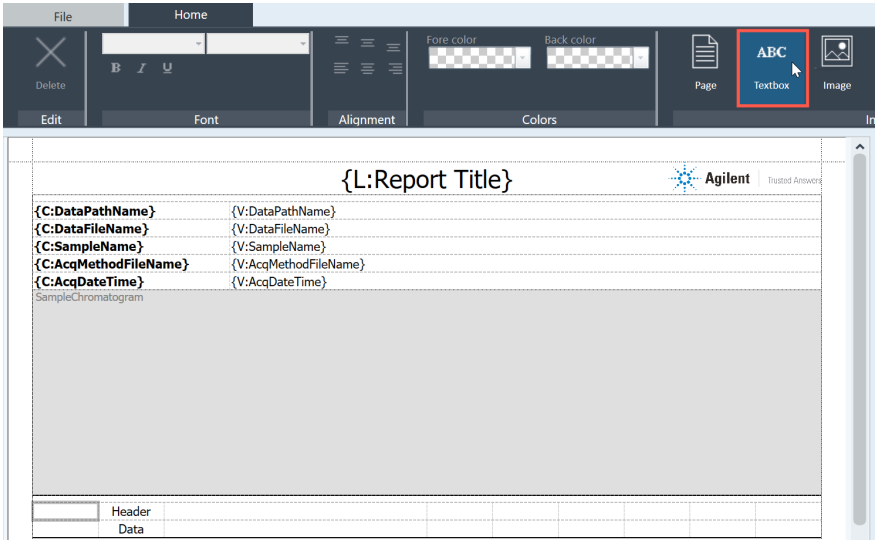
17 Under **Data Bindings**, select **Hit**, and select **Left outer join**. All components and matching hits are now included in the result table.



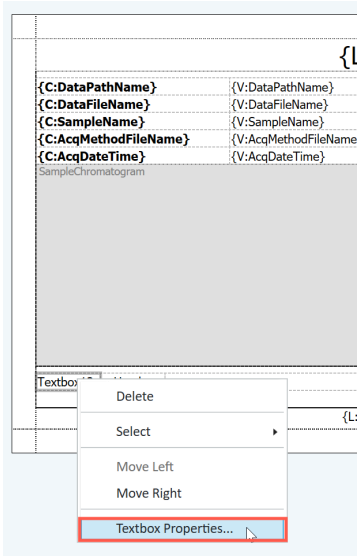
18 Click **OK** to close the **Data Binding** window.



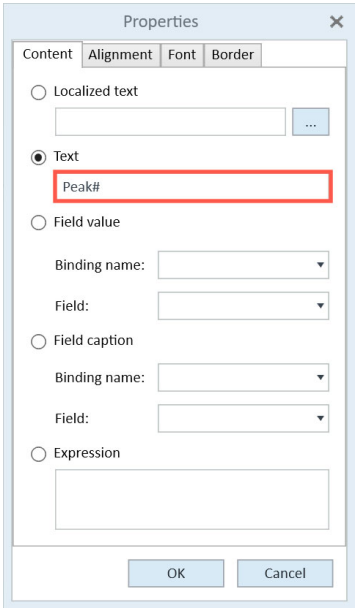
19 Select the first cell in the first row, and click **Textbox**.



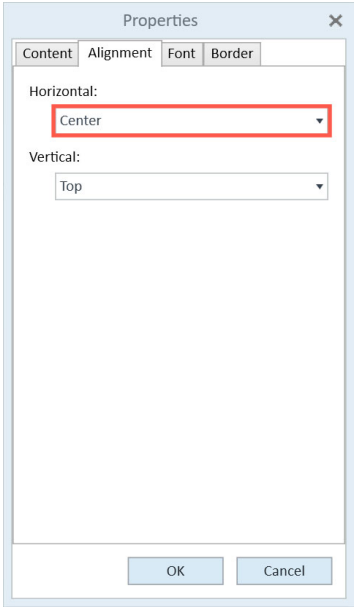
20 Right-click the cell, and select **Textbox Properties**.



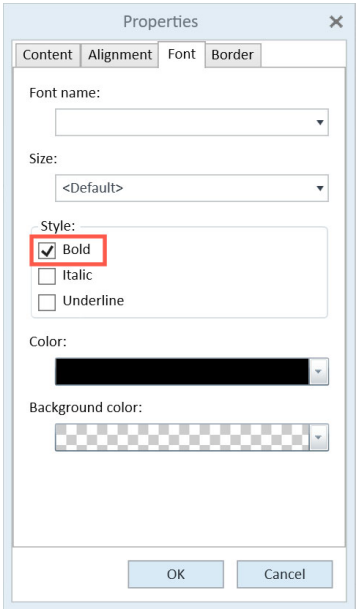
21 Enter **Peak#** in the **Text** field.



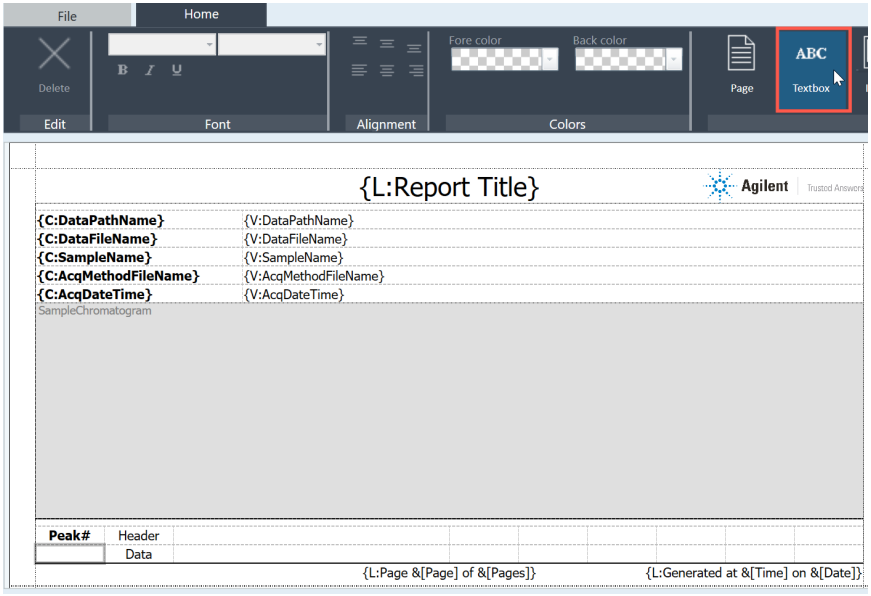
22 On the **Alignment** tab, select **Center** from the **Horizontal** list.



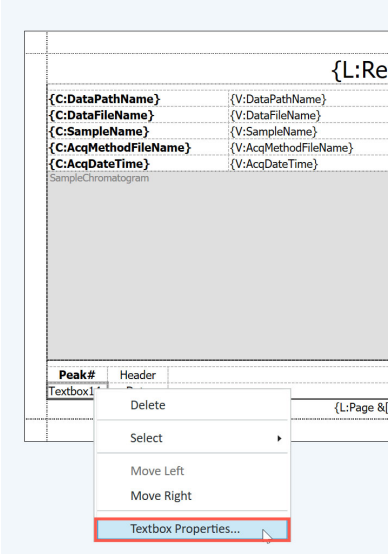
23 On the **Font** tab, select **Bold**. Click **OK**.



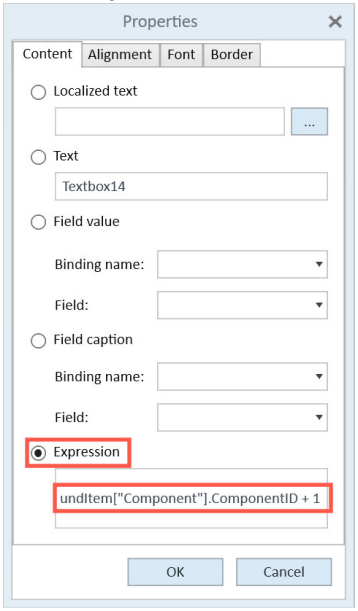
24 Select the first cell in the second row and click **Textbox**.



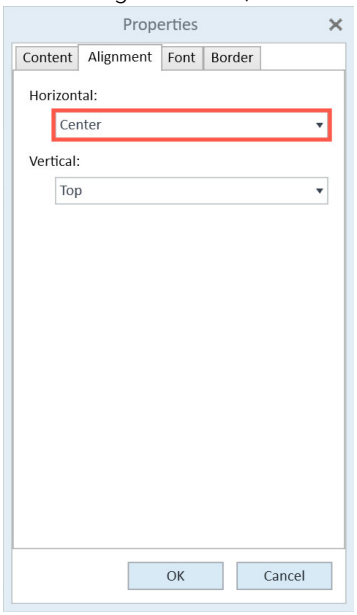
25 Right-click the cell, and select **Textbox Properties**.



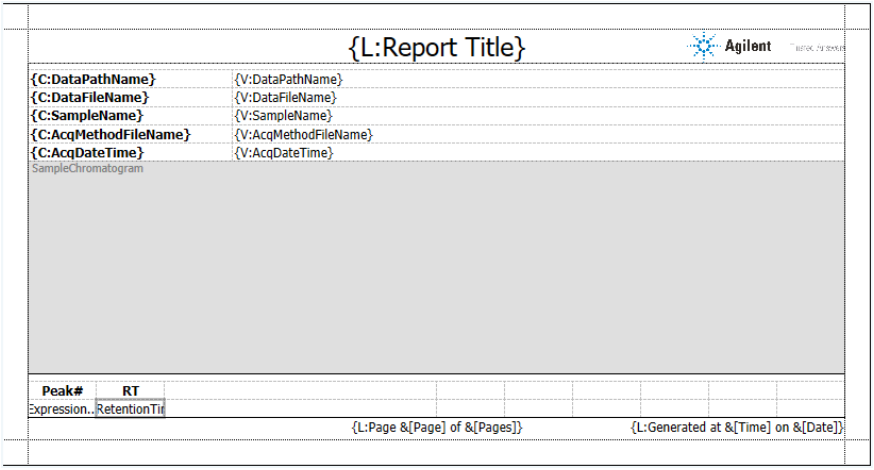
26 Select **Expression**, and enter **BoundItems["Component"].ComponentID + 1**.



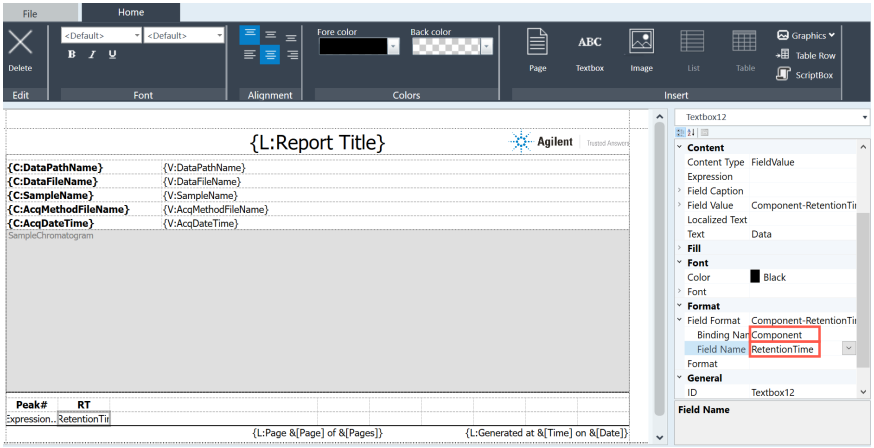
27 On the Alignment tab, select **Center** from the **Horizontal** list.



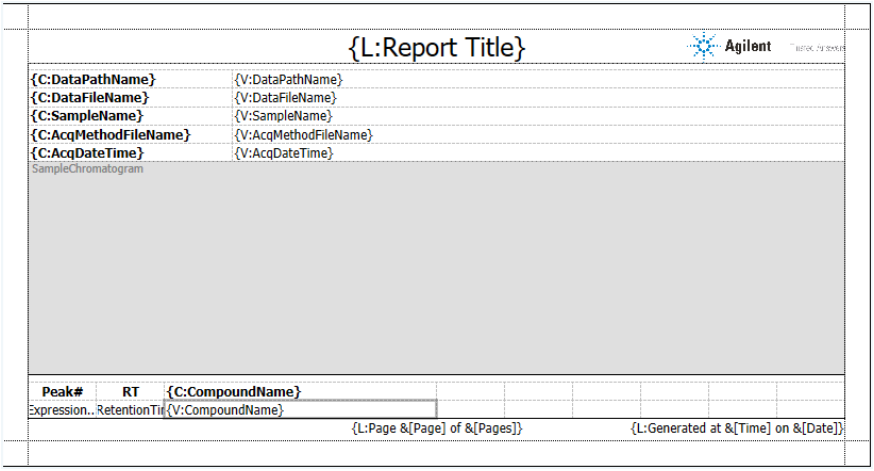
28 For the cells in the second column, enter **RT** in the **Text** field for the cell in the first row and set the font to **Bold**. For the cell in the second row, select **Field value**, select **Component** from the **Binding name** list, and select **RetentionTime** from the **Field** list. Set the horizontal alignment of both cells to **Center**.



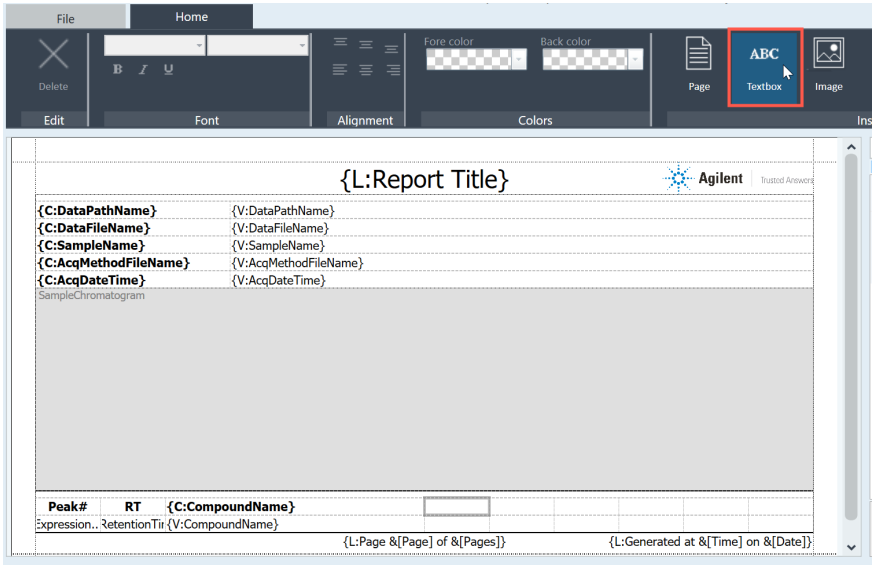
29 To use the same format in the **{V:RetentionTime}** cell as is found in the Quantitative Analysis software, double-click **Field Format** in the Properties pane, and select **Component** from the **Binding Name** list, and **RetentionTime** from the **Field Name** list.



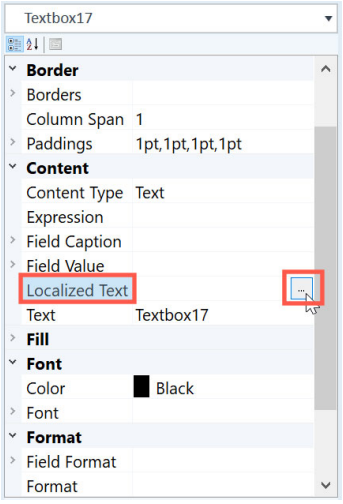
30 For the cells in the third column, use the instructions in the previous steps to select **Hit** and **CompoundName** for the **Field Caption** of the cell in the first row, and **Hit** and **CompoundName** for the **Field Value** of the cell below it. Bold the text of the cell in the first row, and change the horizontal alignment of both cells to **Left**.



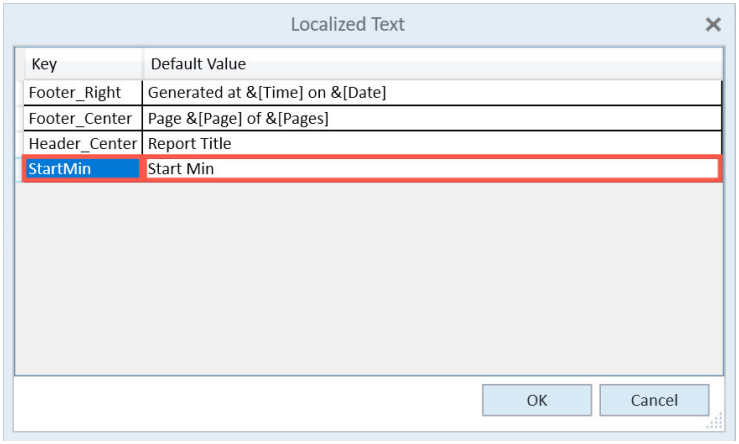
31 Select the cell in the first row of the fourth column, and click **Textbox**.



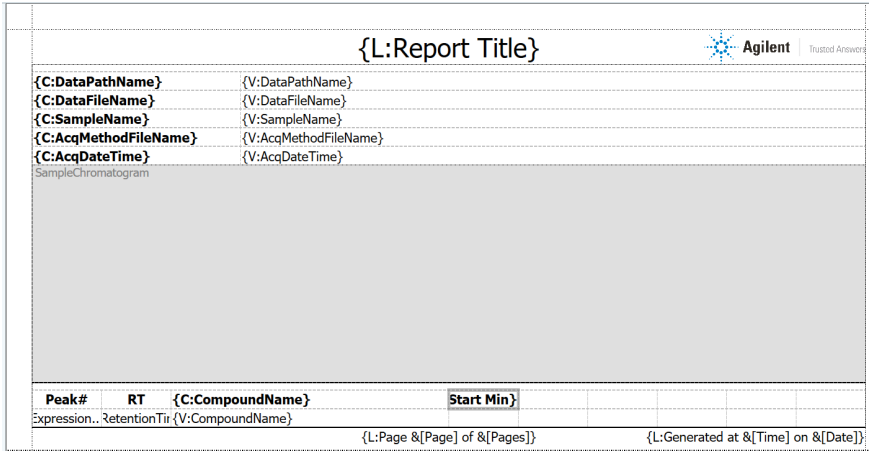
32 Click **Localized Text** in the Properties pane, then click the ellipsis.



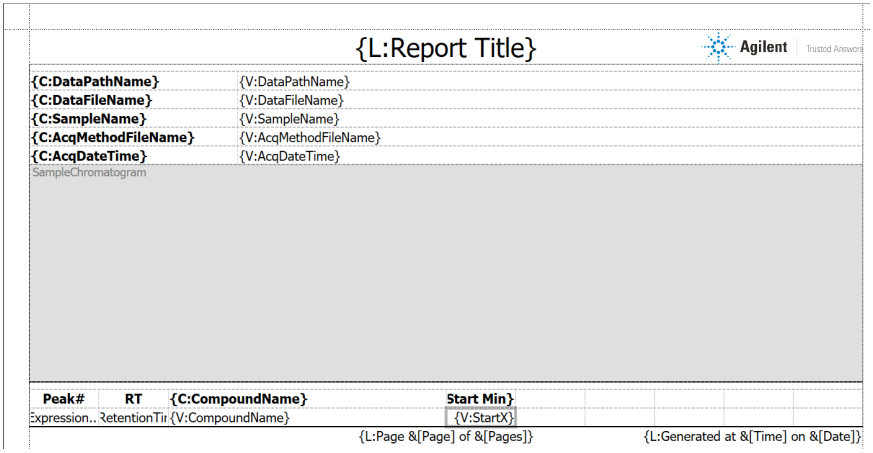
33 On the fourth row, enter **StartMin** in the **Key** column, and **Start Min** in the **Default Value** column. Click **OK**.



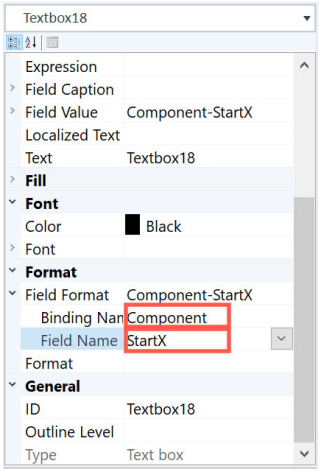
34 In **Textbox Properties**, bold the text, and set the horizontal alignment to **Right**.



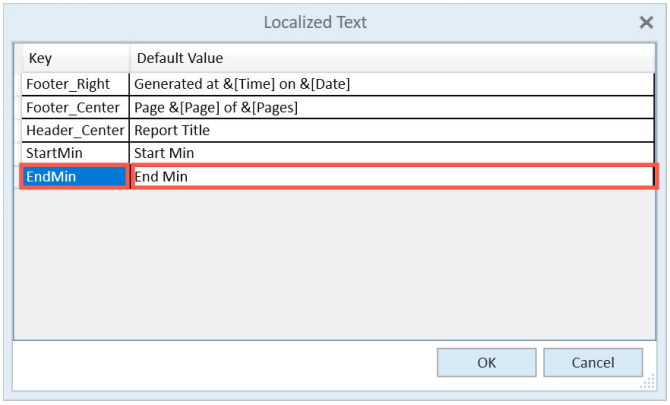
35 For the cell in the second row of the fourth column, select **Component** and **StartX** for **Field Value**, set the horizontal alignment to **Right**, and click **OK**.



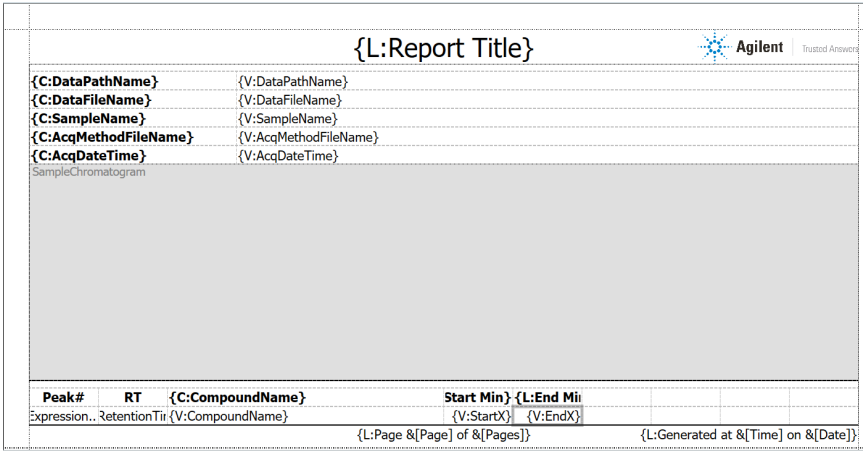
36 Select the **{V:StartX}** cell, double-click **Field Format** in the Properties pane, and select **Component** from the **Binding Name** list and **StartX** from the **Field Name** list.



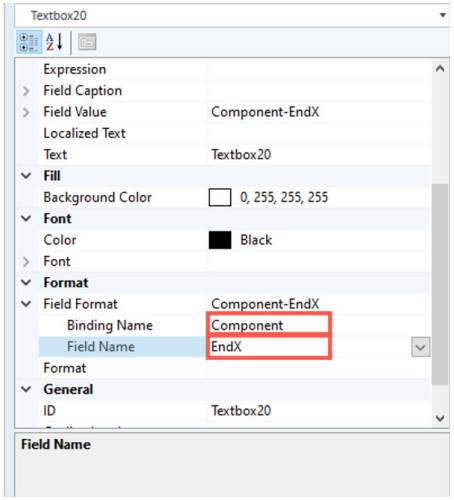
37 For the cell in the first row of the fifth column, in the **Localized Text** window, enter **EndMin** in the **Key** column, and **End Min** in the **Default Value** column, and click **OK**.



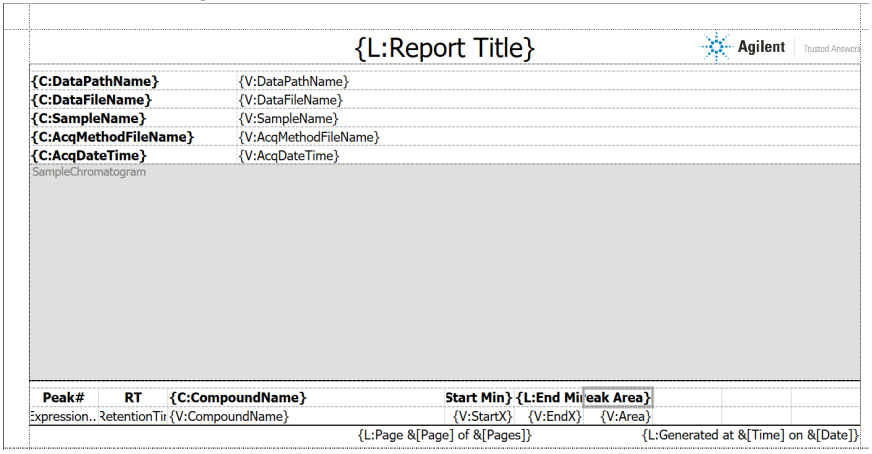
38 For the cell below it, select **Component** and **EndX** for **Field Value**. Bold the text of the cell in the first row, and change the horizontal alignment of both cells to **Right**.



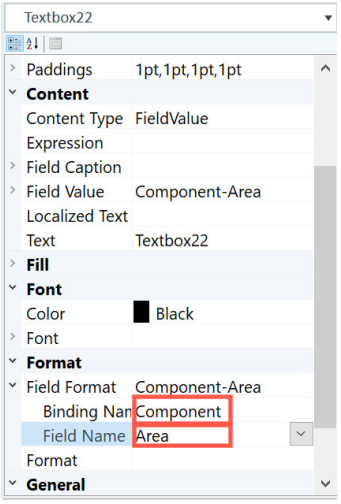
39 Select the cell containing **{V:EndX}**, double-click **Field Format** in the Properties pane, and select **Component** from the **Binding Name** menu, and **EndX** from the **Field Name** menu.



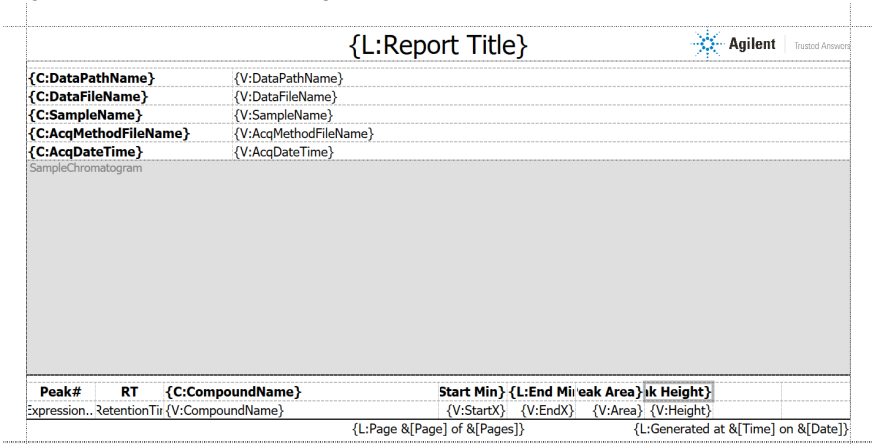
40 For the cells in the sixth column, enter **PeakArea** for **Key**, and **Peak Area** for **Default Value** in the **Localized Text** window for the cell in the first row, and select **Component** and **Area** for the **Field Value** of the cell in the second row. Bold the text of the cell in the first row, and change the horizontal alignment of both cells to **Right**.



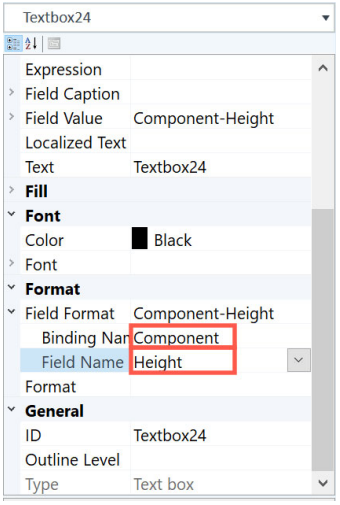
41 Select the **{V:Area}** cell, and select **Component** and **Area** in the **Field format** of the Properties pane.



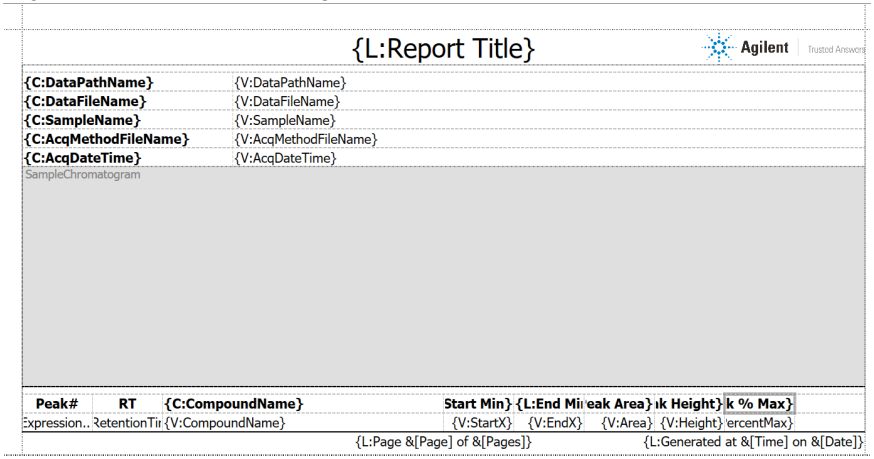
42 For the cells in the seventh column, enter **PeakHeight** for **Key**, and **Peak Height** for **Default Value** in the **Localized Text** window for the cell in the first row, and select **Component** and **Height** for the **Field Value** of the cell in the second row. Bold the text of the cell in the first row, and change the horizontal alignment of both cells to **Right**.



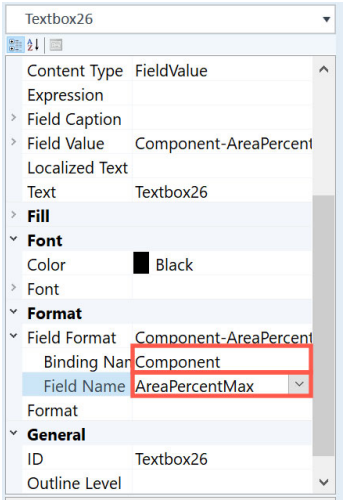
43 Select the **{V:Height}** cell, and select **Component** and **Height** in the **Field format** section of the Properties pane.



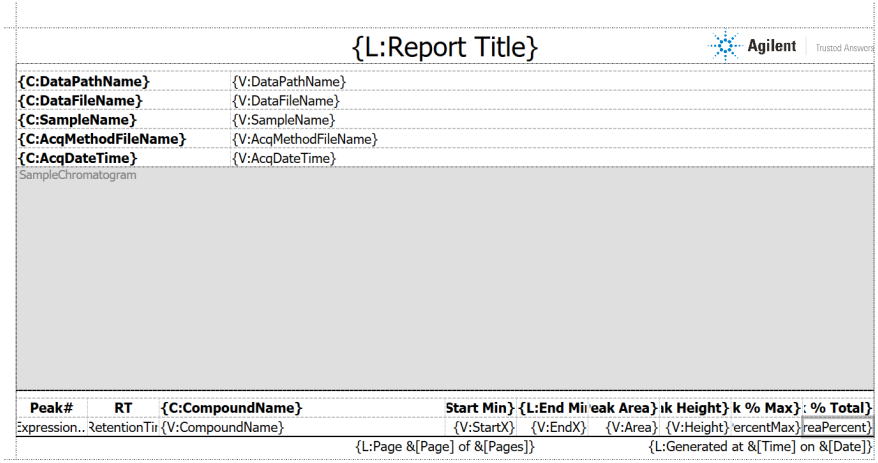
44 For the cells in the eighth column, enter **Peak%Max** for **Key**, and **Peak % Max** for **Default Value** in the **Localized Text** window for the cell in the first row, and select **Component** and **AreaPercentMax** for the **Field Value** of the cell in the second row. Bold the text of the cell in the first row, and change the horizontal alignment of both cells to **Right**.



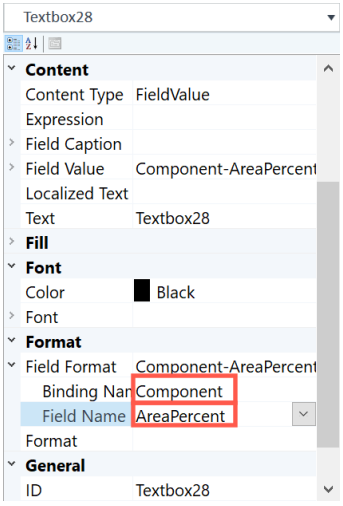
45 Select the **{V:AreaPercentMax}** cell, and select **Component** and **AreaPercentMax** in the **Field format** section of the Properties pane.



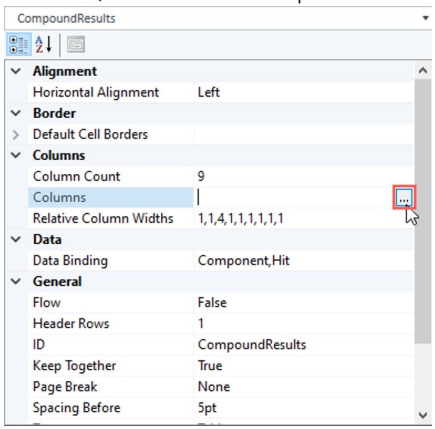
46 For the cells in the ninth column, enter **Peak%Total** for **Key**, and **Peak % Total** for **Default Value** in the **Localized Text** window for the cell in the first row, and select **Component** and **AreaPercent** for the **Field Value** of the cell in the second row. Bold the text of the cell in the first row, and change the horizontal alignment of both cells to **Right**.



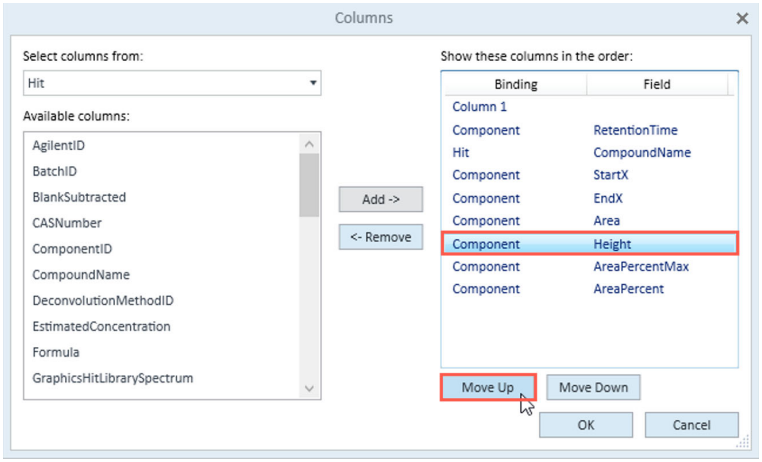
47 Select the **{V:AreaPercent}** cell, and select **Component** and **AreaPercent** in the **Field format** section of the Properties pane.



48 Select **CompoundResults** from the list at the top of the Properties pane. Click **Columns**, then click the ellipsis.

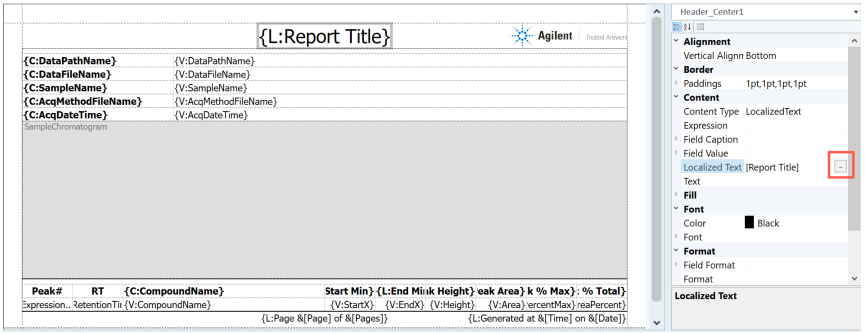


49 In the **Columns** window, select **Height**, and click **Move Up**. Click **OK**.

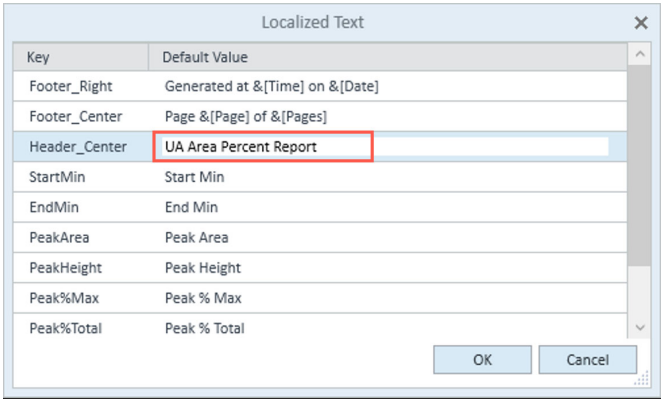


Add a report title

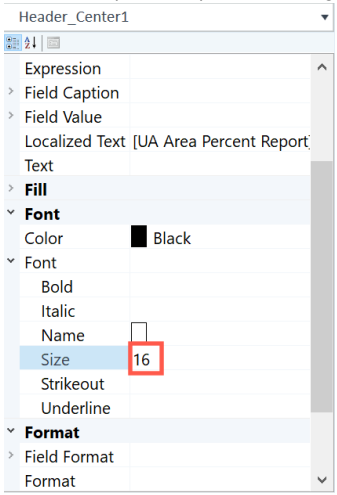
1 Select the **{L:Report Title}** cell in the page header. Click **Localized Text** in the Properties pane, then click the ellipsis.



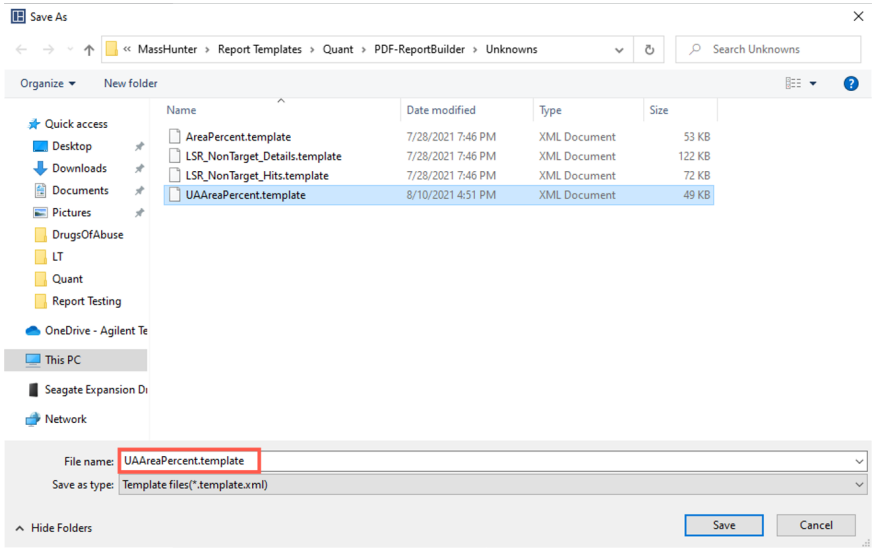
2 Enter **UA Area Percent Report** in the **Default Value** column for **Report Title**. Click **OK**.



3 In the Properties pane, change the font size to **16**.



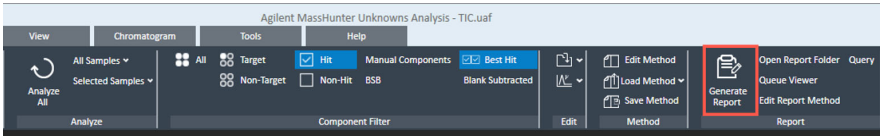
4 Click **File > Save As**, and save the template as **UAAreaPercent.template.xml**.



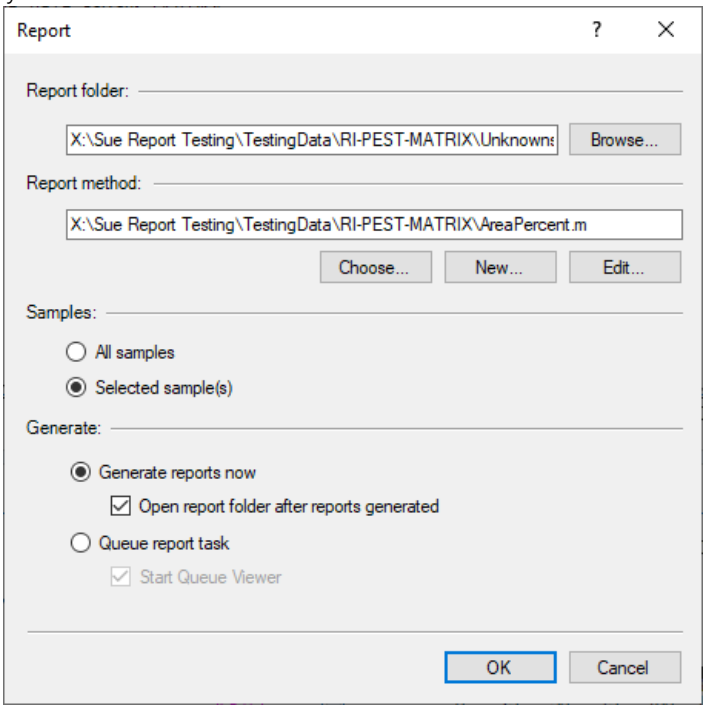
Generate a report

1 Open a TIC analysis in MassHunter Unknowns Analysis.

2 Click **Home > Generate Report**.



3 Under **Report method**, click **Choose**, navigate to the relevant folder, and load your method.

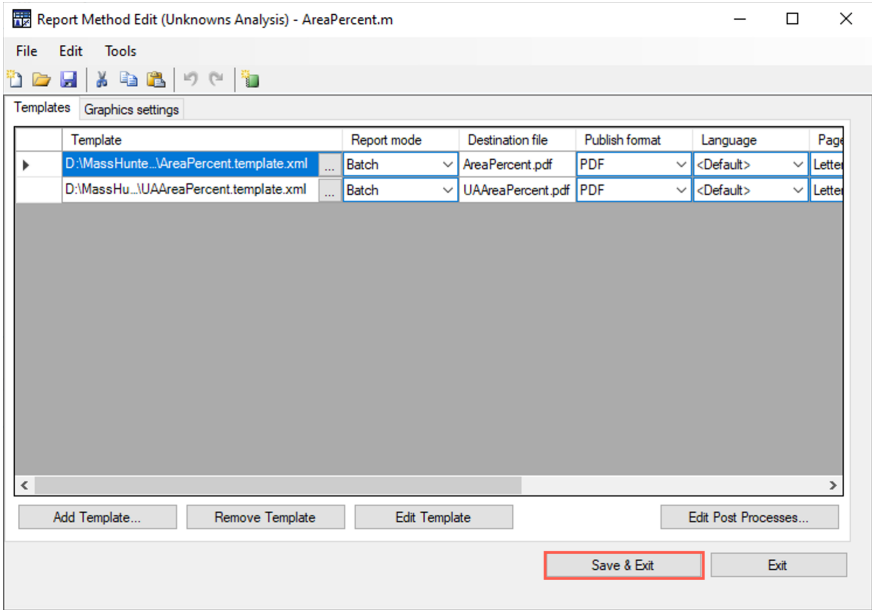


4 Under **Report method**, click **Edit**.

5 Click **Add Template**.

6 Search for and select your report template, and click **Open**.

7 Click **Save & Exit**.

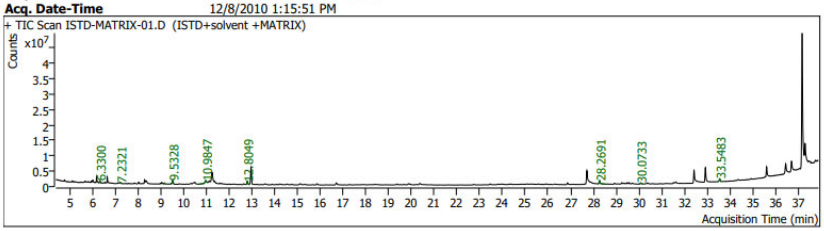


8 Click **OK** at the bottom of the **Report** window. A PDF report is generated using the selected batch files.

UA Area Percent Report

Agilent | Trusted Answers

Path Name	D:\MassHunter\Data\QuantExamples\MS\RI-PEST-MATRIX
File Name	ISTD-MATRIX-01.D
Sample Name	ISTD+solvent +MATRIX
Acq. Method File	unknown ChemStation method
Acq. Date-Time	12/8/2010 1:15:51 PM



Peak#	RT	Compound Name	Start Min	End Min	Peak Height	Peak Area	Peak % Max	Peak % Total
1	4.5471		4.5169	4.6217	111620.1	400754.0	0.30	0.074
2	4.7766		4.7246	4.8525	425676.1	1056317.8	0.78	0.196
3	4.9475		4.9316	5.0008	103819.8	162110.0	0.12	0.030
4	5.1129		5.0811	5.1503	363378.4	801907.4	0.59	0.149
5	5.1716		5.1503	5.2090	296977.9	538325.2	0.40	0.100
6	5.2464		5.2090	5.3371	173600.1	700716.0	0.52	0.130
7	5.5079		5.4496	5.5506	124176.3	489995.1	0.36	0.091
8	5.6841		5.5506	5.7695	532281.3	2796552.9	2.07	0.519
9	5.8122		5.7695	5.9190	397344.8	2053917.3	1.52	0.381
10	5.9457		5.9190	5.9884	552101.6	1555946.5	1.15	0.289
11	6.0150		5.9884	6.1538	939583.6	3533420.0	2.61	0.656
12	6.1859		6.1538	6.2926	1996357.4	4772464.6	3.53	0.886
13	6.3300	4-Isopropylaniline	6.2926	6.4261	780110.3	2219151.3	1.64	0.412
14	6.4528		6.4261	6.4901	99831.8	225882.6	0.17	0.042
15	6.5488		6.4901	6.5809	343728.5	980698.6	0.73	0.182
16	6.6556		6.6076	6.7463	2010795.4	4593388.0	3.40	0.853
17	6.7730		6.7463	6.8478	247699.8	931148.1	0.69	0.173
18	6.8691		6.8478	6.9617	128186.5	513046.6	0.38	0.095
19	7.1734		7.0079	7.1947	268803.2	1179532.3	0.87	0.219
20	7.2321	Promecarb artifact [5-isopropyl-3-methylphenol]	7.1947	7.3201	412183.4	1387288.1	1.03	0.258
21	7.3602		7.3360	7.3869	59278.0	106871.1	0.08	0.020
22	7.4723		7.3869	7.5146	138226.0	363796.0	0.27	0.068
23	7.5684		7.5373	7.6058	177809.2	354774.4	0.26	0.066
24	7.6431		7.6058	7.6743	138834.7	307501.9	0.23	0.057
25	7.7392		7.6889	7.7873	80327.5	258435.6	0.19	0.048
26	7.8406		7.7873	7.9421	268633.3	1125971.0	0.83	0.209
27	8.0328		7.9635	8.1129	583026.8	1849105.8	1.37	0.343
28	8.1449		8.1129	8.1716	136463.8	343106.4	0.25	0.064
29	8.2250		8.1716	8.2517	142361.4	555019.6	0.41	0.103
30	8.2944		8.2517	8.3264	1385881.9	3360444.4	2.49	0.624
31	8.3691		8.3264	8.6307	984507.4	5648265.6	4.18	1.049
32	8.7321		8.6734	8.7647	73854.2	261227.1	0.19	0.048
33	8.8121		8.7774	8.9136	87565.5	445246.9	0.33	0.083
34	8.9776		8.9136	9.0096	298768.8	735845.2	0.54	0.137
35	9.0470		9.0096	9.1324	574933.0	2075184.2	1.54	0.385
36	9.1645	Tetrahydrophthalimide, cis-1,2,3,6-	9.1324	9.2285	384897.8	1073670.1	0.79	0.199
37	9.2659		9.2285	9.3406	99177.7	413634.1	0.31	0.077
38	9.5328	Cashmeran	9.4527	9.6175	1303243.9	4089720.4	3.03	0.759
39	9.8103		9.7641	9.9224	171585.9	792690.1	0.59	0.147
40	9.9972		9.9224	10.0452	61705.8	280784.5	0.21	0.052
41	10.1093		10.0627	10.1947	92637.5	486768.1	0.36	0.090
42	10.3281		10.1947	10.3762	310478.0	1691707.9	1.25	0.314
43	10.4936		10.3762	10.6751	688415.5	5348863.8	3.96	0.993

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3 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.

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.

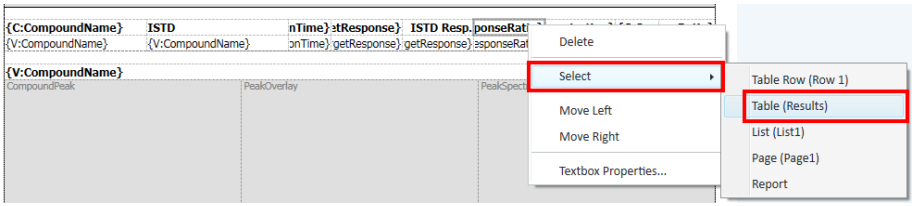
Replace a Column in the Report

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

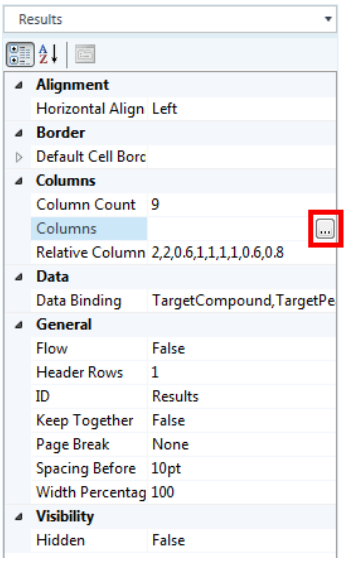
Replace a column using the Columns window

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

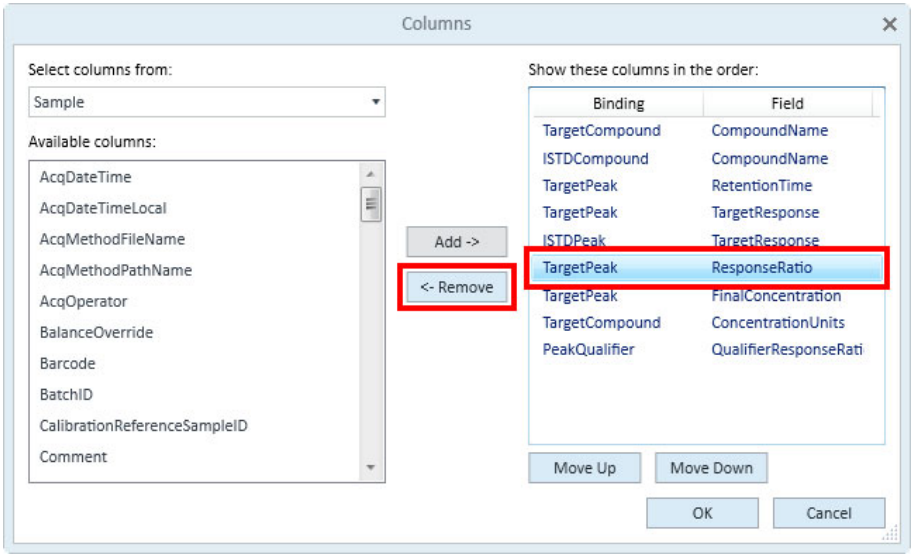
2 Right-click the **ResponseRatio** column header, and select **Select > Table (Results)**.



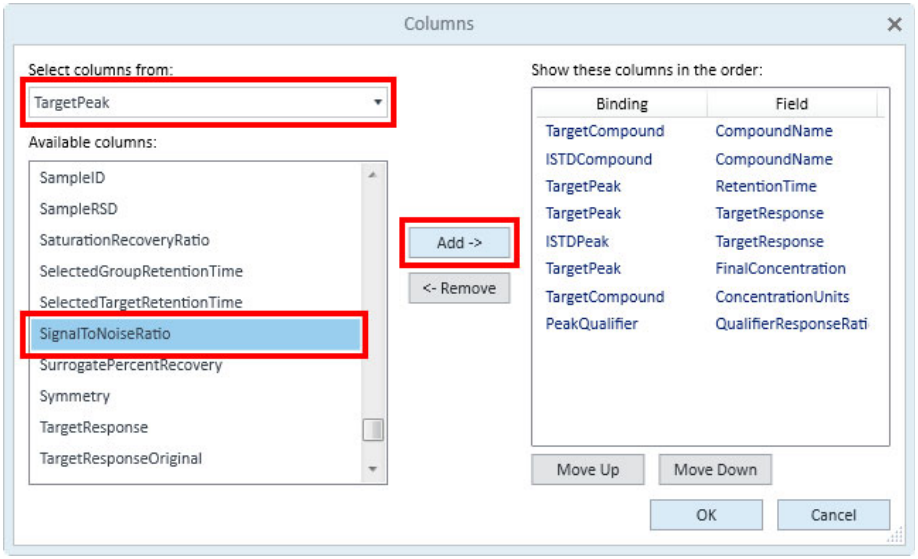
3 In the **Columns** field in the **Properties** pane, click the ellipsis.



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**.



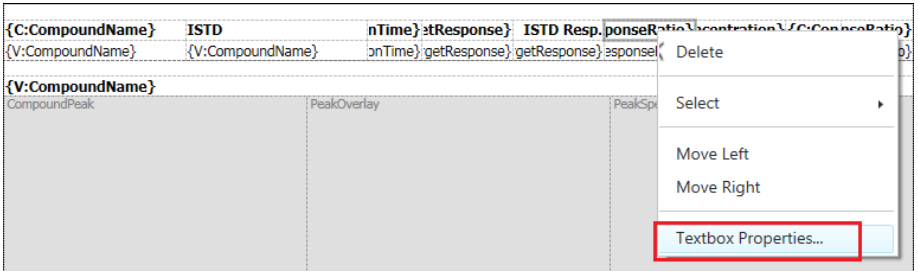
6 Click **Move Up** or **Move Down** to move the column to the desired location.

7 Click **OK**. The **ResponseRatio** column is replaced by the **SignalToNoiseRatio** column.

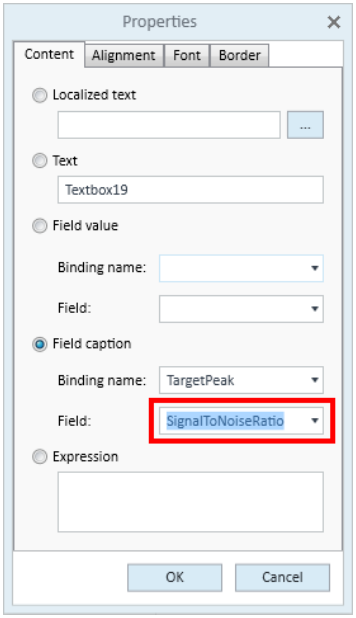
Replace a column using the Textbox Properties window

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

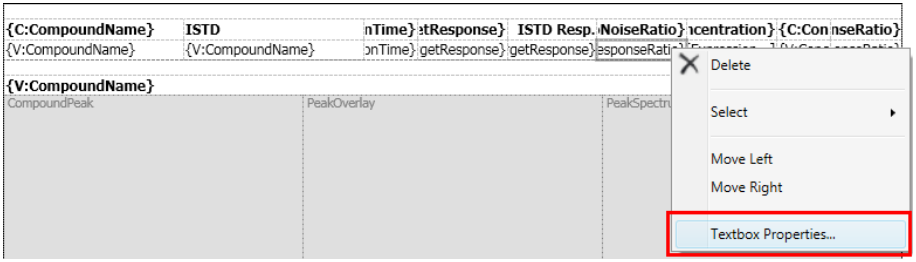
2 Right-click the **ResponseRatio** column header, and select **Textbox Properties**.



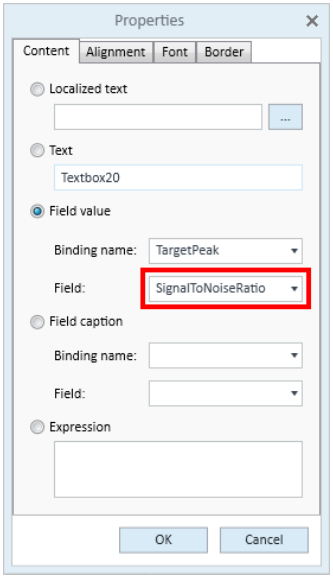
3 Select **SignalToNoiseRatio** from the **Field Caption > Field** list, and click **OK**.



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



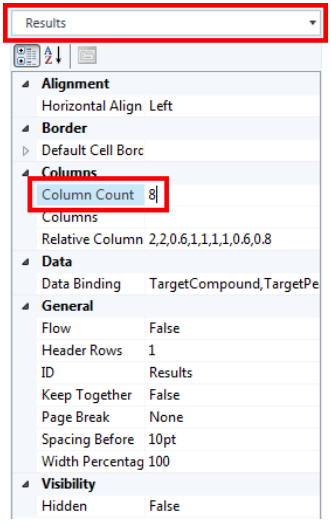
5 Select **SignalToNoiseRatio** from the **Field Value > Field** list, and click **OK**



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.

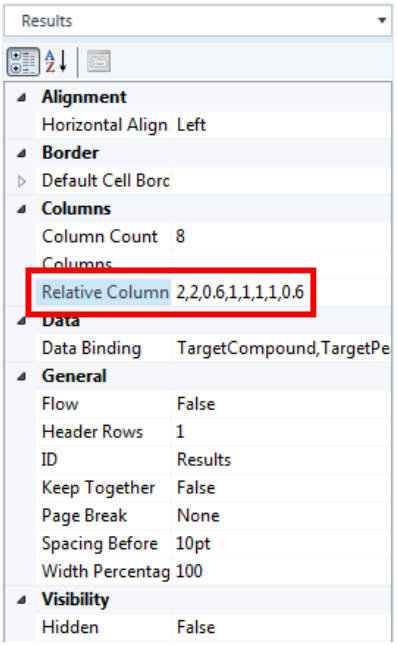
To remove a column that is not the last column in the table:

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.

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.

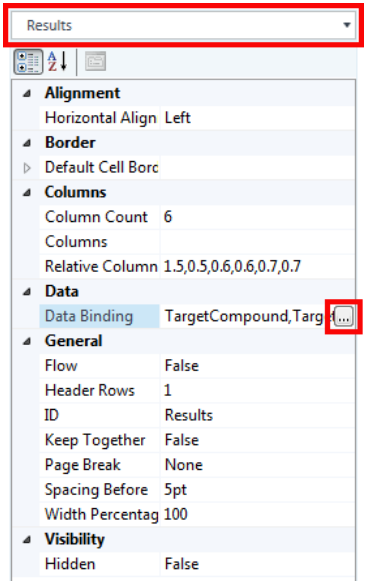
Filter Results Using Special Conditions

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

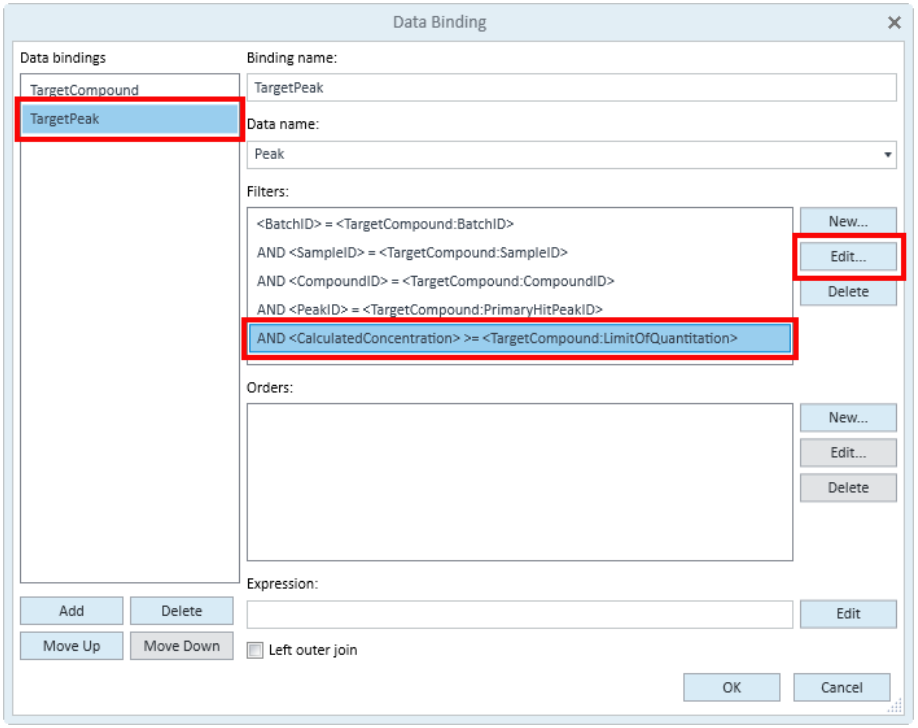
   This report filters results lower than the LOQ. Use this procedure to modify the data binding to filter results lower than the LOD.

2. Select the **Results** table in the **Properties** pane, and click the ellipsis in the **Data Binding** field.

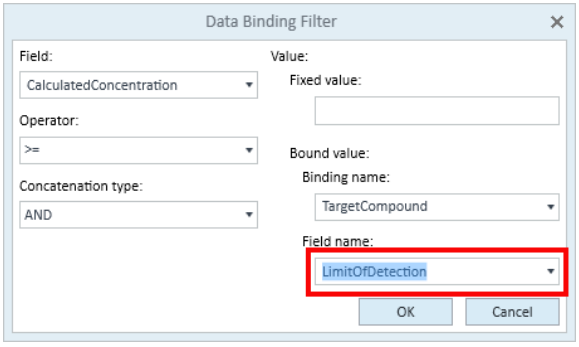
3. In the **Data Binding** window, select **Target Peak**, and then select **AND <CalculatedConcentration> >= <TargetCompound:LimitOfQuantitation>**.



4 Click **Edit**.



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

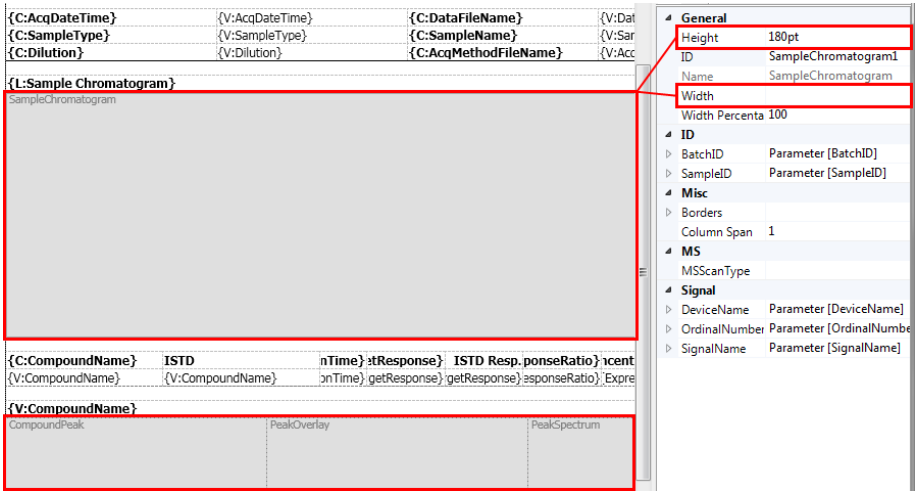


6 Click **OK**.

7 Save the template.

Adjust the Size of a Graphic

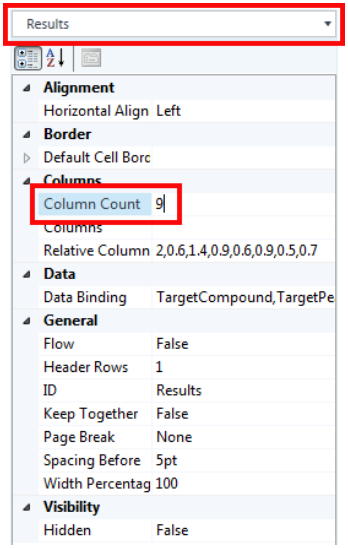
1. Navigate to **D:\MassHunter\Report Templates\Quant\PDF-ReportBuilder\Quant**, and open **Gen_Samples_ISTD.template.xml**.
2. Select the graphic to resize.
3. In the **Height** and **Width Percentage** fields in the **Properties** pane, change the values to adjust the size of the graphic.



4. Save the template.

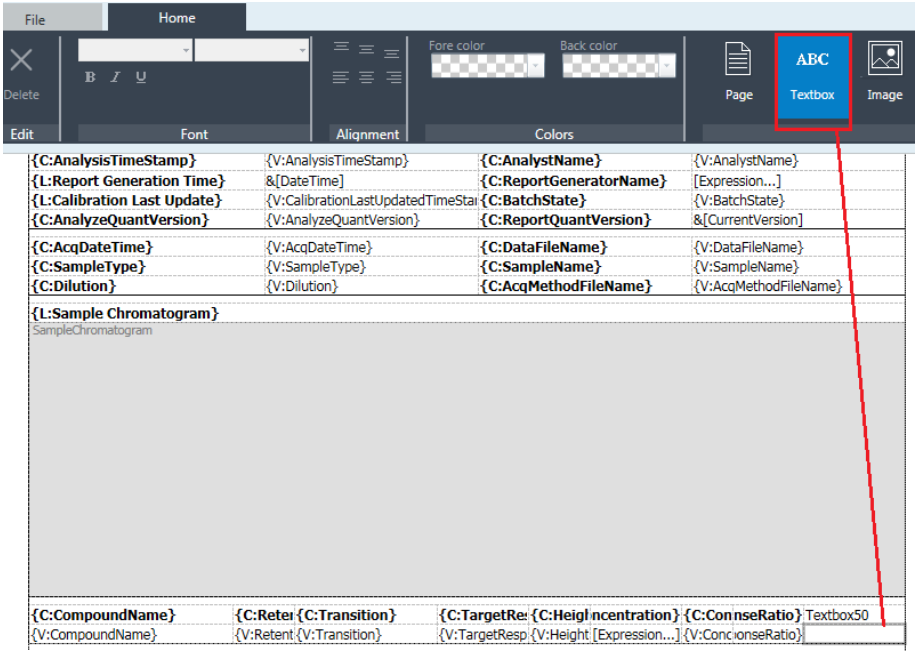
Add a New Column to an Existing Report

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**.



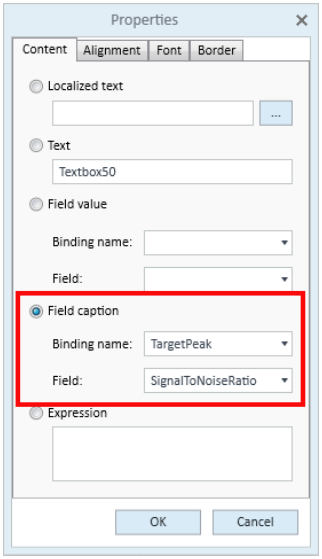
A new empty column is added to the end of the table.

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**.

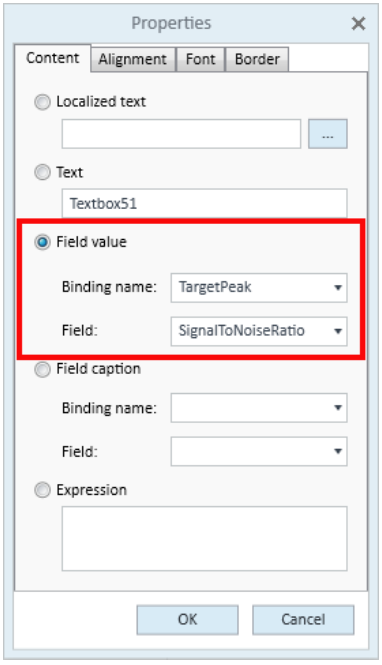
5 Select **Field caption**, select **TargetPeak** from the **Binding name** list, and then select **SignalToNoiseRatio** from the **Field** list.



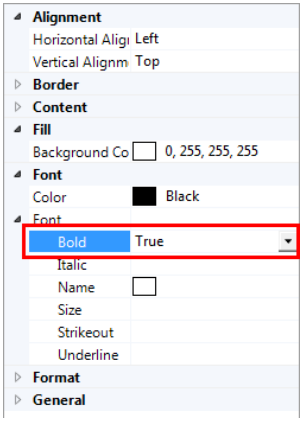
6 Click **OK**.

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.

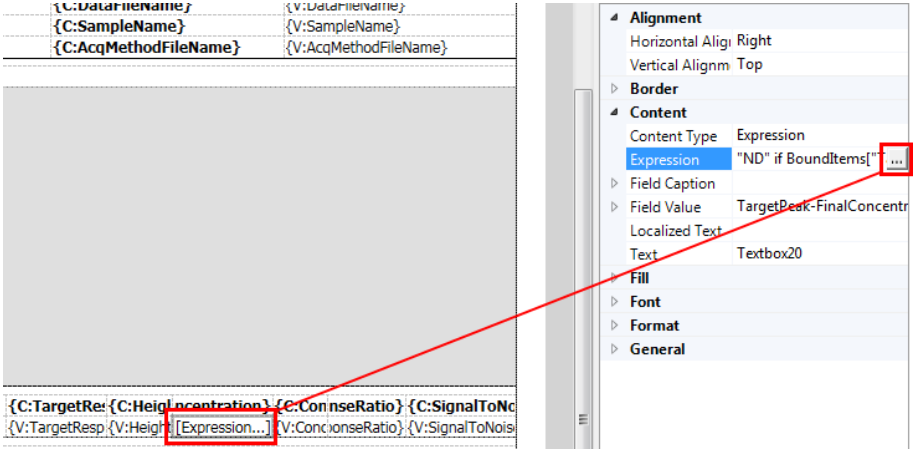


10 Save the template.

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**.

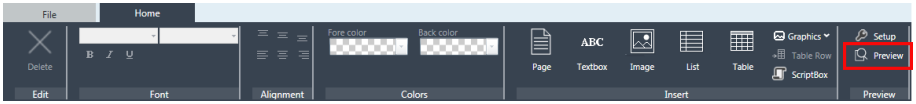
4 Save the template.

Preview the Report

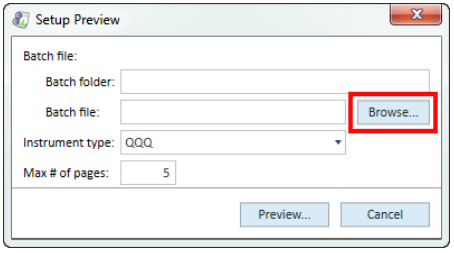
After changes have been made to the report template, you can preview the report by setting up the Report Builder with your dataset.

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

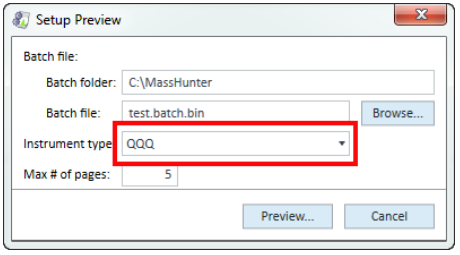
2 Click **Preview**.



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

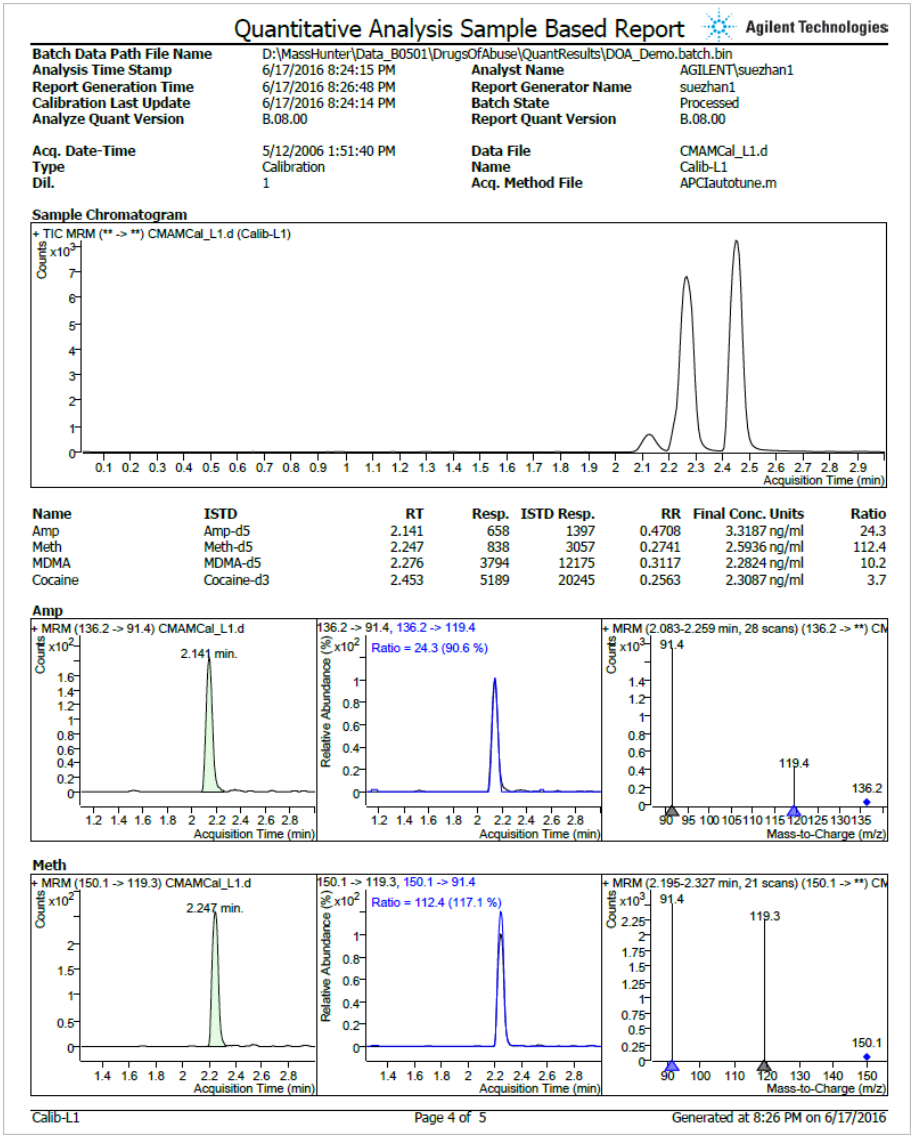


4 Select the **Instrument type** to match your dataset.



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 **DrugsofAbuse** dataset.



Quantitative Analysis Sample Based Report — Agilent Technologies

Batch Data Path File Name	D:\MassHunter\Data_B0501\DrugsOfAbuse\QuantResults\DOA_Demo.batch.bin		
Analysis Time Stamp	6/17/2016 8:24:15 PM	**Analyst Name**	AGILENT\suezhan1
Report Generation Time	6/17/2016 8:26:48 PM	**Report Generator Name**	suezhan1
Calibration Last Update	6/17/2016 8:24:14 PM	**Batch State**	Processed
Analyze Quant Version	B.08.00	**Report Quant Version**	B.08.00
Acq. Date-Time	5/12/2006 1:51:40 PM	**Data File**	CMAMCal_L1.d
Type	Calibration	**Name**	Calib-L1
Dil.	1	**Acq. Method File**	APCIautotune.m

Sample Chromatogram

+ TIC MRM (** -> **) CMAMCal_L1.d (Calib-L1)

Name	ISTD	RT	Resp.	ISTD Resp.	RR	Final Conc. Units	Ratio
Amp	Amp-d5	2.141	658	1397	0.4708	3.3187 ng/ml	24.3
Meth	Meth-d5	2.247	838	3057	0.2741	2.5936 ng/ml	112.4
MDMA	MDMA-d5	2.276	3794	12175	0.3117	2.2824 ng/ml	10.2
Cocaine	Cocaine-d3	2.453	5189	20245	0.2563	2.3087 ng/ml	3.7

Amp

+ MRM (136.2 -> 91.4) CMAMCal_L1.d — 2.141 min.

136.2 -> 91.4, 136.2 -> 119.4 — Ratio = 24.3 (90.6 %)

+ MRM (2.083-2.259 min, 28 scans) (136.2 -> **) CM — 91.4, 119.4, 136.2

Meth

+ MRM (150.1 -> 119.3) CMAMCal_L1.d — 2.247 min.

150.1 -> 119.3, 150.1 -> 91.4 — Ratio = 112.4 (117.1 %)

+ MRM (2.195-2.327 min, 21 scans) (150.1 -> **) CM — 91.4, 119.3, 150.1

Calib-L1 Page 4 of 5 Generated at 8:26 PM on 6/17/2016

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