Report Template Editor

Concepts Guide

Agilent Technologies

Notices

Manual Part Number

G4635-90014

Edition

01/2013

Printed in Germany

Agilent Technologies
Hewlett-Packard-Strasse 8
76337 Waldbronn

This product may be used as a component of an in vitro diagnostic system if the system is registered with the appropriate authorities and complies with the relevant regulations. Otherwise, it is intended only for general laboratory use.

Software Revision

This guide is valid for revision A.01.05 of Agilent OpenLAB CDS.

Warranty

The material contained in this document is provided "as is," and is subject to being changed, without notice, in future editions. Further, to the maximum extent permitted by applicable law, Agilent disclaims all warranties, either express or implied, with regard to this manual and any information contained herein, including but not limited to the implied warranties of merchantability and fitness for a particular purpose. Agilent shall not be liable for errors or for incidental or consequential damages in connection with the furnishing, use, or performance of this document or of any information contained herein. Should Agilent and the user have a separate written agreement with warranty terms covering the material in this document that conflict with these terms, the warranty terms in the separate agreement shall control.

Technology Licenses

The hardware and/or software described in this document are furnished under a license and may be used or copied only in accordance with the terms of such license.

Restricted Rights Legend

If software is for use in the performance of a U.S. Government prime contract or subcontract, Software is delivered and licensed as "Commercial computer software" as defined in DFAR 252.227-7014 (June 1995), or as a "commercial item" as defined in FAR 2.101(a) or as "Restricted computer software" as defined in FAR 52.227-19 (June 1987) or any equivalent agency regulation or contract clause. Use, duplication or disclosure of Software is subject to Agilent Technologies' standard commercial license terms, and non-DOD Departments and Agencies of the U.S. Government will receive no greater than Restricted Rights as defined in FAR 52.227-19(c)(1-2) (June 1987). U.S. Government users will receive no greater than Limited Rights as defined in FAR 52.227-14 (June 1987) or DFAR 252.227-7015 (b)(2) (November 1995), as applicable in any technical data.

Safety Notices

CAUTION

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

WARNING

A WARNING notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in personal injury or death. Do not proceed beyond a WARNING notice until the indicated conditions are fully understood and met.

In This Guide...

This guide contains information for template developers. It describes the concepts and advanced features of the Report Template Editor (RTE).

For information on basic tasks and the user interface please refer to the RTE online help.

1 Overview

This chapter provides an overview of the possibilities of the Report Template Editor.

2 Text Fields and Data Fields

This chapter describes the characteristics and usage of text fields and data fields in RTE.

3 Tables

This chapter describes the characteristics and usage of tables in RTE.

4 Matrices

This chapter describes the characteristics and usage of matrices in RTE.

5 Composite Groups

This chapter describes the characteristics and usage of Composite Groups in RTE.

6 Images

This chapter describes the characteristics and usage of images in RTE.

7 Chromatograms

This chapter describes the characteristics and usage of chromatograms in RTE.

8 Calibration Curves

This chapter describes the characteristics and usage of calibration curves in RTE.

9 Spectra

This chapter describes the characteristics and usage of spectra in RTE.

10 Charts

This chapter describes the characteristics and usage of charts in RTE.

11 Method Information

This chapter describes the characteristics and usage of method information in RTE.

13 Expressions

This chapter describes the characteristics and usage of expressions in RTE.

14 Calculation Variables

This chapter describes the characteristics and usage of calculation variables in RTE.

19 Appendix

This chapter contains a list of all operators and functions available in the Expression Editor.

Contents

1 Overview

This chapter provides an overview of the possibilities of the Report Template Editor.

Overview

Data provided by different applications

You can use report templates in different applications, for example, in OpenLAB ECM Intelligent Reporter, OpenLAB CDS ChemStation, or OpenLAB CDS EZChrom edition. With report templates, a user can create reports with a specific design, such as a sequence overview with a sequence table and statistics, or a cross-sequence summary. The reports will contain the data selected in the current session of the respective program.

File format of report templates

All report templates are based on the Report Definition Language (RDL), which is a standardized XML format provided by Microsoft®.

Creating and editing report templates

To create report templates, you can either use the Report Template Editor (RTE) or Microsoft SQL Server Business Intelligence Development Studio (BI Studio):

- *RTE* provides an easy-to-use interface that helps you create report templates in a few steps. It supports all types of report items and most of the respective configuration options. The RTE user interface is adapted to handle OpenLAB CDS data.

  With RTE, you cannot edit templates that have been created with BI Studio.

- *BI Studio* provides the complete range of functions (for example, you can create custom code for complex calculations or advanced expressions). BI Studio is a general tool, that does not specifically address analytical data.

  In BI Studio, you can edit any report template, no matter whether it was created with RTE or with BI Studio.

  However, working with BI Studio requires advanced knowledge of template development. For more information, please refer to the *Manual for Advanced Report Template Designers*. This manual also contains detailed descriptions of the Agilent report templates that are delivered with OpenLAB ECM Intelligent Reporter.

NOTE These templates are specifically designed for usage in BI Studio and contain most of the advanced features that are not available in RTE.

Snippets

RTE provides various preconfigured report items — so-called *snippets* — that you can use in your templates. The items are organized in folders that reflect the content. The folders and subfolders under which the snippets are located are determined by the snippet itself and cannot be changed.

Report Template Documentation

Report Template Documentation Tool is a standalone application to view the description of the RTE supported report templates. It can also save this description in PDF format. The description about the report template includes layout of report items along with their parameter details, such as calculation variables, report parameters, expressions used, filter condition, sort condition, audit trail etc.

To launch the Report Template Documentation Tool, run the TemplateDocumentation.exe file. By default, it is located in c:\chem32\core for ChemStation Edition or c:\Program Files\Agilent Technologies\EZChrom for EZChrom Edition. When the application is launched, an Open dialog allows you to select a report template.

Report Types

Each template is of specific report type. Depending on this report type, the template is connected to a particular database view. Therefore, different data fields are available in a report template, depending on the report type. In addition, RTE displays the report items differently depending on the report type. The following report types are available:

- **Single Injection**: You can use any information associated with the sample acquisition (sequences/samples/injections/instruments), the results (signals/peaks/compounds/calibration curves), and the project administration (file/project).

  With this report type, RTE automatically creates a list of all injections in the current data scope, and then shows the report items from the template separately for each injection. Therefore, you do not need to worry about repeating composite groups on injection IDs. On the other hand, you cannot compare results from different injections in one table or matrix.

- **Single Sequence Summary**: You can use the same information as in a Single Injection report.

  With this report type, RTE automatically creates a list of all sequences in the current data scope, and then shows the report items from the template separately for each of the sequences. Therefore, you do not need to worry about repeating composite groups on sequence IDs. On the other hand, you cannot compare results from different sequences in one table or matrix.

- **Cross-Sequence Summary**: You can use the same information as in a Single Injection report.

  With this report type, the data is *not* automatically grouped. Therefore, you must pay more attention to the grouping of your report items, but in return you can create report items that compare data from different sequences.

Working With Templates

To add and configure report items

1. In the **Report Items** browser, open the tree for the required item type, and drill down to the report item level.
2. Drag the report item to the template.
3. Grab the handles to resize the item, or grab the gray border to move the item.
4. To configure the report item, right-click the item and select **Properties** from the context menu. Alternatively, you can double-click the report item.

   If you double-click a text field, you can directly enter the *Value*.

   If you double-click a data field, you can directly enter the *Label* of the field.

   If you double-click a table header, you can directly enter the header text.

   If you double-click other report items, the corresponding **Properties** dialog opens.
5. Adjust the properties according to your requirements.
6. Select **File > Save** or **File > Save as** to save the report template.

To move or resize report items

To move a report item:

- Grab the report item border with the mouse, and drag it to the new position.

  - or -
- Select the report item, and use the arrow keys.

To resize a report item:

- Grab the handles of the report item border, and drag them to the required new size.

  - or -
- Select the report item, and press **Shift+Arrow key**.

To align report items

NOTE

- Aligning and spacing options are not applicable for report items inside locked composite groups.
- Sizing options are not applicable for locked report items.
- Spacing options are not applicable for multiple report items selected across different regions (that is, body, header, or footer).

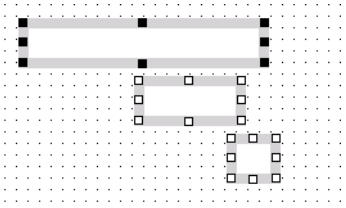
To align multiple report items relative to each other

To align multiple report items, either none of the selected items must be in a composite group, or all items must be in the same composite group.

1 Click the report item you want to use to align the other report items.

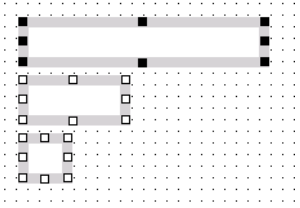
2 Hold the **Ctrl** key while clicking the items you want to align.

The first selected report items is highlighted with black squares. All other selected items are highlighted with white squares.



3 Right-click one of the selected items, and select the appropriate **Align** command from the context menu.

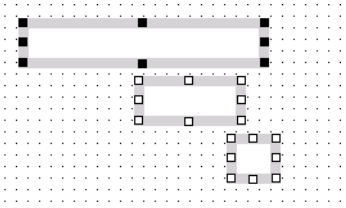
All items are aligned to the first selected item. The following figure shows the report items after aligning the left margins.



To set the same size for multiple report items

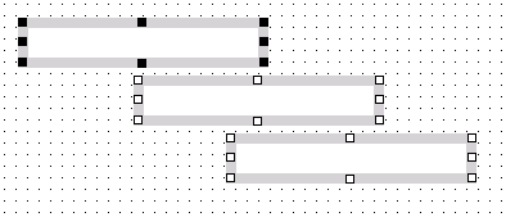
1 Click the text field or data field from which you want to use the width or height.

2 Hold the **Ctrl** key while clicking the text fields or data fields that you want to adjust.



3 Right-click one of the selected items, and select the appropriate **Make Same Size** command from the context menu.

The width or height or both are adjusted to the size of the first selected item. The following figure shows the report items after setting the same *width* to all items.



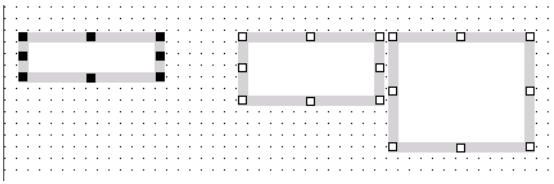
To set equal horizontal spacing

To adjust the spacing between multiple report items, either none of the selected items must be in a composite group, or all items must be in the same composite group.

1 Select the text fields or data fields for which you want to adjust the spacing. The order in which you select the items is irrelevant.

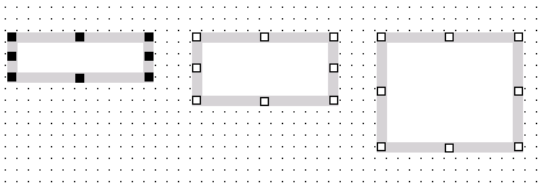
2 Align the items horizontally (**Tops**, **Middles** or **Bottoms**).

The following figure shows an example with aligned tops.



3 Right-click one of the selected items, and select **Horizontal Spacing > Make Equal** from the context menu.

The same horizontal spacing is used between all selected items.

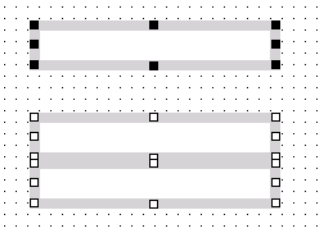


To set equal vertical spacing

1 Select the text fields or data fields for which you want to adjust the spacing. The order in which you select the items is irrelevant.

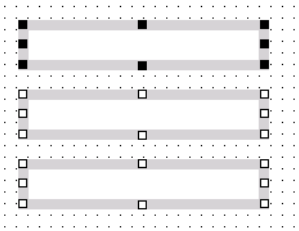
2 Align the items vertically (**Lefts**, **Rights**, or **Centers**).

To following figure shows an example with same widths and aligned lefts.



3 Right-click one of the selected items, and select **Vertical Spacing > Make Equal** from the context menu.

The same vertical spacing is used between all selected items.



To dock the Report Items browser

You can dock the **Report Items** browser to the left or to the right of the Editing Pane.

1 Drag the title bar of the **Report Items** browser to the other side of the Editing Pane.

The **Report Items** browser snaps to the right or to the left side, depending on the position of the mouse when you release the title bar.

To show or hide the Report Items browser

You can either show the **Report Items** browser permanently, or collapse it and show it dynamically on demand. By default, the **Report Items** browser is permanently visible.

To collapse the Report Items browser:

1 Click  .

The **Report Items** browser collapses. It is shown as a vertical label on the side of the Editing Pane.

2 Click the vertical label, or simply move the mouse over it, to show the **Report Items** browser on demand.

The **Report Items** browser is shown. If you move the mouse away, it will collapse again.

To permanently show the Report Items browser:

1 The title bar of a dynamically shown **Report Items** browser contains a horizontal pushpin  . Click this pin.

The pushpin changes to vertical  . The **Report Items** browser is now permanently visible.

To change the page width and margins

1 In Report Properties, change the values under **Page Layout**.

With **Page Height** and **Page Width**, you set the paper size. With **Top Margin**, **Bottom Margin**, **Left Margin**, and **Right Margin**, you set the margins on the paper.

2 Save your settings.

The area shown in the Editing Pane already considers the margins configured in the report properties. When you generate the report, RTE will automatically add these margins.

If the new page width is too small for all report items to be printed, the area that exceeds the page size is shown with a light gray background. If there is a gray area, additional pages will be printed.

3 If required, delete, resize, or move the report items from the gray area.

4 To remove the gray area: Move the mouse over the right border of the gray area. When the pointer becomes a double-headed arrow, drag the pointer to the left.

2
Text Fields and Data Fields

This chapter describes the characteristics and usage of text fields and data fields in RTE.

About Text Fields and Data Fields

Available fields

The assortment of data fields in the **Report Items** browser depends on the following factors:

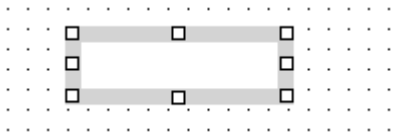
- The selected report type
- The chromatography data system

Field types

The Report Template Editor provides the following types of fields:

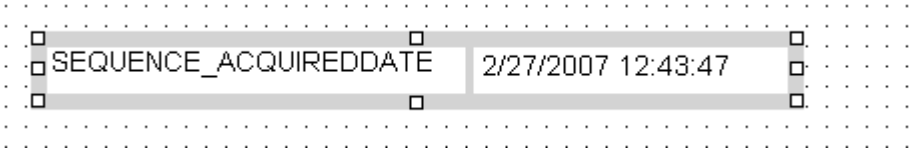
- *Text fields* are basically simple textboxes that can contain either static text or dynamic expressions. Text fields are, for example, used to display static headlines in a report template.

  In the **Report Items** browser, you find the **Text field** in the **Special Objects** category.



- *Data fields* are divided into two parts, label and value. The label contains a static text, the value contains a dynamic expression. Data fields are typically used to show specific data, for example the sequence name or the sample name. You can, however, modify both label and value according to your requirements.

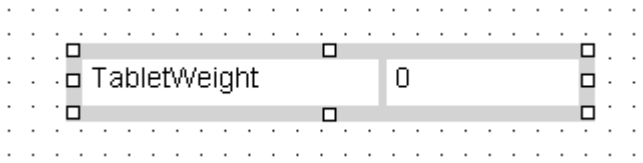
  In the **Report Items** browser, you find all available data fields in the **Fields** category.



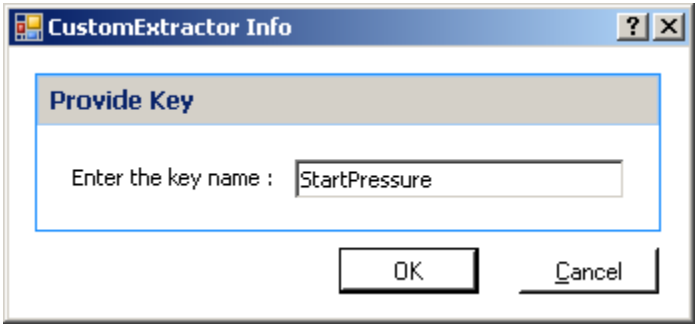
- *Custom fields* are a special type of data field. You configure the custom fields in the chromatography data system, for example, in the method definition in ChemStation. Custom fields allow you to create customized information (both labels and values) which belongs to a specific context, for example, to a sample or to a compound. RTE allows you to perform calculations with custom fields.

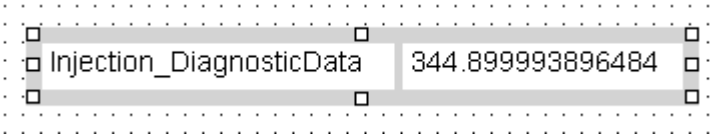
  In contrast to the regular data fields, the label shown for custom fields is not the data field name (e.g. **Sample_CustomField01**) but rather the customized label information (e.g. "TabletWeight"). This is achieved by a combination of the *Trim*, *Choose*, and *Split* functions in the expression for the value. RTE automatically creates this expression.

  You can configure both label and value in your chromatography data system.



- *Complex custom fields* are data fields that do not contain a single value but an entire XML structure. This XML structure contains various key/value pairs. If you drag such a field to the template, a dialog asks you for the key of the information you want to access. As a result, RTE creates a data field where the label is the name of the complex custom field, and the value is the specific value stored under the given key. This value is accessed with the help of the
  `CFE` function. RTE automatically creates this expression.





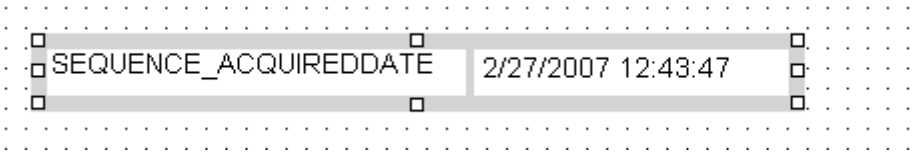
Depending on the chromatography data system, the following complex custom fields may be available:

- **Injection > DiagnosticData**: information on the injection, for example start pressure, stop pressure, or air temperature. The keys depend on the chromatography data system used (see "Keys in Diagnostic Data" on page 173).
- **Sequence > CustomFields**: all labels and values contained in the data fields **Sequence_CustomField01** to 10 (or higher, if there are more than 10 ten custom fields).
- **Sample > CustomFields**: all labels and values contained in the data fields **Sample_CustomField01** to 10 (or higher, if there are more than 10 ten custom fields).
- **Injection > CustomFields**: all labels and values contained in the data fields **Injection_CustomField01** to 10 (or higher, if there are more than 10 ten custom fields)
- **Compound > CustomFields**: all labels and values contained in the data fields **Compound_CustomField01** to 10 (or higher, if there are more than 10 ten custom fields)

Using Fields

To adjust the width of the label part

Data fields are divided in two parts, label and value:



To adjust the width of the label part, move the mouse over the boundary line between label and value, and drag the line to the required width.

To enter text directly

In text fields, you can edit the text directly by double-clicking the text field in the Editing Pane. The entered text corresponds to the **Value** configured in the item properties. You can enter either static text or dynamic expressions (starting with an equals sign).

In data fields, you can only edit the label part directly, by double-clicking it.

To add a line break

You have various options for entering line breaks:.

- Edit the text directly in the Editing Pane, and press **Ctrl**+**Enter**.
- Edit the **Value** of the text field in the **Expression Editor**, and press **Ctrl**+**Enter**.
- Edit the **Value** of the text field in the **Expression Editor**, and enter the Visual Basic constant *vbNewLine*. For example, the expression can look like the following:

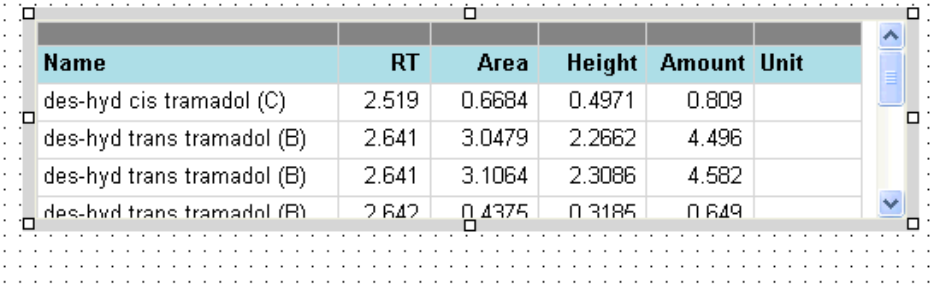
  ="Retention" + vbNewLine + "Time"

3 Tables

This chapter describes the characteristics and usage of tables in RTE.

About Tables

With tables, you can display results in a 2-dimensional format. Tables are used, for example, to summarize the results of samples/sequences. The amount of columns and the headlines are static, the number of rows corresponds to the number of records in the dataset.



Name	RT	Area	Height	Amount	Unit
des-hyd cis tramadol (C)	2.519	0.6684	0.4971	0.809	
des-hyd trans tramadol (B)	2.641	3.0479	2.2662	4.496	
des-hyd trans tramadol (B)	2.641	3.1064	2.3086	4.582	
des-hyd trans tramadol (B)	2.642	0.4375	0.3185	0.649	

Basically, each table contains a specific dataset that is determined by the type of the base template (see "Report Types" on page 12). Thus, without any further configuration, the table would show one row for each record in the dataset, where the records are unsorted, ungrouped, and unfiltered. In order to organize and structure the data, you have the following options for configuring a table:

- **Repeat Table On**: Display the table several times, where each table only contains the data according to the value of specific key information. The particular values (for example, compound names) are used as table headers.
- **Grouping**: The detail rows are arranged according to the distinct values of a given key information (for example, the distinct sample names).
- **Sorting**: The detail rows are sorted according to a given key information.
- **Filtering**: Exclude specific data from the table content.
- **Area Rejection**: Exclude information on peaks that are too small.
- **Show Peak Types**: Specify the type of peaks to be shown in a table (for example, **Identified Peaks** or **Unknown Peaks**).

The table report items available in the **Report Items** browser are all preconfigured in a specific way, so you can use them with only a few adjustments.

Using Tables

To add and remove columns

In the Editing Pane (drag and drop):

1 Select the table in the Editing Pane.

2 In the **Fields** category in the **Report Items** browser, select the information you want to add to the table, and drag the field to the table.

While you move the mouse across the table columns, RTE selects the respective columns. When you release the mouse button, RTE will add the new column to the right of the currently selected column.

In the Editing Pane (context menu)

1 In the Editing Pane, select the table column next to which you want to add the new column.

2 Right-click that column, and select **Insert Column to Left** or **Insert Column to Right** from the context menu.

A sub menu opens with all data categories. The categories contain all data fields that are available for the report type of the current template

3 Select the data field that you want to show in the new table column.

In the Table Properties dialog:

1 Select the table.

2 In the **Table Properties**, select the **Columns** page.

3 Double-click the required data field in the **Available Fields** tree.

OR

Alternatively, you can select the field and click >.

The corresponding table column is inserted to the right of the selected column.

To remove columns

In the Editing Pane:

1 In the Editing Pane, select the table column you want to delete.

2 Right-click the column, and select **Delete Column** from the context menu.

In the Table Properties dialog:

1 In the **Table Properties**, select the **Columns** page.

2 In the **Table Layout**, click the required column to select it.

3 Click <.

The column is removed from the table.

To change the order of table columns

In the Editing Pane:

1 Select the table in the Editing Pane.

2 In the dark gray bar at the top of the table header fields, select the column and drag it to the new position.

While dragging the column, new positions are indicated by a thin blue line.

In the Table Properties dialog:

1 Open the **Table Properties** dialog.

2 Select the **Columns** page.

3 In the dark gray bar at the top of the table header fields, select the column and drag it to the new position.

While dragging the column, new positions are indicated by a thin blue line.

To adjust the column widths

For columns containing any type of value:

1 Select the table in the Editing Pane.

2 In the dark gray bar at the top of the table header fields, drag the column borders with the mouse.

For columns containing string values:

1 Select the table in the Editing Pane.

2 In **Table Properties**, select the **Columns** page.

3 Select the column that you want to adjust.

4 Click **Column Properties**.

The **Column Properties** dialog opens.

5 In the **Column Properties** dialog, select the **Value Format** page.

6 Enter the required width (number of characters) in the **Column Width** field.

7 Save the settings.

To adjust the colors and fonts in a table

You have the following options for adjusting the colors and fonts used in a table:

- Select a table style for the entire table.
- Set the colors and fonts manually for a specific column or for the entire table. You can set the colors/fonts separately for the table headings and the table data.
- Configure conditional formatting for a specific column (see "To highlight outliers using conditional formatting" on page 33).

The settings are applied in the order shown here. Thus, the table style is overruled by the color and font specifications, which are overruled by the conditional formatting.

To select a table style:

1 In **Table Properties**, select the **Format** page.

2 Select one of the styles in the **Format Styles** list box.

The corresponding appearance is shown under **Preview**.

3 Save the settings.

To set colors and fonts for the entire table:

1. In **Table Properties**, select the **Style** page.
2. Under **Data Font Properties For All Columns**, adjust the settings for the table data.
3. Under **Header Font Properties For All Columns**, adjust the settings for the table headers.
4. Save the settings.

To set colors and fonts manually for a specific column:

1. In **Table Properties**, select the **Columns** page.
2. Select the column for which you want to change the colors or fonts.
3. Click **Column Properties**.

   The **Column Properties** dialog opens.
4. In **Column Properties**, select the **Font** page.
5. Adjust the settings for the table data and the table header.
6. Save the settings.

To highlight outliers using conditional formatting

You can use conditional formatting, for example, to highlight outliers in a data overview. Values that are outside a specified range or meet other specific conditions are displayed in a different color or font.

1 In **Column Properties**, select the **Conditional Formatting** page.

2 Scroll to the color or font property you want to use for highlighting the outliers. For example, if you want to use bold fonts for the outliers, scroll to the **Font Weight** section.

3 Enter the expression that determines the condition. For example, if you want to highlight all compound amounts greater than 4, enter the following expression:

Expression	Operation	Value
Compound_Amount	>	4

If the expression is true for, the given format is activated.

4 Save the settings.

To adjust the table borders

You have the following options for adjusting the table borders:

- Select a table style for the entire table. The table style determines the style of inside borders and outside edges.
- Manually configure the outside edges of a table. The manual settings overrule the table style settings.

To choose a table style:

1 In **Table Properties**, select the **Format** page.

2 Select one of the styles in the **Format Styles** list box.

The corresponding appearance is shown under **Preview**.

3 Save the settings.

To configure the outside edges of a table:

1 In **Table Properties**, select the **Style** page.

2 Adjust the default settings or the settings of each individual border.

3 Save the settings.

To change the column header

To change the headers directly in the Editing Pane:

1 Double-click the table header in the Editing Pane.

You can now edit the header text directly.

2 To confirm the new text, press **Enter** or click outside the header.

To change the headers in Table Properties:

1 In **Table Properties**, select the **Columns** page.

2 In **Table Layout**, double-click the header you want to edit.

You can now edit the header text directly.

3 To confirm the new text, press **Enter** or move the mouse over the **Available Fields** area.

To change the headers in Column Properties:

1 In **Table Properties**, select the **Columns** page.

2 Select the column that you want to adjust.

3 Click **Column Properties**.

The **Column Properties** dialog opens.

4 In the **Column Properties** dialog, select the **Value** page.

5 Under **Header**, change the text in the **Header Text** field.

6 Save the settings.

To create a line break in a table header

If you want to add a line break in a table header, you can use the *vbNewLine* constant, which is provided by Visual Basic. For example, if you want to add a line break between the words *Retention* and *Time*, the expression in the table header will look like this:

="Retention" + vbNewLine + "Time"

This type of line break is not shown in the Editing Pane, but will be applied when you generate the report.

To create a second table row

To create a second row in the table header

1 In the **Table Properties**, select the **Columns** page.

2 Under **Multiple Table Rows**, select the **Enable Additional Header Row** check box.

3 Select the column for which you want to set the heading, and click **Column Properties**.

The **Column Properties** dialog opens.

4 On the **Value** page, provide a header text for the second header row in the **Additional Header Text** field.

5 On the **Header Format** page, configure the format of the table header.

Both header rows will have the same format.

To create a second row in the table details

1 In the **Table Properties**, select the **Columns** page.

2 Under **Multiple Table Rows**, select the **Enable Additional Detail Row** check box.

3 Select the column for which you want to set the heading, and click **Column Properties**.

NOTE We recommend using only one table details row for the first column, and adding a second table row only to the other columns. This will make it easier to identify the table rows belonging to each other in the generated report.

The **Column Properties** dialog opens.

4 On the **Value** page, provide an expression for the second detail row in the **Additional Value** field.

5 On the **Value Format** page, configure the format of the two detail rows.

The basic formatting will be the same for both detail rows. You can, however, set a different number format for each detail row.

6 On the **Summary Calculations** page, you can configure specific summary calculations for each detail row. From the drop-down list, choose the detail row that you want to configure.

However, for a better overview of the results, we recommend creating a summary calculation only for one specific detail row.

7 On the **Conditional Formatting** page, you can format each detail row separately. From the drop-down list, choose the detail row that you want to configure.

You can format each detail row separately. From the drop-down list, choose the detail row that you want to configure.

Name	RT [min]	Area	Height	RF	Amount [ng/ul]
	Width	Area %	Height %	Tail Factor	Type
Uracil	1.355	32.5637	19.8944	0.34477	11.227
	0.024	8.7571	12.1936	0.70556	BB
Ethyl paraben	5.062	53.4534	24.3948	0.25073	13.402
	0.034	14.375	14.9520	1.0723	BB
Propyl paraben	5.897	48.8092	21.6386	0.27072	13.214
	0.035	13.126	13.2627	1.0765	BB
Heptyl paraben	8.806	61.0532	25.2993	0.39365	24.034
	0.037	16.419	15.5064	1.1023	BB

Figure 1 Example of a double-row table

To change the text alignment in a table

1 In **Table Properties**, select the **Columns** page.
2 Select the column that you want to adjust.
3 Click **Column Properties**.

The **Column Properties** dialog opens.

4 To adjust the alignment of the table header, select the **Header Format** page. To adjust the alignment of the value, select the **Value Format** page.
5 Adjust the horizontal/vertical alignment and the other cell properties as needed.
6 Save the settings.

To adjust the number format in a table

1 In **Table Properties**, select the **Columns** page.
2 Select the column that you want to adjust.
3 Click **Column Properties**.

The **Column Properties** dialog opens.

4 In the **Column Properties** dialog, select the **Value Format** page.
5 Under **Number Format**, adjust the settings according to your requirements.

The **Preview** area shows the appearance of the currently selected settings.

NOTE The **Number Format** section is only visible if the selected column contains numbers.

6 Save the settings.

To configure a table footer

You can add various functions to the table footer. These functions summarize the data of the entire table.

1 Select the column that you want to summarize, then click **Column Properties**.

The **Column Properties** dialog opens.

2 In the **Column Properties** dialog, select the **Summary Calculations** page.

3 Select the functions that you want to use in the table footer. Each function will appear in a separate row.

4 Adjust the number format for each function used.

a Under **Number Format for Summary Calculations**, select the relevant function.

b Adjust the number format as required.

The **Preview** area shows the appearance of the currently selected settings.

5 Save the settings.

The selected functions are added to the table as footer rows. Each function is shown in its own footer row.

NOTE If you add a summary calculation, the table will expand downwards in the generated template. However, the layout of the report item is not automatically adjusted in the Editing Pane! You need to resize the table layout to allow for the additional footer lines. Otherwise, the subsequent report items may overlay the table footer in the generated template.

NOTE If a table column shows an expression that contains a calculation variable or a report parameter, you cannot add a summary calculation for this column.

To sort a table

You can provide sorting expressions for any report item that lists multiple pieces of information, such as tables or composite groups. This procedure explains how to change the sorting expression for a table, but it basically applies also to the other report items.

1 In the properties dialog, select the **Sorting** page.

2 In the **Expression** drop-down list, select the data field you want to use for sorting.

For example, you can sort by the following expressions:

- **Fields > Peak > RetentionTime** if you want to sort by the retention time
- **Fields > Sample > OrderNo** if you want to sort by the order of the samples in the sequence table
- **Fields > Injection > OrderNo** if you want to sort by the order in which the injections took place

The correct name of the respective data field is shown with an equals sign in front of it. For example: **=Peak_RetentionTime**.

3 In the **Direction** drop-down list, select whether you want to sort the entries in an ascending or descending order.

4 If required, you can add expressions to sort by more than one field.

The sorting expressions will be applied from top to bottom.

5 If required, change the order of the sorting expressions with the arrow buttons  and  .

To filter a table

If you want to create a table that shows only specific data, you need to filter the table accordingly. This procedure shows you how to filter for a sample name, sample type, or compound name.

1 In **Table Properties**, select the **Filtering** page.

2 In the **Expression** drop-down list, select the data field that you want to use for filtering:

- **Fields > Sample > NAME** if you want to filter for a specific sample name
- **Fields > Sample > TYPE** if you want to filter for a specific sample type
- **Fields > Compound > NAME** if you want to filter for a specific compound name

The correct name of the respective data field is shown with an equals sign in front of it. For example: =*Sample_Name*.

3 In the **Operation** drop-down list, select **Equals**.

4 Select the **Value** field.

If you start typing, you replace the entire existing content of the field. If you press **F2**, the cursor is shown, and you can edit the existing content.

5 Enter the required value.

NOTE In the **Value** field, text strings must be enclosed in quotes to be recognized as text. If you do not add quotes, RTE adds them for you when you close the dialog.

Numbers are written without quotes.

NOTE If you filter for an enumeration, you must enter the required number in the **Value** field. See "Enumerations" on page 162 for an overview of all enumerations.

For example:

- *"Standard L1"* as a sample name
- *1* as a sample type, in this case the calibration samples
- *"TRAMADOL"* as a compound name

6 Click **OK** to confirm the settings.

The table in the generated report now contains only the data that passed the filter condition. As the editor uses built-in example data to preview the table in the Editing Pane, this preview may show no contents at all.

To filter for peak area or area%

To exclude small peaks

1 In **Table Properties**, select the **Peaks and Repeating** page.

2 Under **Area Rejection**, select the check boxes to exclude peaks with area or area% less than a specific value.

3 Enter a value for area or area%. This value is used as a minimum value. Only peaks with an area or area% equal to or greater than this value are included in the report.

To exclude large peaks

1 In **Table Properties**, select the **Filtering** page.

2 Enter a filter expression to filter for peaks with an area or area% equal to or greater than a specific value. For example, you can use the following expressions:

Expression	Operation	Value
=Peak_Area	>=	3
=Peak_AreaPercent	>=	3

NOTE

After reloading a template in the Editing Pane, RTE may automatically map the filter condition to the **Area Rejection** property. This happens, if you use the *Greater Than (>)* or *Equals (=)* operators. The filter expression is then removed from the **Filtering** page and is visible in the **Peaks and Repeating** page instead.

To repeat a table

This procedure shows you how to repeat a table on the compound name.

1 In **Table Properties**, select the **Peaks and Repeating** page.

2 In the **Repeat Table On** drop-down list, select **Fields > Compound > NAME**

The name of the according data field is shown, with an equals sign in front of it: =Compound_Name.

3 Click **OK** to confirm the settings.

In the table preview in the Editing Pane, a headline is added for the compound name. If you generate the report, the table will be repeated for each compound name available in the current scope.

About Table Groups

With table groups, you can structure the detail rows of a table. You can define specific header rows, and show footer rows with summary information specifically for that group.

For example, if you used two detector wavelengths for signal detection, you get two signals for each detected compound. In this case, you can create a table group for the detector wavelengths in order to show all signals of one wavelength under each other, with a group header above and a summarizing footer below the details rows.

RT	Compound Name	Area	Area%	Resol. USP	Tail Factor
	*** SIGNAL ***				
0.877	o-desm tramadol (D)	0.121	0.0791	0.122	1.4
0.878	o-desm tramadol (D)	0.1178	0.0759	0.117	1.2
1.432	trans- tramadol (A)	0.1397	0.0989	0.23	0.9
1.565	TRAMADOL	729.3899	262.0219	1015.418	2.4
2.519	des-hyd cis tramadol (C)	0.1674	0.1157	0.192	1.2
2.644	des-hyd trans tramadol (B)	0.1491	0.1087	0.22	0.9
	Sum	730.0849	262.5002		
	Avg			169.383	1.3
	*** SIGNAL ***				
1.565	TRAMADOL	209.7591	75.4511	1015.418	2.2
1.566	TRAMADOL	209.6631	74.9885	1014.953	2.3
	Sum	419.4222	150.4396		
	Avg			1015.185	2.3

Usage of table groups is limited to max. three groups. The order of grouping is defined by the position of the group in the list.

Two groups will be shown with header/footer lines in the report template, the third group will only be used to organize the detail rows in the table.

Preparation for using table groups

Using table groups can make the table quite complex, especially if there is more than one group. It is important that you plan the table groups in advance and know exactly how the groups will structure your data. Otherwise, you might get unexpected results and will not know which properties of which group must be changed to correct the table.

Use the following guidelines before creating table groups:

- What is the top-level element in your report template? Use this element for the **Repeat Table On** setting.
- Which field should be used to group the detail data? Which (static) sub headline should be used for the groups? Use this information for the **Group On** setting in the table group.
- Which fields should be used to sort the detail data inside each group? Use this information in the properties of the table itself. The table sorting will overrule the table group sorting.
- Which footers do you need needed for each table group? The use of headers or footers is optional. It may be useful to provide a summary of statistical information on a specific table group.

Using Table Groups

To configure a table group

1. In **Table Properties**, select the **Grouping** page.
2. Click **Add** to create a new table group.

   The **Group Properties** dialog opens. The **Group Name** is generated automatically.
3. In **Group Properties**, provide a **Group On** expression.

   This expression will be used to group the table detail rows.
4. If required: Select the **Columns** page and specify the group header and group footer information.

   To create a group header, enter a string in the **Group Header** column. To create a group footer, select one or more of the provided check boxes.
5. If required: Select the **Filtering** page and specify a filter expression for the distinct group values.
6. If required: Select the **Sorting** page and specify a sorting expression for the distinct group values. This sorting can differ from the sorting of the table detail rows!

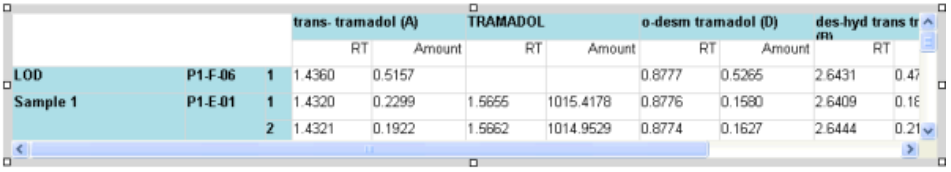
NOTE The sorting of table group data is only applied within each single group. The order of the different groups in the table depends on the table sorting.

4 Matrices

This chapter describes the characteristics and usage of matrices in RTE.

About Matrices

Matrices are like pivot tables or crosstabs in a spreadsheet. As we have seen in the previous chapters, *tables* contain a variable number of rows, depending on the dataset contents, and a fixed number of columns with detail information. *Matrices*, however, also contain a variable number of columns. The number of columns depends on the dataset contents. In a table, for example, you can show a list of all compounds found in a specific injection, and the columns show the specific properties (such as amount or retention time) of each compound. In a matrix you can show a list of all injections; the number of columns corresponds to the number of detected compounds in the injected samples.



			trans- tramadol (A)		TRAMADOL		o-desm tramadol (D)		des-hyd trans tr (R)	
			RT	Amount	RT	Amount	RT	Amount	RT	
LOD	P1-F-06	1	1.4360	0.5157			0.8777	0.5265	2.6431	0.47
Sample 1	P1-E-01	1	1.4320	0.2299	1.5655	1015.4178	0.8776	0.1580	2.6409	0.18
		2	1.4321	0.1922	1.5662	1014.9529	0.8774	0.1627	2.6444	0.21

NOTE If your data contains multiple signals, the matrix items in the Report Template Editor will only show the main signal.

About Matrix Groups

The most important thing about matrices is that everything in a matrix is based on groups. In contrast to tables, matrices contain two different types of groups: row groups and column groups. In the snippets available in the **Report Items** browser, these row groups and column groups are preconfigured. You can only partially change these settings. The options that you can change may vary from snippet to snippet.

Row groups

Row groups define the data in the left part of the matrix. If a matrix contains several row groups, there are several specific columns in this left part, where each column is defined by its own row group. The following figure shows the principle:

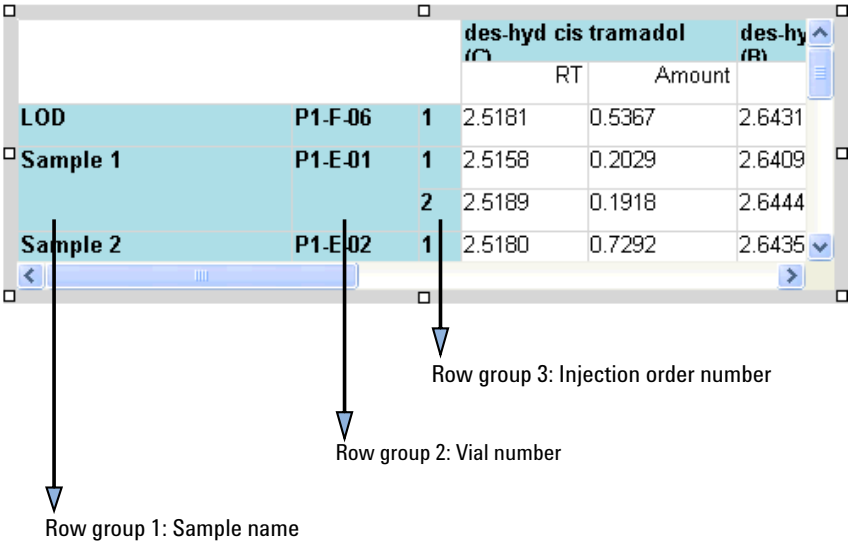


Figure 2 Row groups

The number of row groups and the width of the corresponding columns is defined by the snippet. You can not change these settings in the Report Template Editor.

Column groups

The column group defines the data that makes up the columns in the right part of the matrix. In some matrix snippets, you can adjust the value used to build the columns. The following figure shows the principle:

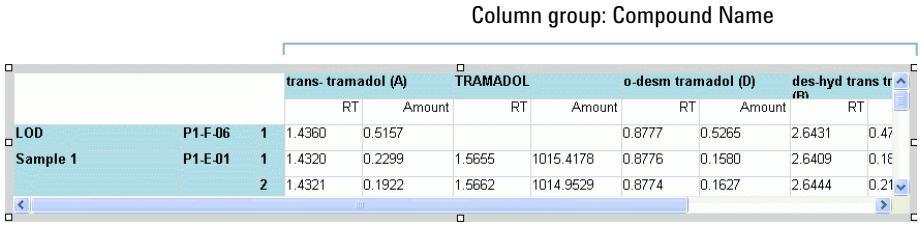


Figure 3 Column groups

Data properties

The detail data is always displayed in the cells defined by the row groups and column groups. The details cells can be split in order to show several different values that belong to the same groups. These multiple details cells can be shown either in columns (side by side) or in rows (on top of each other). The layout type is defined by the snippet and can not be changed in the Report Template Editor. The number of details cells and their content can be configured in the matrix properties.

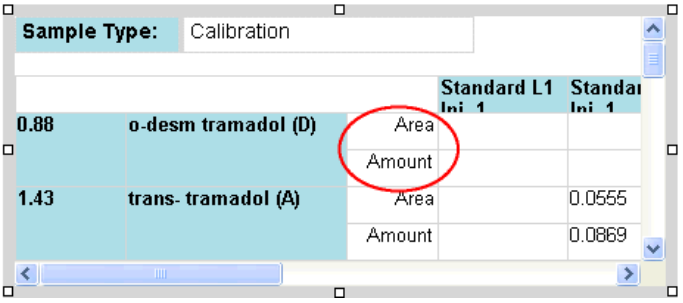
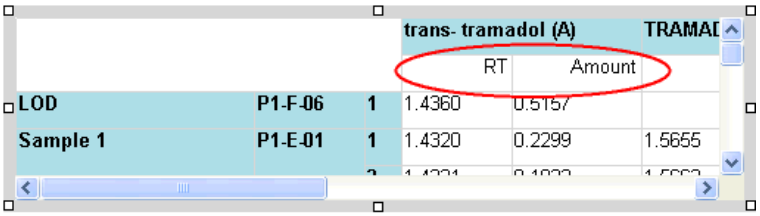


Figure 4 Details cells shown on top of each other



			trans- tramadol (A)		TRAMAD
			RT	Amount	
LOD	P1-F-06	1	1.4360	0.5157	
Sample 1	P1-E-01	1	1.4320	0.2299	1.5655

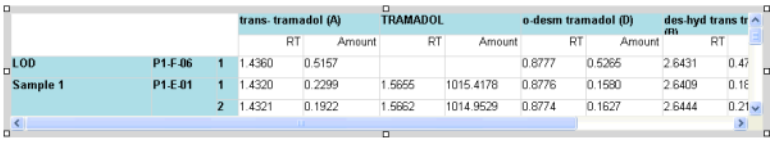
Figure 5 Details cells shown side by side

Using Matrices

To create a matrix

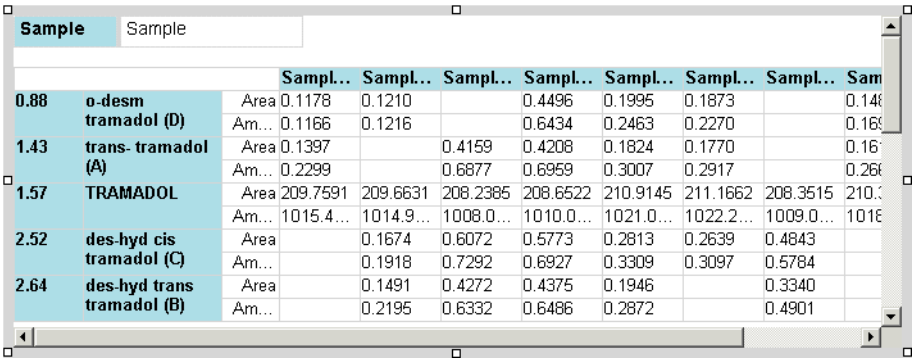
With the available matrix snippets, you can create overviews for different scenarios:

- With the **Compound Summary RT Amount** snippet, you generate an overview of the retention times and amounts for each detected compound. The compounds are shown as columns; the sample names, vial locations, and injection numbers are shown as rows. The snippet also contains summary calculations in the footer (average, standard deviation, and relative standard deviation).



			trans- tramadol (A)		TRAMADOL		o-desm tramadol (D)		des-hyd trans tr (B)	
			RT	Amount	RT	Amount	RT	Amount	RT	
LOD	P1-F-06	1	1.4360	0.5157			0.8777	0.5265	2.6431	0.47
Sample 1	P1-E-01	1	1.4320	0.2299	1.5655	1015.4178	0.8776	0.1580	2.6409	0.18
		2	1.4321	0.1922	1.5662	1014.9529	0.8774	0.1627	2.6444	0.21

- There are two **Sample Summary** snippets. With these snippets, you generate an overview of the retention time and compound amount for each sample. The sample names are shown as columns; the compound names and their respective retention times are shown as rows.



Sample	Sample		Sampl...	Sampl...	Sampl...	Sampl...	Sampl...	Sampl...	Sampl...	Sam
0.88	o-desm tramadol (D)	Area	0.1178	0.1210		0.4496	0.1995	0.1873		0.14
		Am...	0.1166	0.1216		0.6434	0.2463	0.2270		0.16
1.43	trans- tramadol (A)	Area	0.1397		0.4159	0.4208	0.1824	0.1770		0.16
		Am...	0.2299		0.6877	0.6959	0.3007	0.2917		0.26
1.57	TRAMADOL	Area	209.7591	209.6631	208.2385	208.6522	210.9145	211.1662	208.3515	210.
		Am...	1015.4...	1014.9...	1008.0...	1010.0...	1021.0...	1022.2...	1009.0...	101
2.52	des-hyd cis tramadol (C)	Area		0.1674	0.6072	0.5773	0.2813	0.2639	0.4843	
		Am...		0.1918	0.7292	0.6927	0.3309	0.3097	0.5784	
2.64	des-hyd trans tramadol (B)	Area		0.1491	0.4272	0.4375	0.1946		0.3340	
		Am...		0.2195	0.6332	0.6486	0.2872		0.4901	

- The **Sample Summary Area Amount** snippet is not repeated on a specific field. Thus, it shows all samples in the same overview. If there are many samples, the matrix width may become quite large. This snippet is typically used to obtain an overview of a specific set of samples.
- The **Sample Summary per Type** is repeated on **Sample_Type**. Thus, the matrix is repeated several times, and each repetition shows only samples of the same sample type.

To sort a matrix

There is no **Sorting** page available for the matrix itself. Any sorting information must be provided separately for the respective row group or column group!

1 In the **Matrix Properties**, select the **Grouping** page.

2 To change the sort order of a row group, click **Edit** in the **Rows** section. To change the sort order of a column group, click **Edit** in the **Columns** section.

For more information on row groups and column groups, see "About Matrix Groups" on page 49.

3 Select the **Sorting** page.

4 In the **Expression** drop-down list, select the data field you want to use for sorting.

For example, you can sort by the following expressions:

- **Fields > Peak > RetentionTime** if you want to sort by the retention time
- **Fields > Sample > OrderNo** if you want to sort by the order of the samples in the sequence table
- **Fields > Injection > OrderNo** if you want to sort by the order in which the injections took place

The correct name of the respective data field is shown with an equals sign in front of it. For example: **=Peak_RetentionTime**.

5 In the **Direction** drop-down list, select whether you want to sort the entries in an ascending or descending order.

6 If required, you can add expressions to sort by more than one field.

The sorting expressions will be applied from top to bottom.

7 If required, change the order of the sorting expressions with the arrow buttons  and  .

To adjust the column widths

You can adjust the width of both the the static columns shown in the left part of the matrix and the width of the dynamically created columns in the right part of the matrix.

To change the width of static columns:

1 In **Matrix Properties**, select the **Grouping** page.

2 Select the appropriate row group, and click **Edit.**

3 In **Group Properties**, select the **Format** page.

4 Enter a suitable number of characters for the column width.

5 Save your settings.

To change the width of dynamically created columns:

1 In the **Matrix Properties**, select the **Data** page.

2 Select the appropriate column, and click **Column Properties**.

3 In **Column Properties**, select the **Format** page.

4 Under **Column Width**, enter a suitable number (in points) for the column width.

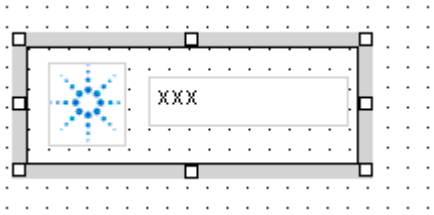
5 Composite Groups

This chapter describes the characteristics and usage of Composite Groups in RTE.

About Composite Groups

A composite group is a conglomeration of report items of any type that are always used together. In the **Report Items** browser, you find predefined composite groups in the **Sequences** category and in the **Samples** category. These groups contain a collection of data fields with basic header information on a sequence or sample.

In the Editing Pane, composite groups are marked by a surrounding rectangle.



Save locally

If you save the composite group in the Report Template Editor, the composite group is listed in the **Report Items** browser under the **Composite Groups** category. You can then reuse it for other report templates.

The xml file associated to the composite group is saved in your local file system, so that you can transfer the xml file to other computers and reuse the composite group there as well. The location depends on the host application and the operation system. For example, with OpenLAB CDS ChemStation Edition and Windows XP, the xml file is saved under C:\Documents and Settings\[username]\Application Data\Agilent Technologies\Agilent ChemStation\[version]\IntelligentReporter\CompositeGroups.

Repeat on

Composite groups can be repeated on a specific key information. The entire group is then displayed several times - once for each value of the selected information. For example, a group containing information on samples may be repeated for each sample in a sequence.

Composite groups correspond to lists in Microsoft Business Intelligence Studio.

Using Composite Groups

To create a Composite Group

Prerequisites

You have placed several report items in the template that should always be used together. These may be report items of any type, including other composite groups.

To prepare the group:

1 Select all of the report items that you want to combine to form a composite group. You can select multiple report items in different ways:

- Drag the mouse over the relevant items.

  - or -

- Select the first item, then hold down **Ctrl** and click the other required items one after each other.

  All of the required items are now selected.

2 Click  in the toolbar.

  A rectangle is added that encloses the selected report items.

3 To configure the group properties, right-click anywhere inside the group, and select **Properties** from the context menu. Be careful not to click any specific report item, as this would select the specific item instead of the group.

  The **Composite Group Properties** dialog opens.

To save the group:

1 Right-click anywhere inside the group, and select **Save Composite Group** from the context menu. Be careful not to click any specific report item, as this would select the specific item instead of the group.

2 Enter a suitable name for the group.

NOTE Existing composite groups cannot be overwritten. You must always provide a new name when saving a composite group.

The new composite group is now available in the **Report Items** browser under the **Composite Groups** category.

To repeat a composite group

The following procedure shows you how to repeat a composite group on the sample name.

1 In the **Composite Group Properties**, select the **Grouping** page.

2 In the **Group Repeat** drop-down list, select **Fields > Sample > NAME**.

The name of the respective database field is shown, with an equals sign in front of it: **=Sample_Name**.

3 Click **OK** to confirm your settings.

To create a nested composite group

A composite group may contain any type of report item, even other composite groups. This way it is possible to create nested groups where, for example, the outer group is repeated on the sample type, and the inner group is repeated on the sample name. The following procedure shows you how to create a nested group.

1. Create and save a composite group with sample information that is repeated on the sample name (see "To create a Composite Group" on page 58).
2. Add the field **Sample_Type** to your template. Place it above the previously created composite group.
3. Select both the **Sample_Type** field and the previously prepared composite group.
4. Create a new composite group containing the two selected items.
5. Repeat the new composite group on **Sample_Type**.

   If you generate the report, the different sample types are shown as headings. Under each sample type, the respective samples are listed.

NOTE Nested composite groups correlate to "lists in lists" in Microsoft Business Intelligence Studio.

To filter a composite group

The filter of a composite group is only active if the composite group is repeated on a specific value.

If you need to filter a composite group that is not repeated at all, enter the expression
`=-1` as the **Group repeat on value.** With -1, the composite group is shown only once, but the filter is active nonetheless.

6 Images

This chapter describes the characteristics and usage of images in RTE.

About Images

RTE offers you the possibility to add images, such as your company logo, to the report template. Images are typically added to the report header, but you can also place them in the report body or report footer.

You find the image items in the **Report Items** browser under the **Special Objects** category. The default image is an Agilent logo, but you can change the image source and also the image size in the **Image Properties** dialog. The file selection dialog for the image source automatically opens when you drop the predefined image item onto the template.

If you save a template in which you use an image item, this image is automatically added to the **Special Objects** for the current template. Thus, if you want to add the image also at a different place in the same template, you can easily access the same image.

7 Chromatograms

This chapter describes the characteristics and usage of chromatograms in RTE.

About Chromatograms

With chromatogram report items, you can print signals from the detectors of the chromatographic system on the report. The report item shows the results for all injections that are included in the selected data. There is at least one signal per injection. If the detector was configured to give multiple measurements, for example a diode-array or multi-wavelength detector, the chromatogram accordingly contains multiple signals per injection.

NOTE The data shown in the chromatogram also depends on whether the chromatogram is placed in a composite group and on the grouping and filtering of the composite group.

Depending on the configuration of the report item, the *signals* may be shown in separate graphs, overlaid graphs, stacked graphs, or as Iso plots.

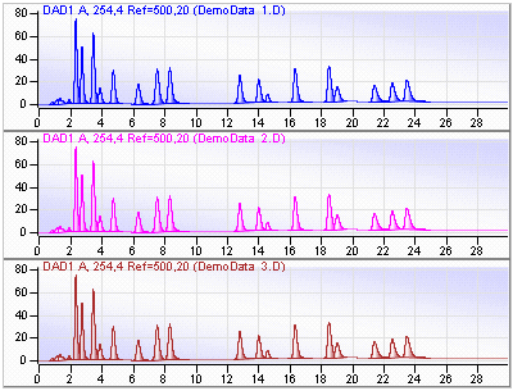


Figure 6 Example: chromatogram with three signals in separate graphs

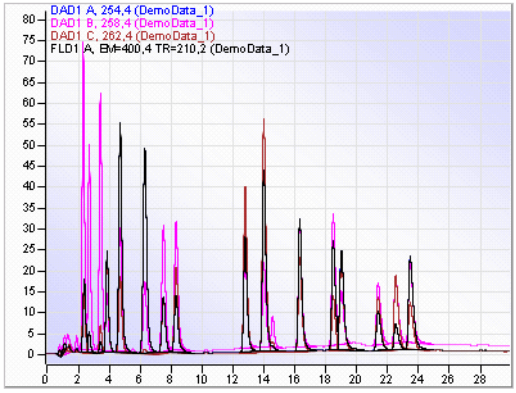


Figure 7 Example: chromatogram with multiple signals in an overlaid graph

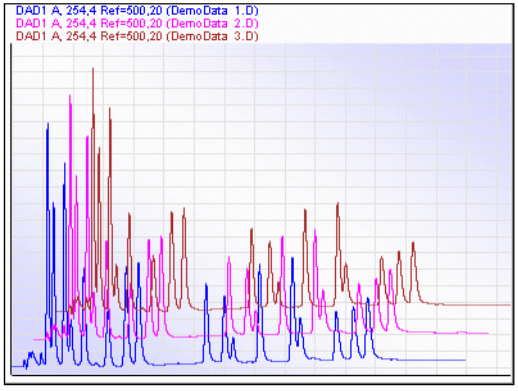


Figure 8 Example: chromatogram with multiple signals in a stacked graph

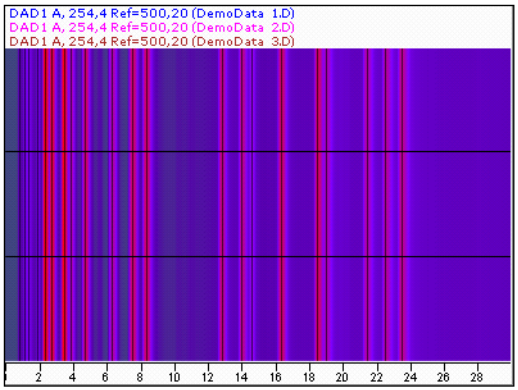


Figure 9 Example: chromatogram with multiple signals shown as iso plot

Single Signal Plot and Multi Signal Plot

In the **Report Items** browser, different types of snippets are available for the chromatogram:

- The **Single Signal Plot** snippet always shows only one detector signal. The chromatogram is automatically repeated on the signal ID. Therefore, if the data contains multiple signals (for example, from multiple injections or from a multi-wavelength detector), the chromatogram is repeated several times.
- The **Multi Signal Plot** snippets show all signals in the same chromatogram report item. You can configure the display format and group settings.

Using Chromatograms

To show only specific samples or signals

Specific samples

If you want to show only the signals for a specific sample (here: the sample *SSRSD1*) in a chromatogram, you can filter for the sample name.

Expression	Operation	Value
=Sample_Name	=	"SSRSD1"

In order to compare the signals for two different samples, add a second expression for the other sample name. The two expressions will automatically be linked by *Or*. Alternatively, you can use the **Contains**operator and a wildcard in the **Value** field:

Expression	Operation	Value
=Sample_Name	**Contains**	"SSRSD *"

Specific signals

If you want display only the signals from a specific detector, you can filter for the detector name (here: *DAD1*). The detector name is usually contained in the first characters of the signal name. Therefore you filter for all signals where the relevant characters are contained in the signal name.

Expression	Operation	Value
=Signal_Name	**Contains**	"DAD1"

If you want to filter for one specific signal, use the complete signal name (here: *DAD1 A, Sig=270,8 Ref=500,100*) in the filter expression.

Expression	Operation	Value
=Signal_Name	=	"DAD1 A, Sig=270,8 Ref=500,100"

To show only a specific sample type

This procedure shows you how to create an overlaid chromatogram that displays only the samples of a specific sample type.

To create one chromatogram for each sample type:

1 Add the data field **Fields > Sample > Type** to the report template.

2 Add the **Multi Signal Plot Overlaid** snippet to the report template.

3 Select the two items and click  to create a composite group.

4 Repeat the composite group on **Sample_Type**.

5 If you used multiple signals, filter the chromatogram for one specific signal. For example, the filter expression would be:

Expression	Operation	Value
Signal_Name	**Contains**	"DAD 1A*"

To create a template with only one chromatogram for one sample type:

1 Add the **Multi Signal Plot Overlaid** snippet to the template.

2 Filter for the sample type, and if required, for a specific signal. For example, the filter expression would be:

Expression	Operation	Value
Sample_Type	=	3
Signal_Name	**Contains**	"DAD 1A*"

NOTE If you filter for an enumeration (such as **Sample_Type**), you must enter the required number in the **Value** field. See "Enumerations" on page 162 for an overview of all enumerations.

To label also the missing compounds

By default, only the identified compounds are labeled in the chromatogram. If you want to add labels for the missing compounds at the respective retention times, proceed as follows:

1 In **Multi Signal Plot Properties**, select the **Peak Labels** page.

2 Make sure the **Show Peak Labels** check box is selected.

3 Select the **Undetected Compounds** check box.

4 Save the settings.

NOTE The report item preview in the Editing Pane is based on built-in data, not on the actually selected data. The labels for undetected compounds will therefore be visible only after generating the report.

To switch on/off peak labeling depending on the peak

If you want to label the peaks depending on certain peak properties, you must create a customized expression for the peak labels.

1 In **Multi Signal Plot Properties**, select the **Peak Labels** page.

2 Make sure, the **Show Peak Labels** check box is selected.

3 Under Peak Labels, select **No Label** for the labels 2 to 4.

4 Click **fx...** to create a customized expression for **Label 1**.

The **Expression Editor** opens.

5 Enter one of the following expressions, according to your requirements.

Expression	Description
=Iif(Peak_Area> 5, Str(Round(Peak_RetentionTime, 2)), "")	Shows the retention time rounded to two decimals, but only for peaks with a calculated area greater than five.
*=Iif(UCase(Compound_Name)="TRAMADOL", "*** Tramadol found ***", "")*	Shows the label *"*** Tramadol found ***"* for the Tramadol peak. All other peaks remain unlabeled.

6 Save the settings.

To show only peaks with a certain minimum area

If you want to show only peaks with a certain minimum area, you can filter for the peak area. For example, you can show only peaks with Area% greater than 5.

Expression	Operation	Value
=Peak_AreaPercent	>	5

NOTE If all peaks are filtered out, no signal is displayed.

To scale on the peak height of a certain compound

If you want scale on the peak of a certain compound, and you do not know how many other compounds there are and which peak heights they have, you can use a customized expression to scale on the correct peak.

1 In the **Multi Signal Plot Properties**, select the **Signal Axis** page.

2 Under **Scaling**, select **All Signals in Given Scale**.

3 Click **fx...** to the right of the **To** field.

The **Expression Editor** opens.

4 Enter the following expression:

Expression	Description
*=Iif(UCase(Compound_Name)="TRAMADOL", Peak_Height*1.05, "")*	This expression returns the height of the Tramadol peak, multiplied by 1.05. "Tramadol" may be written in uppercase or lowercase in the method.

5 Save the settings.

To create a single peak plot

1 Create a composite group that is repeated on **Peak_ID** (see "To create a Composite Group" on page 58)

With this group, you ensure that only one single peak is shown in each chromatogram.

NOTE If you want to create a single peak plot for only one compound, you can filter the composite group for the required compound.

2 Add a chromatogram to the composite group.

3 Configure the **Signal Axis** of the chromatogram.

a Under **Scaling**, select **All signals in given scale**.

b Enter the following expressions for the upper limit of the signal axis:

Use for	Expression	Description
To	=Peak_Height*1.05	This expressions returns the peak height multiplied by 1.05.

4 There are different ways to configure the **Time Axis** page. With the following settings, the signal axis is labeled with absolute values, and the upper limit in each graph will correspond to the height of each peak.

a Under **Scaling**, select **All Time Axes with Same Scale**, and select the **Custom scale** check box.

b Enter the following expressions for the lower and upper limit of the time axis:

Use for	Expression	Description
From	=*Round(*Peak_BeginTime-*0.05**(*Peak_EndTime - Peak_BeginTime*), 1)*	This expressions returns the peak begin time, minus five percent of the peak duration.
To	=*Round(*Peak_EndTime + *0.05**(*Peak_EndTime - Peak_BeginTime*), 1)*	This expressions returns the peak end time, plus five percent of the peak duration.

5 Save your settings.

To create a multi page plot

If you want to divide a chromatogram into two parts, you need to add two chromatogram items to your report template. If you place them inside a composite group, make sure both chromatograms are placed inside. Also, the filter conditions for each of the chromatograms must be identical.

The only difference between the two chromatograms is the time range:

- First chromatogram: from 0 to 50% (or to 52.5% to get a small overlap)
- Second chromatogram: from 50 to 100% (or from 47.5% to get a small overlap)

NOTE When creating multi-page plots, carefully consider which option you select under **Search Scale Within** for the scaling of the signal axis. If you select the **Given Time Axis Range** option, you will obtain different signal axes for each separate plot.

To show an instrument curve

You can display various instrument curves, depending on the modules you use. This procedure shows you how to add the pump pressure instrument curve to your report.

1 In the **Chromatogram Properties**, select the **Instrument Curves** page.

2 Select the **Include Instrument Curves** check box.

3 Under **Filter List**, click into the **Expression** field.

The expression **SIGNAL NAME** is automatically set.

4 In the **Operation** field, select **Contains**.

5 In the **Value** field, enter `*Pressure*`.

6 Save the settings.

7 Preview the report.

Each chromatogram in the report contains the associated pressure curve. If you used two pumps, two pressure curves will be displayed.

The display format (such as **Overlaid** or **Separate**) depends on the settings in the **Multi Signals** page of the **Chromatogram Properties**.

NOTE In order to find out which other instrument curves are available, remove any filters in the **Instrument Curves** page and preview the report. The available signal names are shown in a legend.

8
Calibration Curves

This chapter describes the characteristics and usage of calibration curves in RTE.

About Calibration Curves

With calibration curves, you can place the visual presentation of the calibration results on your report template. The graph shows the results for all compounds and calibration samples that are included in the selected data.

NOTE In order to obtain a calibration curve, you must have configured the respective samples as calibration samples in the sequence table, and you must have configured the calibration table.

Depending on the configuration of the report item, the multiple curves may be shown in separate, overlaid, or stacked graphs.

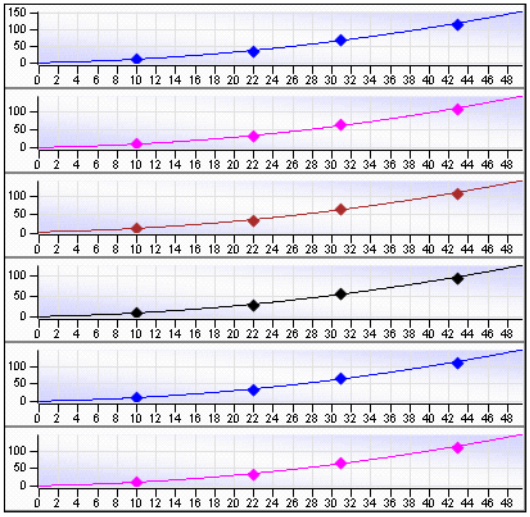


Figure 10 Example: calibration curve with separate graphs

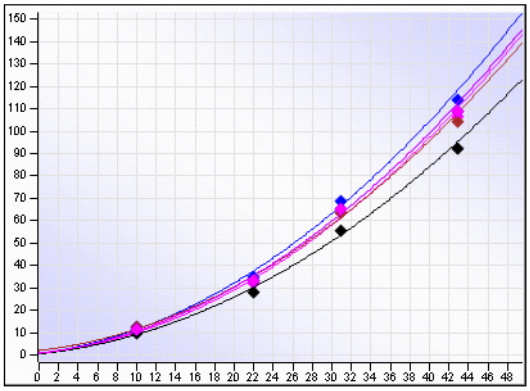


Figure 11 Example: calibration curves in an overlaid graph

Types of calibration curves

In the **Report Items** browser, the following snippets are available for the calibration curve:

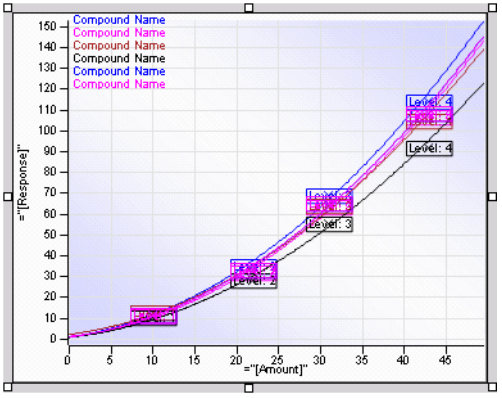
- **Calib Curve Plot by Compound** contains a composite group with a calibration curve and additional information such as the formula or the correlation coefficient. The composite group is automatically repeated on the compound name. Therefore, if your data contains multiple calibrated compounds, the information is repeated several times.
- **Calibration Curves Overlaid** adds a single calibration curve item. In this item all curves contained in the current scope (defined by data selection, grouping, filtering, etc.) are shown overlaid in the same graph. You can configure the display format and group settings.

Using Calibration Curves

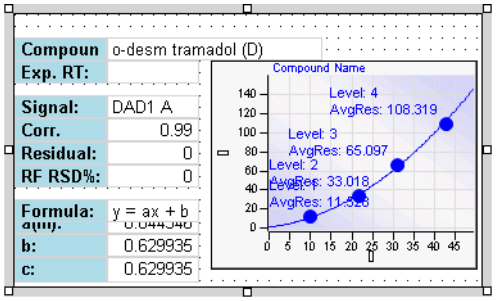
To create a calibration curve

With the available calibration curve snippets, you can create calibration curves for different scenarios. See the following examples:

- In order to create an overlaid calibration curve with data from multiple compounds, simply add the **Calibration Curves Overlaid** snippet to your report. The report will show only one graph in which the curves of all compounds are overlaid.



- To show the calibration curves for single compound, you have the following options:
  - Add the **Calibration Curves Overlaid** snippet and filter the calibration curve item for the required compound (for example, **Compound_Name**=*"TRAMADOL"*). Only one calibration curve will be shown in the report.
  - Add the **Calib Curve Plot by Compound** snippet. A composite group will be shown that is repeated on the compound name. The composite group also contains some more information on the calibration curve, such as the formula or the correlation coefficient.



NOTE If a ChemStation data file was processed with a non-matching calibration table, the report shows an empty calibration curve, and no peaks are identified. This happens if the calibration table has been set up for one signal, but data have been recorded for a different signal. Ensure that the signal description in the calibration table exactly matches the DAD signal set up in the used method (for example, *DAD1A 254,4 Ref 360,600*).

To place multiple curves in a row

Calibration curves are shown one under each other by default. However, you can configure the report item so that multiple curves are shown side by side in the same row.

To place multiple curves in a row

1. Add a calibration curve report item to your template.
2. In **Calibration Curve Properties**, select the **Multi Curves** page.
3. Under **Display format**, select **Separate**.

   Only separate graphs can be shown side by side in the same row.
4. In **Calibration Curve Properties**, select the **Layout** page.
5. In the **# Graphics** field, enter the number of curves to be shown in one row. For example, enter 4 to show four curves in one row.
6. Save your settings.

   The given number of curves is now shown in the same row.

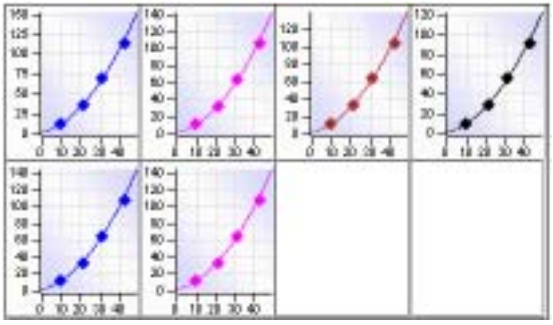


Figure 12 4 calibration curves in the same row

9 Spectra

This chapter describes the characteristics and usage of spectra in RTE.

About Spectra

With spectra report items, you can place the visual output of an optical 3D detector (for example, a diode array detector) on your report template. The spectra shown in the graph correspond to your selection of the positions in each peak. You can extract spectra, for example, at the start, at the apex, or at the end of a peak. In addition, you can filter the data shown in a spectrum using the filter list.

Depending on the configuration of the report item, multiple spectra may be shown in separate graphs, overlaid graphs, stacked graphs, or as Iso plots. If there are spectra for different compounds, you can group the spectra by compound name.

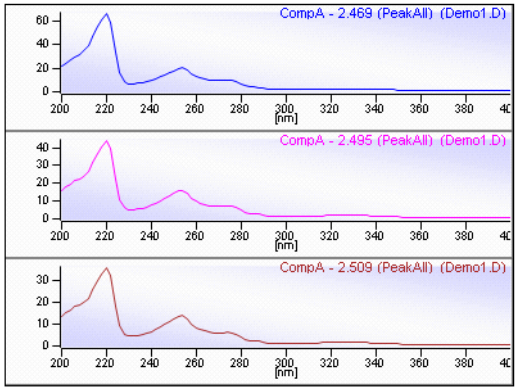


Figure 13 Example: three spectra in separate graphs

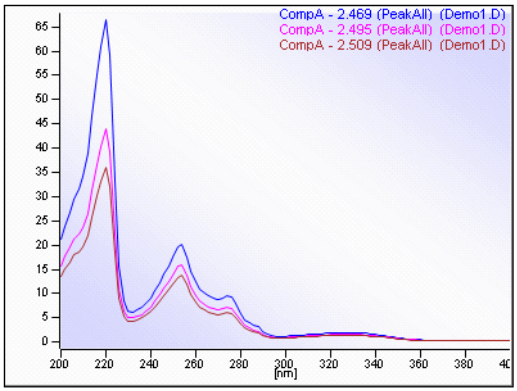


Figure 14 Example: three spectra in an overlaid graph

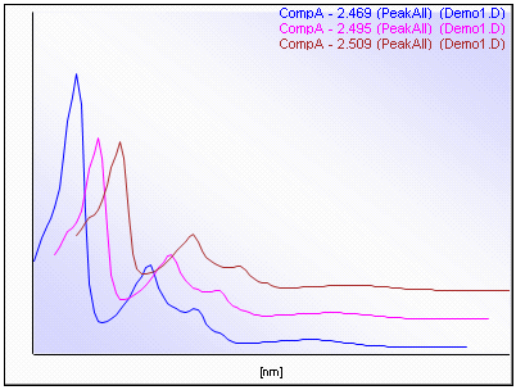


Figure 15 Example: three spectra in a stacked graph

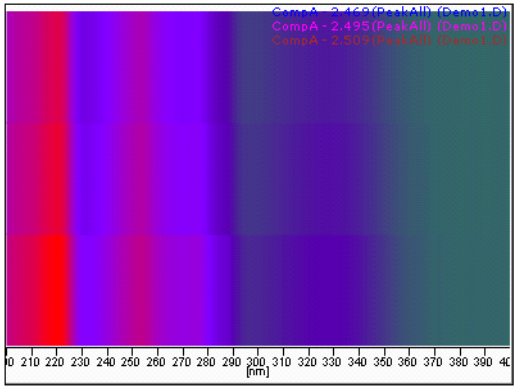
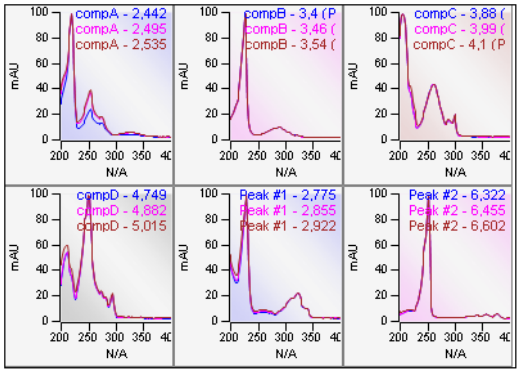


Figure 16 Example: three spectra shown as Iso plot

Using Spectra

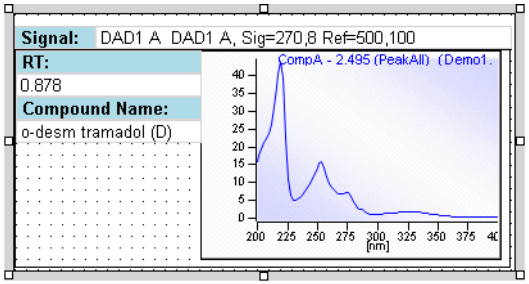
With the available spectra snippets, you can create graphs for different scenarios:

- The **Spectra Plot** snippet contains a plot where all available spectra are shown in an overlaid format. By default, the spectra are grouped by peak, and multiple spectra selected from the same peak are shown in an overlaid graph.

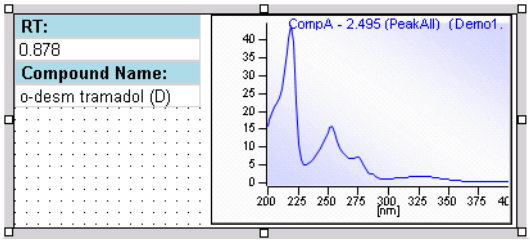


This snippet is typically used in combination with a composite group that is repeated on a specific information, depending on your requirements. You can, for example, create a composite group that is repeated by sample name; inside this composite group, the Spectra Plot snippet will show one graph for each peak, with overlaid spectra for all injections of the current sample.

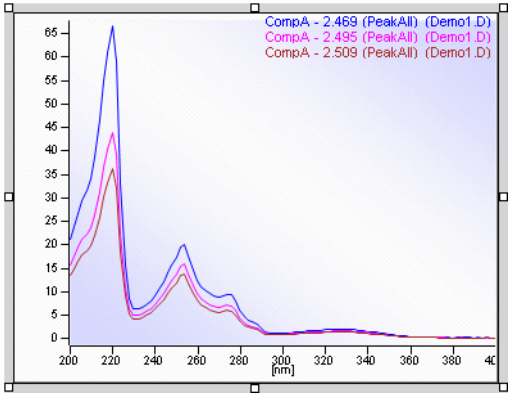
- The **Spectra Plot All Peaks** snippet contains a plot that is embedded in two composite groups. The first composite group is repeated on the signal name, the second composite group is repeated on the peak ID. Thus, you obtain a single spectrum for each peak and signal.



- The **Spectra Plot Compounds** snippet contains a plot that is embedded in a single composite group. The composite group is repeated on the peak ID, and it also contains the retention time and the compound name for each peak. If there are multiple signals, this snippet uses only the peaks of the main signal.



- The **Spectra Plot per Peak** snippet is repeated by peak, that is, the entire report item is displayed once for each peak in the generated report. You cannot remove the repeating by peak in the report item properties. Multiple spectra selected from the same peak are shown in an overlaid graph.



10 Charts

This chapter describes the characteristics and usage of charts in RTE.

About Charts

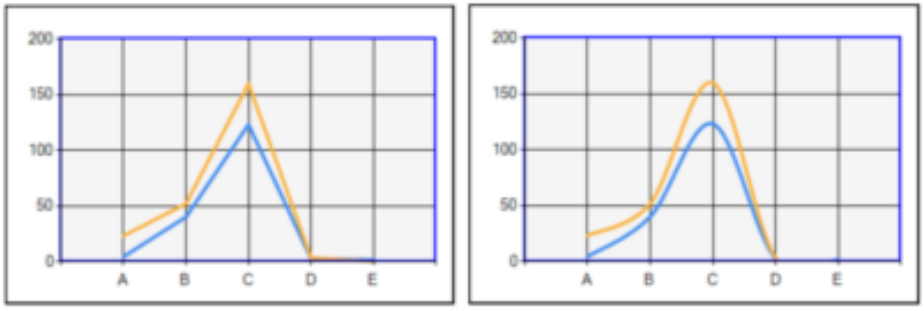
Charts are very useful for graphic display of data. As in tables or matrices, you can present aggregated data.

The following chart types are available in RTE:

- *Line chart*

  With line charts you can visualize categorized data using a direct line to connect the values. The category values are used to label the x-axis. For example, you can categorize the data by the sample name, calibration level or compound name. Different series of data are shown as several lines in different colors.

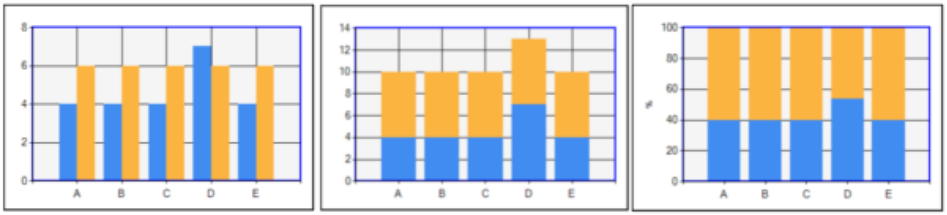
  Line - Simple and **Line - Smooth**:



- *Column chart*

  Column charts are very similar to line charts. You can also visualize categorized data, but the data is shown as column bars instead of being connect with a line. The category values are used to label the x-axis. For example, you can categorize the data by the sample name, calibration level or compound name. Different series of data are shown as several bars in different colors.

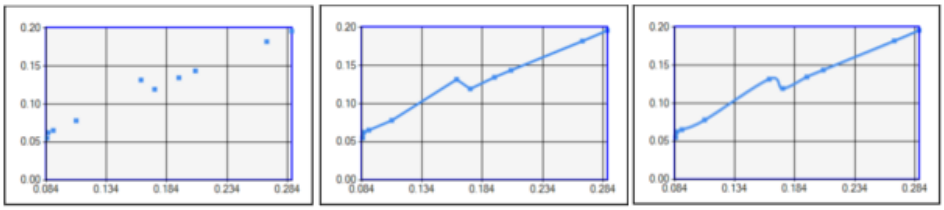
Column - Simple, **Column - Stacked**, and **Column - Stacked 100%**:



- *Scatter chart*

  In scatter charts, the location of the data points is determined by x and y-values. The x-values are typically numeric values or date/time values. For example, you can show the ratio of compound amount to peak area in an accuracy plot.

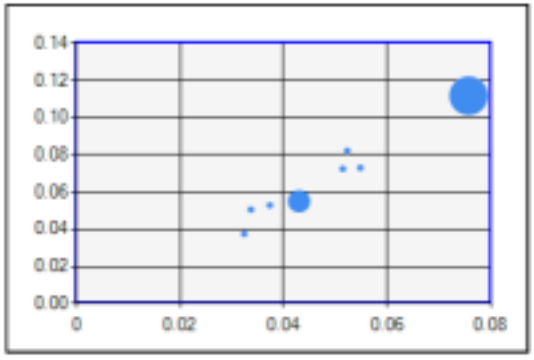
  Scatter - Simple, **Scatter - Lines**, and **Scatter - Smooth Lines**:



- *Bubble chart*

  As in scatter charts, the location of the data points is determined by x and y-values. In addition, the size of the bubbles is determined by a separate numeric value.

  Bubble:



Preparing the Data

Using charts, especially scatter or bubble charts, can be quite complex. It is important that you plan the axis scaling, category group and series group expression in advance and know exactly how they will structure your data. Otherwise, you might get unexpected results and will not know which properties you must change in order to correct the result.

NOTE

The data shown in the chart also depends on the report type and on whether the chart is placed in a composite group:

- In Single Injection reports, the entire template content is repeated for each single injection. It is therefore impossible to compare data from several injections in the same chart with a Single Injection report.
- In composite groups you can group, sort, and filter the data that will be available in a chart.

Read and understand the following before creating a chart:

- Which chart type suits your requirements?
  - If you want to label the x-axis with string values such as *Sample 1*, *Sample 2*, *Sample 3*, you will typically create a line chart or column chart.
  - If you want to label the x-axis with numeric values such as the retention time or the compound amount, you will typically create a scatter chart or bubble chart.
- How many data points do you want to show in the chart? For example, one for each sample, one for each compound, or one for each peak? Which expression can you use to distinguish the data? Use this expression for the category group.
- Do you need to distinguish the data aggregated by the category group? For example, the category group may distinguish the samples names, but you used two signals and want to display one data point per signal and sample name. Use the additional expression (in this example, the signal name) as a series group expression.
- Do you need to filter the data? For example, filter the data to show only specific compounds or only specific signals.

- Which values do you want to plot on the y-axis? These values must be numeric. We recommend using aggregating functions, as the category group may contain multiple values.
- For scatter charts and bubble charts: Which values do you want to plot on the x-axis? The x-values are typically numeric or date/time values. However, it is also possible to plot text values on the x-axis.

NOTE For line and column charts, the category values are identical to the x-axis values. For scatter and bubble charts, the category group only has an impact on the amount of displayed data — the x-axis values are set separately and can differ from the category values.

- Do you need to sort the data? We recommend using the same expression for sorting and grouping the category group. In line and column charts, this sorts the labels on the x-axis. For scatter charts using lines, the line connects the data points in the order given by the category group.
- For bubble charts: Which value should influence the bubble size?

Category Group

For *all* chart types, the category group has an impact on the amount of displayed data. You can choose a category group expression that groups multiple subsets of data together. For example, if your data contains multiple injections of the same sample, you can choose the sample name for the grouping expression. The chart will then show only one data value for each distinct sample, such as the average compound amount.

The impact of the category group on the x-axis labels depends on the chart type:

- For *line* and *column* charts, the category values are identical to the x-axis values.
- For *scatter* and *bubble* charts, the category group only has an impact on the amount of displayed data – the x-axis values are set separately and can differ from the category values.

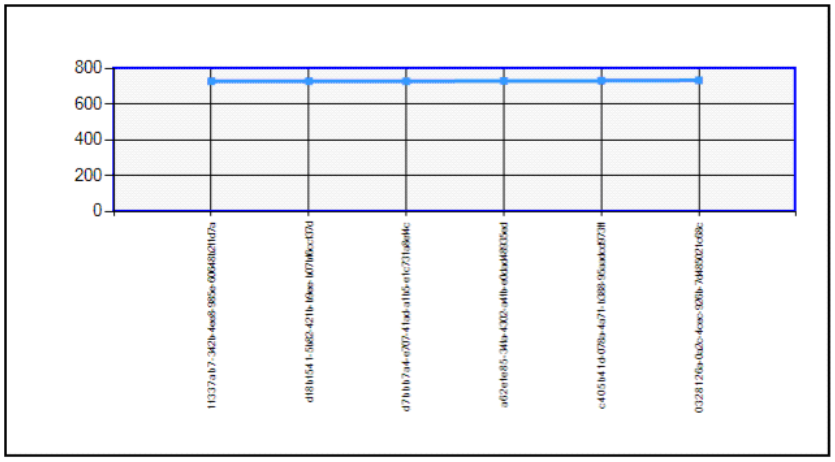
Category Group Example

For example, your data may include 3 samples, where each of the samples has been injected 2 times. If you select **=Injection_ID** as a grouping expression, the diagram will contain 6 data points. If you select **=Sample_ID**, the diagram will only contain 3 data points. Each data point may show, for example, the average of the 2 peak areas.

- Line chart with the following settings:

  y-value: =Peak_Area

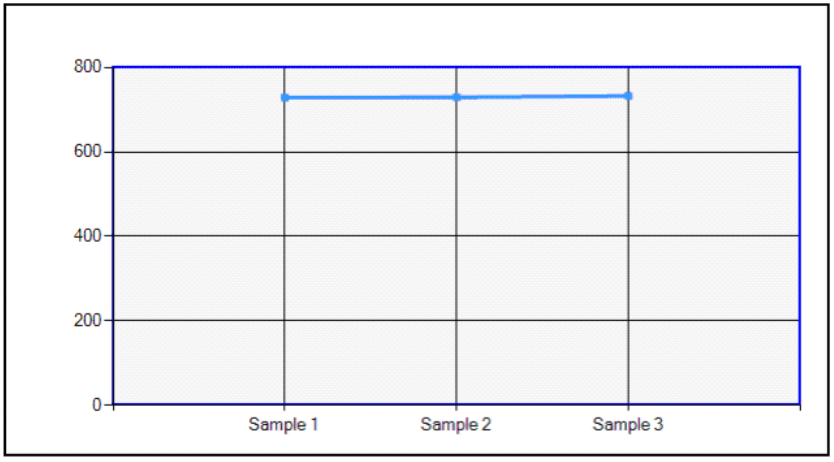
  Category group expression: =Injection_ID



- Line chart with the following settings:

  y-value: =Avg(Peak_Area)

  Category group expression: =Sample_ID

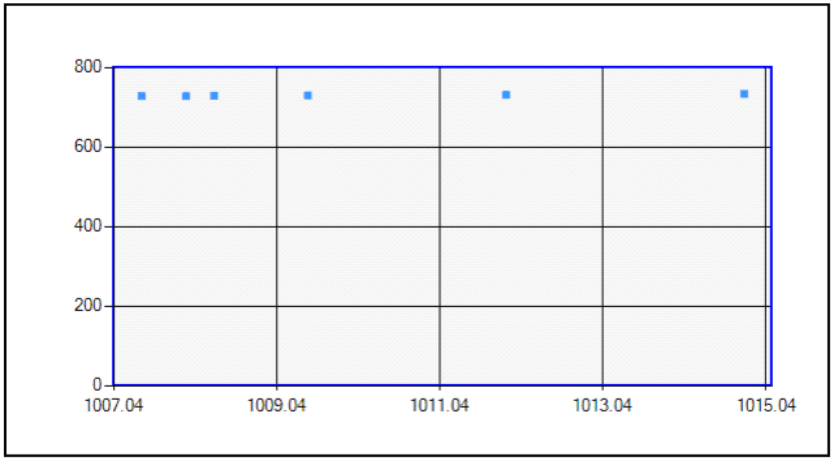


- Scatter chart with the following settings:

  y-value: =Peak_Area

  x-value: =Compound_Amount

  Category group expression: =Injection_ID

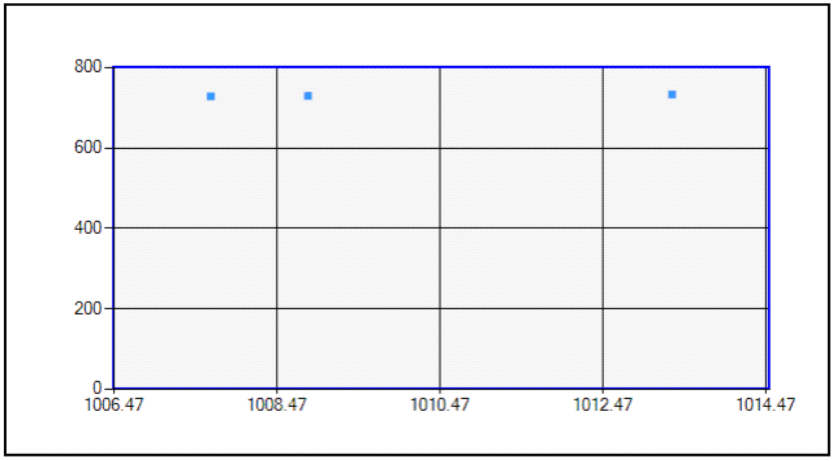


- Scatter chart with the following settings:

  y-value: =Avg(Peak_Area)

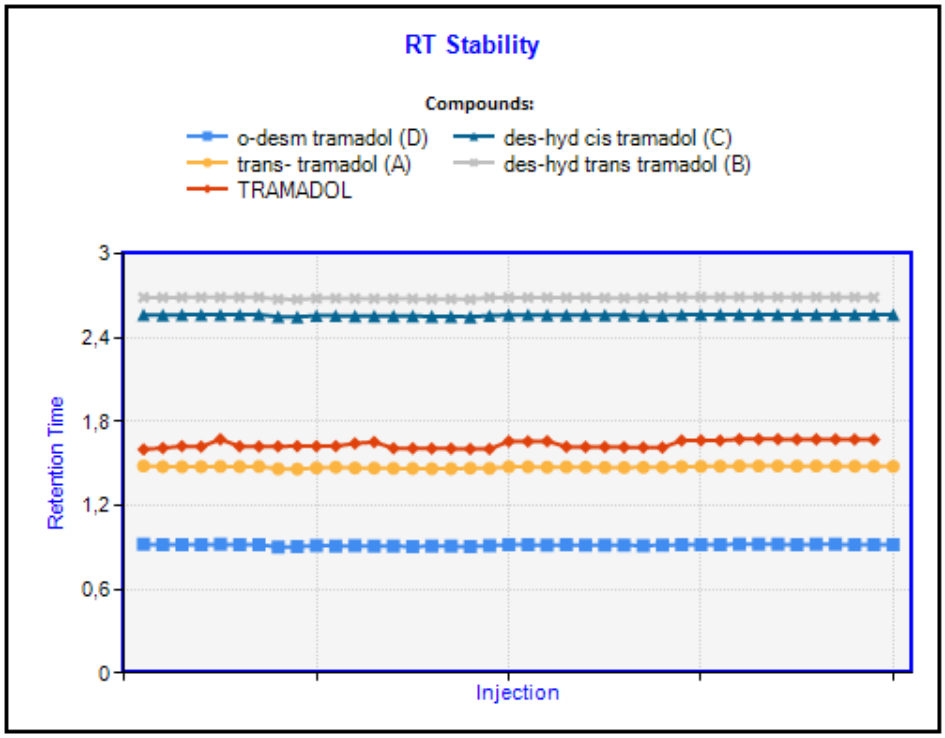
  x-value: =Avg(Compound_Amount)

  Category group expression: =Sample_ID



Series Group

You can place several series of data in the same chart. For example, you may want to create a chart that shows the stability of retention times over a set of injections. If there are several compounds, you can show a separate line for each compound. In this case, create a category group based on the injection ID, and a series group which is grouped by the compound name. The result may resemble the following line chart.



Y-value: **=Peak_RetentionTime**

Format code for y-axis label: F1

Category group expression: **=Injection_ID**

Category sorted by: **=Injection_AcquiredDate**

Series group expression: **=Compound_Name**

Using Charts

To change the chart title and axes titles

1. In the **Chart Properties**, select the **Chart** page.
2. Under **Titles**, click the **fx** button for the title you want to change.
3. In the **Expression Editor**, enter the title. You can use static titles without an equals sign or dynamic expressions starting with an equals sign.
4. Save the settings.

To change the values plotted on the y-axis

1. In the **Chart Properties**, select the **Data** page.
2. Under **Data Values**/**Select Y-Value**, select the required data field or expression that you want to plot on the y-axis. As the y-value must be numeric, only data fields returning numeric values are available in the list.
3. Click  to move the selected expression to the active settings, which are shown on the right side.
4. Select the previously used expression on the right side, and click  to remove it from the active settings.
5. Save the settings.

To change the y-axis labels

1 In the **Chart Properties**, select the **Data** page.

2 Under **Data Values**, click **Data Value Properties**.

3 In the **Data Value Properties**, select the **Label** page.

4 If you want to completely hide the y-axis labels, clear the **Show Y-Axis Labels** check box.

5 If you want to use a different format for the numbers defined by the y-value expression, click **fx** to enter the required Format Code (see "Format Codes" on page 116).

6 Save the settings.

To change the values plotted on the x-axis

For line charts or column charts

1 In the **Chart Properties**, select the **Data** page.

2 Under **Category Properties**/**Select Grouping for X-Axis**, select the required data field or expression that you want to plot on the x-axis.

This expression is used both to group the data and to label the x-axis. The expression may return string values or numeric values.

3 Save the settings.

For scatter charts and bubble charts

1 In the **Chart Properties**, select the **Data** page.

2 Under **Data Values**/**Select X-Value**, select the required data field or expression that you want to plot on the x-axis (typically a numeric value).

3 Save the settings.

To change the x-axis labels

1. In the **Chart Properties**, select the **Data** page.
2. Under **Category Group**, click **Category Properties**.
3. In the **Category Properties**, select the **Label** page.
4. If you want to completely hide the x-axis labels, clear the **Show X-Axis Labels** check box.
5. The usage of the expression for x-axis labels depends on the type of diagram:
   - *For line charts and column charts:*

     If you want to use different labels than the ones resulting from the category group expression, click **fx** and enter the required expression in the **Expression Editor**.

     Use an expression that is based on an identifier equivalent to the identifier of the category group expression. For example, if the category is grouped on the sample ID, you could display the sample name. Displaying the sequence name or the injection order number would lead to ambiguous x-axis labels.
   - *For scatter charts and bubble charts:*

     If you want to use a different format for the numbers defined by the x-value expression, click **fx** to enter the required Format Code (see "Format Codes" on page 116).
6. Save the settings.

To change the legend title

1. In the **Chart Properties**, select the **Legend** page.
2. Under **Visibility**, make sure the **Show Legends** and **Show Legend Title** check boxes are selected.
3. Click **fx** to enter a legend title.
4. Save the settings.

To change the series labels

To check the type of series label

1 In the **Chart Properties**, select the **Data** page.

2 Under **Data Values**, click **Data Value Properties**.

3 In the **Data Value Properties**, select the **Label** page.

4 Check the status of the **Show Series Expression** check box.

If you clear this check box, RTE will use default series labels such as **Series 1**, **Series 2**, **Series 3** and so on.

If you select this check box, RTE will use a dynamic expression for the series labels. See the following steps to change this expression.

5 Save the settings.

To change the expression for series labels

1 In the **Chart Properties**, select the **Data** page.

2 Under **Series Group**, click **Series Properties**.

3 In the **Series Properties**, select the **Label** page.

4 Click **fx** to change the expression.

By default, this expression is empty. With an empty series label expression, the series labels are built using the series expression from the **Data Fields** page in the **Chart Properties**.

5 Save the settings.

To plot different y-values in the same chart

The category group and series group expressions define the basic set of data. However, you can provide multiple expressions as y-values and thus plot different y-values for the same data.

1 In the **Chart Properties**, select the **Data** page.

2 Under **Category Group**, select the category group expression.

3 If required, select a series group expression under **Series Group**.

NOTE As multiple y-values are displayed the same way as multiple series values, using both options at the same time may lead to an overcrowded chart.

4 Under **Data Values**/**Select Y-Value**, select the required data fields and click  to move them to the active settings.

5 If required: Under **Data Values**/**Select X-Value**, select the same number of data fields as for the y-value. You can select the same x-value expression multiple times. X-values are only available for *Scatter* and *Bubble* charts.

6 If required: Under **Data Values**/**Select Size**, select the same number of size expressions as for the y-value. You can select the same size expression multiple times. Size expressions are only available for *Bubble* charts.

7 Save the settings.

11
Method Information

This chapter describes the characteristics and usage of method information in RTE.

About Method Information

With the **Method Information** snippets, you can add information on the used methods to your report. This includes information on the method parameters and instrument settings such as the signals, flow rates, or pressure limits.

The method information is structured in up to five levels. Each level may contain single data fields, tables, or a combination of both. The content of each level depends on the system generating the method file. The data in each level is organized in sections with specific section names. You can create filter expressions using these section names.

To filter for a specific section

Find out in which level the section is contained

1 In the **Method Properties**, select the **Setpoint** page.

2 Select only one of the levels.

3 Save the settings.

4 Generate the report.

5 Check whether the required section is included in the report. If it is not, repeat the procedure with the next level.

NOTE If you clear the higher levels and select only one of the lower levels, for example only level 5, the report still includes the section names contained in the higher levels. The detail information is shown only for the selected level. If you want to hide the section as well, create a filter for the required sections.

Filter for the required section

If you want to show only a specific section, you can create a filter for the section name as described in the following procedure. This will remove all sections, including their sub sections, that do no match the filter expression.

1 In the **Method Properties**, select the **Filter** page.

2 Under the level that you identified above, create a filter expression for the required section. The filter expression is always **SECTION NAME**.

For example: *SECTION NAME=Signals*

3 Save the settings.

12
Instrument Information

Early Maintenance Feedback (EMF) Counters

Certain GC instrument drivers provide Early Maintenance Feedback (EMF) information. This information includes, for example, the number of injections for a front inlet septum, the number of runs with a column, or the total time a lamp has been switched on. If the values exceed the Service Due limits, the EMF counters return a *value exceeded* information. The exact keys and values depend on the instrument driver.

Instrument Modules

The **Instrument Modules** snippet (only available in the context of ChemStation) shows information on the modules such as the module name, serial number, or firmware version.

NOTE You cannot configure the **Instrument Modules** snippet. There is no Properties dialog available.

13 Expressions

This chapter describes the characteristics and usage of expressions in RTE.

About Expressions

Expressions are used to define the value of a data field or text field item, the values shown in a table column, specific properties such as the background color of an item, or for many other purposes. The most basic expression is a reference to a specific data field, but expressions can also contain mathematical functions on different data fields.

An expression always starts with an equals sign. The most basic expression is one that refers to a specific data field, for example the sequence name: =*Sequence_Name*.

However, you may need to create more complex expressions during template development. For example, you may filter for sample names with a certain prefix, compare numbers with a certain threshold value, or calculate one value from another using a custom formula.

The **Expression Editor**, which is part of RTE, helps you build dynamic expressions that include data fields and logical or mathematical functions.

NOTE

All expressions are written in Microsoft Visual Basic. Therefore, you can use any function available in Visual Basic. The only consequence may be that the Expression Editor shows a red, serrated line, if the used functions are not modelled by RTE. In addition, the preview on the report item in the properties dialog or in the Editing Pane may not be shown correctly. However, when the report template is generated, the functions are nevertheless used correctly.

For more information on Microsoft Visual Basic, refer to http://msdn.microsoft.com/en-us/library/sh9ywfdk.aspx.

NOTE

The notation of functions or data fields in the **Expression Editor** is *not case-sensitive*.

Operators

Arithmetic

Table 1 Arithmetic

Name	Syntax	Description
^	NUMBER^POWER	Raises a number to the power of another number.
*	NUMBER1*NUMBER2	Multiplies two numbers.
/	NUMBER1/NUMBER2	Divides two numbers and returns a floating-point result.
Mod	NUMBER1 Mod NUMBER2	Divides two numbers and returns only the remainder.
+	NUMBER1 + NUMBER2	Adds two numbers.
-	NUMBER1 - NUMBER2	Substracts one number from another, or indicates the negative value of a numeric expression.

Comparison

Table 2 Comparison

Name	Description
<	Less than
<=	Less than or equal to
>	Greater than
>=	Greater than or equal to
=	Equal to
<>	Not equal to
Like	Compares two strings. The string to be compared with must contain wildcards: • ? matches any single character. • * matches any number of adjacent characters.

Logical

Table 3 Logical

Name	Description
`And`	Performs a logical conjunction on two Boolean expressions.
`Not`	Performs logical negation on a Boolean expression.
`Or`	Performs a logical disjunction on two Boolean expressions.

Concatenation

Table 4 Concatenation

Name	Description
`&`	Generates a string concatenation of two expressions.
`+`	Concatenates two strings.

Functions

Program Flow

Table 5 Program Flow

Name	Syntax	Description
`Choose`	`choose(NUMBER, "argument_1", "argument_2", [...], "argument_n")`	Selects and returns a value from a list of arguments.
`Iif`	`Iif(CONDITION, THEN-VALUE, ELSE-VALUE)`	Returns one of two values, depending on the evaluation of the condition.

Aggregate

Table 6 Aggregate

Name	Syntax	Description
Avg	Avg(FIELDNAME)	Returns the average of all non-null values of the specified field.
Count	Count(FIELDNAME)	Returns a count of non-null values of the specified field.
CountDistinct	CountDistinct(FIELDNAME)	Returns a count of the distinct values of the specified field.
CountRows	CountRows()	Returns the number of rows, including rows with null values.
Max	Max(FIELDNAME)	Returns the maximum value from all values of the specified field.
Min	Min(FIELDNAME)	Returns the minimum value from all non-null values of the specified field.
StDev	StDev(FIELDNAME)	Returns the standard deviation of non-null values based on a sample of the entire population: $s = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}\left(x_i - \bar{x}\right)^2}$
StDevP	StDevP(FIELDNAME)	Returns the standard deviation of non-null values based on the entire population: $s = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(x_i - \bar{x}\right)^2}$
Sum	Sum(FIELDNAME)	Returns a sum of the values of the specified field.
First	First(FIELDNAME)	Returns the first of the values of the specified field.
Last	Last(FIELDNAME)	Returns the last of the values of the specified field.

NOTE There is no specific function for the relative standard deviation. This must be manually calculated as (Stdev/Avg*100).

Aggregating functions always refer to all records in a scope and return only one value. This value is either calculated from those records or selected according to specific criteria. Therefore, aggregating functions are automatically used, for example, for the creation of table headers or footers. You can use aggregating functions if you need to summarize your data.

Math

Table 7 Math

Name	Syntax	Description
`Abs`	`Abs(NUMBER)`	Returns the absolute value of a single-precision floating-point number.
`Exp`	`Exp(POWER)`	Returns e raised to the specified power.
`Log`	`Log(NUMBER)`	Returns the natural (base e) logarithm of a specified number.
`Log10`	`Log10(NUMBER)`	Returns the base 10 logarithm of a specified number.
`Pow`	`Pow(NUMBER, POWER)`	Returns a specified number raised to the specified power.
`Round`	`Round(NUMBER)`	Rounds a double-precision floating-point value to the nearest integer.
`Sqrt`	`Sqrt(NUMBER)`	Returns the square root of a specified number.
`Int`	`Int(NUMBER)`	Returns an integer, obtained by truncating (not rounding!) the provided number.

Conversion, Date/Time

Table 8 Conversion, Date/Time

Name	Syntax	Description
`Cstr`	`Cstr(...)`	Convert to string
`Val`	`Val("198th Street")`	Returns the numbers contained in a string as a numeric value of appropriate type. If the string does not contain any numbers, 0 is returned.
`CDbl`	`CDbl(...)`	Convert to Double
`CInt`	`CInt(...)`	Convert to Integer

Table 8 Conversion, Date/Time

Name	Syntax	Description
Cdate	CDate("October 19, 1962")	Convert to date.
Str	Str(NUMBER)	Returns a string representation of a number.
Day	Day(DATETIME)	Returns an integer value from 1 to 31 representing the day of the month.
Hour	Hour(DATETIME)	Returns an integer value from 0 to 23 representing the hour of the day.
Month	Month(DATETIME)	Returns an integer value from 1 to 12 representing the month of the year.
MonthName	MonthName(MONTH)	Returns a string value containing the name of the specified month. MONTH is the numeric designation of the month. For example, January is 1, February is 2, and so on.
Now	Now	Returns a date value containing the current date and time according to your system.
Year	Year(DATETIME)	Returns an integer value from 1 to 9999 representing the year part of a specified date.
Today	Today	Returns a date value containing the current date according to your system.

Text

Table 9 Text

Name	Syntax	Description
Chr	Chr(65)	Returns the character associated with the specified ANSI character code.
InStr	InStr(HAYSTACK, NEEDLE)	Returns an integer specifying the start position of the first occurrence of one string (NEEDLE) within another (HAYSTACK).
InStrRev	InStrRev(HAYSTACK, NEEDLE)	Returns the position of the first occurrence of one string (NEEDLE) within another (HAYSTACK), starting from the right end of the string.

Table 9 Text

Name	Syntax	Description
`Lcase`	`Lcase(STRING)`	Returns a string or character converted to lower case.
`Left`	`Left(STRING, LENGTH)`	Returns a string containing a specified number of characters from the left end of a string.
`Len`	`Len(STRING)`	Returns an integer containing the number of characters in a string.
`Right`	`Right(STRING, LENGTH)`	Returns a string containing a specified number of characters from the right end of a string.
`Split`	`Split(STRING, DELIMITER)`	Returns a zero-based, one-dimensional array containing a specified number of substrings. The specified delimiter is used to create the substrings.
`LTrim`, `RTrim`, `Trim`	`Trim(STRING)`	Returns a string containing a copy of a specified string with no leading spaces (LTrim), no trailing spaces (RTrim), or neither leading nor trailing spaces (Trim).
`FormatDateTime`	`FormatDateTime(DATE, FORMAT)`	Returns a string expression representing a date/time value in a specified format. The following formats are available (used without quotes, not case-sensitive): • GENERALDATE: Displays a date and/or time. If there is a date part, it is displayed as a short date. If there is a time part, it is displayed as a long time. If present, both parts are displayed. • LONGDATE: Displays a date using the long date format specified in your computer's regional settings. • SHORTDATE: Displays a date using the short date format specified in your computer's regional settings. • LONGTIME: Display a time using the time format specified in your computer's regional settings. • SHORTTIME: Displays a time using the 24-hour format (hh:mm).

Table 9 Text

Name	Syntax	Description
FormatNumber	FormatNumber(DATE, DIGITSAFTERDECIMAL, LEADINGDIGIT, PARENS, GROUP)	Returns an expression formatted as a number. You can use the following parameters, or use blanks for the default settings: • DIGITSAFTERDECIMAL: Numeric value, indicates how many places are displayed to the right of the decimal. Default: -1, the computer's regional settings are used. • LEADINGDIGIT: True or False, indicates whether a leading 0 is displayed for fractional values. The computer's regional settings are used by default. • PARENS: True or False, indicates whether to place negative values within parentheses. The computer's regional settings are used by default. • GROUP: True or False, indicates whether or not to group numbers using the group delimiter specified in the locale settings. The computer's regional settings are used by default.
FormatPercent	FormatPercent(NUMBER)	Returns an expression formatted as a percentage (that is, multiplied by 100) with a trailing % character.
Mid	Mid(STRING, START, LENGTH)	Returns a string containing a specified number of characters from a string. START defines the starting position of the characters to be returned.
Ucase	UCase(STRING)	Returns a string or character containing the specified string converted to uppercase.

Misc

Table 10 Misc

Name	Syntax	Description
RowNumber	RowNumber(SCOPE) or RowNumber(SCOPE, COUNTGROUP)	Returns a running count of all rows in the specified scope. The scope can be given as single string (Scope as String) or in combination with the group number (Scope as String, CountGroup as String).

Format Codes

With Format Codes, you define the output format of numeric or date/time values. You can either select one of the predefined Format Codes from the given drop-down lists, or enter your own Format Code in the Expression Editor.

NOTE Format Codes do *not* start with an equals sign!

You can use the following placeholders:

Format Code	Description
0	Zero placeholder. The number is always displayed, even if it is 0.
#	Digit placeholder. The number is only displayed if it is different than 0.
.	Decimal point as defined by the country settings.
,	Group separator. Show a thousand separator, if required, as defined by the country settings.
F1	Show the number with 1 digit using the decimal point and group separator as defined by the country settings.
F2	Show the number with 2 digits using the decimal point and group separator as defined by the country settings.
F3	Show the number with 3 digits using the decimal point and group separator as defined by the country settings.
d	Day of the month (1—31).
dd	Day of the month (01—31)
h	Hour (1—12)
hh	Hour (01—12)
H	Hour (1—24)
HH	Hour (01—24)
m	Minute (1—59)
mm	Minute (01—59)

Format Code	Description
M	Month (1—12)
MM	Month (01—12)
MMM	Abbreviation of the Month
ss	Second (01—59)
tt	AM/PM designator
YY	Year (00—99)

The following table shows some examples of how the Format Code defines the output format.

Table 11 Format Codes - Examples

Value	Format String	Output
0.123	#.##	.12
	0.##	0.12
	0.####	0.123
	0.0000	0.1230
	F1	0.1
	F2	0.12
2/27/2007 5:11:30 PM	HH:mm:ss	17:11:30
2/27/2007 5:11:30 PM	dd/MM/YY	02/27/07
2/27/2007 5:11:30 PM	h tt	5 PM

For more information on the Format Codes, refer to the MSDN library (http://msdn.microsoft.com/en-us/library/26etazsy(v=VS.100).aspx).

Using Expressions

To filter data with varying notations (upper/lower case)

If you use expressions that compare the content of a data field with another value (for example, when filtering the table data), be aware that the database contents may contain both uppercase and lowercase. The notation may vary, especially if the entry is provided by the user when preparing the measurement, as, for example, the sample name or sequence name. To ensure that all relevant records are considered, transform the database content to a standardized notation before comparing it.

Table 12 Functions to transform the notation of data fields

Function	Syntax	Description
LCase	*=LCase(fieldname)*	Transforms all characters in the given field to lowercase.
UCase	*=UCase(fieldname)*	Transforms all characters in the given field to uppercase.

The complete entry in the **Filter** page would look like this:

Table 13 Complete entry

Expression	Operation	Value
*=UCase(***Sample_Name***)*	=	"TRAMADOL"

To filter empty fields

Sometimes, you may want to know if a data field contains a value or is empty. For example, you only want to display fields that are not empty. Empty data fields are not always actually empty; sometimes they contain a certain kind of null information. Therefore, it is advisable to use a special syntax to filter for fields with actual content.

To exclude empty *strings*, use the following expression:

Table 14 Expression for excluding empty strings

Expression	Operation	Value
=Len(fieldname)	>	*0*

To exclude empty *numbers*, use one of the following expressions:

Expression	Operation	Value
=fieldname >= 0	=	*True*
=Len(fieldname)	>	*0*

To repeat on sample names beginning with

You can repeat composite groups not only on specific data fields but also on customized expressions. Using expressions you can, for example, repeat the composite group on the first part of a sample name. Let's say that a sequence contains the following samples:

- Sample1_a
- Sample1_b
- Sample1_c
- Sample2_a
- Sample2_b
- Sample2_c

Now let's say you want to repeat the composite group only two times, that is, for Sample1 and Sample2. The first part of the expression must therefore call the *Split* function, that divides the sample name in two parts, using the underscore as a delimiter:

=Split(Sample_Name, "_")

The result of this function is a list containing the following subentries:

- Sample1; a
- Sample1; b
- Sample1; c
- Sample2; a
- Sample2; b
- Sample2; c

The next part of the expression must be a *Choose* function that always returns the first element of a list:

Choose(1, [list])

The list in this example is returned by the Split function:

=Choose(1, Split(Sample_Name, "_"))

This expression returns the following results:

- Sample1
- Sample1
- Sample1
- Sample2
- Sample2
- Sample2

If you use this expression to repeat the composite group, you will get only two composite groups, as there are only two distinct values.

To compare numbers using the Iif function

With the *Iif* function you can, for example, compare a number with a fixed limit, and return either the value itself or an error message. Let's say that you check whether the compound amount is lower than 0.05 µg/ml. If the amount is lower, the actual amount should be displayed. If it is higher, the message "too high" should be displayed.

The general syntax of the *Iif* function is:

=Iif(condition, then-value, else-value)

In this example, the complete expression would be:

=Iif(Compound_Amount < 0.05, Compound_Amount, "too high")

The unit of the amount is not part of the expression. The unit is defined in the chromatographic data system and is stored in a separate data field.

To show the type of injection

In analytical data generated by Agilent ChemStation as a source system, the field **Injection_Volume** may contain positive or negative values:

- Positive values represent the actually injected sample volume.
- Negative values represent several special injection actions. The following values are used:
  - -1: no injection
  - -2: manual injection
  - -3: injector program
  - -4: external injector

To display either the actually injected volume or the appropriate description, you can use the following expression:

=Iif(Injection_Volume >= 0, CStr(Round(Injection_Volume, 4)) & " " & Injection_VolumeUnit, choose(Int(Abs(Injection_Volume)), "no injection", "manual injection", "injector program", "external injector"))

If the original value is positive, it is only rounded off to four decimals. If it is negative, the *Int*, *Abs*, and *Choose* functions are applied.

The *Abs* function removes the algebraic sign. Thus, negative numbers are transformed to positive numbers. Positive numbers are left unchanged.

The *Int* function transforms double-precision floating-point numbers to integer values. It returns the number in front of the decimal point (obtained by truncating, not by rounding).

The *Choose* function selects and returns a value from a list of arguments. The first parameter is a number that indicates the relevant value. In the example above, the *Choose* function returns “no injection” if its first parameter is 1.

To filter for date and time

When filtering for a date or date range, you must enclose the date in hash marks:

Table 15 Filtering for a date

Expression	Operation	Value
=Injection_AcquiredDate	>=	#01/25/2007#

If you do not provide a specific time of day, the system assumes the time #0:00:00#. Therefore, in order to filter for one entire day, you must filter for a date range as follows.

Table 16 Filtering for a date (single day)

Expression	Operation	Value
=Injection_AcquiredDate	>=	#01/25/2007#
=Injection_AcquiredDate	<	#01/26/2007#

It is not possible to filter for a time without using the date.

To calculate with a custom field

You can use the value of a custom field in another expression, just as you can use any value of any data field. However, if you only refer to the field name, the plain content of the custom field is shown, which is composed of a label, a separator, and a value. If you create an expression in which you want to refer only to the value, you need to use the same expression as it is given by default in the custom field value.

In order to calculate with the content, you must first transform the content to a number using the *Val* function.

The following examples show you the results for a sample custom field containing the label *TabletWeight* and the Value *1020*.

Table 17 Expressions referring to a custom field

Expression	Result
=Sample_CustomField01	TabletWeight|1020
=Trim(Choose(1,Split(Sample_CustomField01 ,"|")))	TabletWeight
=Trim(Choose(2,Split(Sample_CustomField01 ,"|")))	1020
*=Val(Trim(Choose(2,Split(Sample_CustomField01 ,"|")))) * 2*	2040

Relative Standard Deviation

No single function returns the value for the relative standard deviation. If you need to display this value, you must calculate it using the following expression:

*=(StDev(fieldname)/Avg(fieldname)*100)*

To filter for similar names

If you have different samples in a sequence, and the samples names differ only by a number (for example, "Sample 1", "Sample 2", "Sample 3" etc.), you can filter for those similar sample names using the **Contains** operator together with wildcards:

Expression	Operation	Value
=Sample_Name	**Contains**	"*Sample*"

This filter returns all samples that contain "Sample" in their name.

The following wildcards are available:

- ? matches any single character.
- * matches any number of adjacent characters.

To show only part of a value

Depending on the value of a data field, you may want to show only part of the value.

For example, the data fields **Sample_DilutionFactor** and **Sample_Multipliers** show five numbers separated by semicolon, but only part of the numbers may be set by the chromatographic data system. Therefore the value may look like *10; 0; 0; 0; 0* if only the first number is set. To display only the number *10* instead of the entire string, you can use the following expression:

=Choose(1, Split(Sample_Multipliers, ";"))

- The *Split* function divides the string in several parts, using the semicolon as a delimiter. In this example, the different parts are the single numbers.
- The *Choose* function selects and returns a specific value from a list of values. In this example, it returns the first value, that is, the number *10*.

14
Calculation Variables

This chapter describes the characteristics and usage of calculation variables in RTE.

About Variables

With calculation variables, you can create a large variety of customized reports. Calculation variables offer you the possibility to store specific values or expression results under a specific name, and reuse the values in other report items in the same template.

There are different scenarios in which you can use calculation variables. Depending on the scenario, the calculation variables are referred to as **Variable**, **Aggregator**, **Category Aggregator**, or **Custom Extractor**:

- With **Variable**, you can store any single numerical value.
- With **Aggregator**, you can store a collection of single values.
- With **Category Aggregator**, you can store a collection of collections.
- With **Custom Extractor**, you can store the key/value pairs contained in the XML content of a complex custom field (for example, **Injection_DiagnosticData** or **Sample_CustomFields**).

To create a new calculation variable, you can either use the **Summary Calculations** feature of a table, or create a suitable expression for a field/table/matrix value and use the **Save Expression Result As...** function in the **Expression Editor**.

Once you have defined the variable, you can refer to it in all *subsequent* report items. You can not refer to a calculation variable in a report item preceding the one in which the variable is defined.

You can see a list of all calculation variables that are available for the current item in the **Expression Editor** under the **Variables** node. A list of all calculation variables used in the entire report template can be found in the **Report Properties** dialog.

The **Report Properties** dialog also allows you to rename existing calculation variables. The renaming includes both the definition and all expressions where the calculation variable is used.

See the following topics for more details on the calculation variable types.

Variable

With **Variable**, you can store any single numerical value. This value is identified by a unique name. You can provide either only a static name for the variable, or use a dynamically generated key in addition (for example, the sample name).

Example

The variable *AvgRetTime* may contain the average retention time of a specific compound found in a specific sample.

Example with Unique Key Value

The variable *AvgRetTime (Sample_Name)* can be created once for each sample in a sequence. With *AvgRetTime("SSRSD1")*, you can show the average retention time in the *SSRSD1* sample. If the variable is embedded in a composite group that is repeated on the sample name, you can automatically list the average retention times for each sample.

Aggregator

With **Aggregator**, you can store a collection of single values. The entire collection is identified by a unique name. You can apply several aggregating functions to the collection. It is not possible to select a single value from the collection.

The **Aggregator** provides the following functions:

- `Sum()`

  This function returns the sum of all values currently contained in the collection.

- `Avg()`

  This function returns the average of all values currently contained in the collection.

- `Stdev()`

  This function returns the standard deviation of all values currently contained in the collection.

- `Prsd()`

  This function returns the relative standard deviation (Stdev/Avg*100) of all values currently contained in the collection.

- `Min()`

  This function returns the lowest value currently contained in the collection.

- `Max()`

  This function returns the highest value currently contained in the collection.

- `Count()`

  This function returns the number of elements in the collection.

- `Clear()`

  This function deletes all values from the collection. At the same time, it returns the number of deleted values.

Example

The aggregator *RetTimeSSRSD1* can contain all retention times of a compound in different injections of the *SSRSD1* sample. You can return the average retention time with *Avg(RetTimeSSRSD1)*, or the standard deviation with *StDev(RetTimeSSRSD1)*.

Example

The aggregator *AvgRetTimes* can contain the average retention times of the same compound in different samples. You can return the standard deviation on the average values with *StDev(AvgRetTimes)*.

Category Aggregator

With **Category Aggregator**, you can store a collection of collections. The entire collection is identified by a unique name. You can apply several aggregating functions to each of the contained collections. It is not possible to select a single value from a specific collection.

The category aggregator provides the following functions (each function takes into account only those values belonging to the currently active value of the given data field):

- `Sum([Field])`

  This function returns the sum of all values currently contained in the collection.

- `Avg([Field])`

  This function returns the average of all values currently contained in the collection.

- `Stdev([Field])`

  This function returns the standard deviation of all values currently contained in the collection.

- `Prsd([Field])`

  This function returns the relative standard deviation (Stdev/Avg*100) of all values currently contained in the collection.

- `Min([Field])`

  This function returns the lowest value currently contained in the collection.

- `Max([Field])`

  This function returns the highest value currently contained in the collection.

- `Count([Field])`

  This function returns the number of elements in the collection.

- `Clear([Field])`

  This function deletes all values from the collection. At the same time, it returns the number of deleted values.

Example

A sample has been injected several times. One specific compound has been detected in each injection. For each sample, a collection of the retention times is created. These collections are addressed via the sample name. All of those collections are contained in a category aggregator named *CatRetentionTimes*.

You can return the average retention time for each sample with *Avg(CatRetentionTimes(Sample_Name))*. The argument in the brackets defines the specific category, that is, the portion of values contained in *CatRetentionTimes* to which the *Avg* function is applied.

You may use this expression, for example, in a composite group that is repeated on the sample name. The average retention times are then automatically calculated and shown for each sample name.

Custom Extractor

There are specific data fields that do not contain a single value but an entire XML structure. This XML structure contains various key/value pairs, where the exact keys and the values depend on the chromatography data system and its configuration (see "Keys in Diagnostic Data" on page 173). With **CustomExtractor**, you can store this XML structure. You can apply several functions to access the single values.

The **CustomExtractor** provides the following functions:

- `GetValue(name)`

  This function returns the value stored under the given name.

- `GetNameValue(index)`

  This function returns a combination of key and value in the form Key=Value. With index=0 the function returns the first key/value pair.

- `GetValueByIndex(index)`

  This function returns the value of the name/value pair at the given position. The first key/value pair is indexed by 0.

- `Count()`

  This function returns the number of key/value pairs in the XML structure.

- `Clear()`

  This function deletes the XML structure from the Custom Extractor and returns the number 0.

Example

You can add an invisible text field to your template with the value **=Injection_DiagnosticData**. If you save this value as a **Custom Extractor** named *CustDiagnosticData*, you can subsequently access the start pressure of a ChemStation LC measurement via the expression:

=CustDiagnosticData(GetValue("StartPressure")).

Using Variables

To activate the use of variables

You can only use calculation variables if they are activated for your report template.

1 Click  to open the report properties.

2 In **Report Properties**, select the **Calculation Variables** page.

3 Select the **Use Calculation Variables in Expressions** check box.

4 Save your settings.

To create a variable based on summary calculation

In this example, you create a table for each compound. Each table shows the retention time of the compound in each sample. A second column shows the difference to the average retention time of the compound in the entire sequence. To accomplish this, you create a composite group which contains one hidden table and one visible table. The hidden table is used to store the average values in a variable.

1 Make sure that variables are activated in your report template (see "To activate the use of variables" on page 132).

2 Add the data field **Fields > Compound > Name** to the template.

3 Add two **Compound Summary** tables to the template.

4 Select all three items and click  to create a composite group.

5 Repeat the composite group on **Compound_Name**.

6 If required, filter the composite group for the main signal (*Peak_Calibrole=1*).

7 Prepare the first table to store the variable.

   a Remove the **Repeat On** setting from the table.

   b In the **Advanced** page, clear the **Visible** check box.

   c On the **Columns** page, select the **RT** column and click **Column Properties**.

   d On the **Summary Calculations** page, select the **Average** function, and enter *VarAvgRT* as the **Variable Name**.

   e Confirm all settings.

   f In the Editing Pane, resize the table so that it requires only minimal space.

8 Prepare the second table to show the difference between retention time and retention time average.

   a Remove the **Repeat On** setting from the table.

   b On the **Columns** page, add a **Custom Field** to the table layout.

   c Move the new column to the right of the **RT** column and adjust its size.

   d In the **Column Properties** of the new column, enter the following expression as a value: *=Peak_RetentionTime - VarAvgRT*

   e On the **Format** page, adjust the number format for the new column to **Number**, **1234.00**, and set **Rounding** to 4 decimal places.

   f Confirm all settings and generate a preview.

   The generated report will show the difference between the individual retention times and the sequence average.

To use a variable

To create a variable:

1 Make sure that variables are activated in your report template (see "To activate the use of variables" on page 132).

2 Add two text fields or a data fields to the template.

3 Select the two fields and click  to create a composite group.

4 Repeat the composite group on **Sample_Name**.

5 Enter a customized expression as a value for one of the fields, for example a correction factor for the sample amount: *=Sample_Amount * 99*

6 Click **Save Expression Result As...**

The **Save Expression Result As** dialog opens.

7 Make sure that the **Variable** option is selected, and enter a **Calculation Variable Name**, for example *VarAmountCorrected*.

NOTE No special characters are allowed in the variable name.

8 Save your settings.

To use the variable in subsequent report items:

1 Resize the composite group to provide space for new report items.

2 Add a table with compound information to the composite group, for example the **Compound Results** table.

3 Add a new column to the table. Enter a customized expression as a value for the new column, for example the compound amount multiplied by the corrected sample amount: *=Compound_Amount * VarAmountCorrected*

To rename a variable

1 Click  to open the report properties.

2 In **Report Properties**, select the **Calculation Variables** page.

3 Select the variable you want to rename.

4 Click **Rename**.

The **Rename Calculation Variable** dialog opens.

5 Enter the new name for the variable.

6 Save your settings.

The variable is now renamed in all expressions in which it is used, in the entire report template.

To use a variable with a unique key

The following example describes how to create a table that compares a compound's retention time in each sample with the average retention time.

To prepare the variable:

1 Make sure that variables are activated in your report template (see "To activate the use of variables" on page 132).

2 Add two text fields to the template.

3 Select the two text fields and click  to create a composite group.

4 Repeat the composite group on **Compound_Name**.

5 In the first text field, enter a static text. For example, *RT Average*.

6 In the second field, enter an expression for the average retention time: *=Avg(Peak_RetentionTime)*

7 Save the expression of the second field as a variable. Use the following settings:

- **Calculation Variables**: **Variable**
- **Calculation Variable Name**: For example, *VarRTAverage*
- **Unique Key Value**: *=Compound_Name*

NOTE In the **Unique Key Value** setting, you must use the same value as you used for repeating the composite group

To use the variable:

1 Underneath the composite group, create a **Compound Summary** table.

2 Add a table column with the following expression: *=Peak_RetentionTime - VarRTAverage(Compound_Name)*

To use an Aggregator

This example describes how to compare the average peak areas for two different sets of samples (for example, calibration samples and checkout samples, or samples with a name containing *SampleA* and samples with a name containing *SampleB*).

To prepare the variables:

1 Add the **Compound Results** table two times to the template.

2 Filter the tables according to the samples for which you want to obtain the average peak areas.

Table 18 To filter for the sample type

Expression	Operation	Value	Description
Sample_Type	=	1	The first table contains only calibration samples.
Sample_Type	=	2	The second table contains only checkout samples.

3 In each table: Open the **Column Properties** dialog of the **Area** column, and save the value as a variable. Use the following settings:

- **Calculation Variables**: **Aggregator**
- **Calculation Variable Name**: For example, *AreaAggregator1* in the first table, and *AreaAggregator2* in the second table.
- **Category**: **[None]**
- **Condition**: **[None]**

To use the variables:

1 Underneath the two tables, create a text field with the following expression: *=Avg(AreaAggregator1) - Avg(AreaAggregator2)*

Instead of the *Avg* function, you can also apply the *Sum*, *Stdev*, *Prsd*, *Min*, *Max*, or *Count* function to the **Aggregator** variables.

NOTE

Clear function

If you create and use the **Aggregator** inside a *composite group*, use the *Clear* function at the end of the group. Add two hidden text fields with the following expressions:

=Clear(AreaAggregator1)

=Clear(AreaAggregator2)

This clears all contents of the **Aggregator**, which ensures that the values are not mixed in subsequent group repetitions.

To use a Category Aggregator

This example describes how to compare the average peak areas for two different sets of samples. In contrast to the other example (see "To use an Aggregator" on page 136), the information is now prepared and shown separately for each compound.

To create the variables:

1 Add the **Compound Results** table to the template twice.

2 Repeat both tables on **Compound_Name**.

3 Filter the tables according to the samples for which you want to obtain the average peak areas.

4 In each table: Open the **Column Properties** dialog of the **Area** column, and save the value as a variable. Use the following settings:

- **Calculation Variables**: **Aggregator**
- **Calculation Variable Name**: For example, *AreaAggregator1* in the first table, and *AreaAggregator2* in the second table.
- **Category**: **Compound_Name**
- **Condition**: **[None]**

NOTE For the **Category** setting, you must use the same value as in the **Repeat On** setting for the tables.

To use the variables:

1 Underneath the tables, add two text fields to the template:

- The first text field shows some static text and the compound name:

  ="Difference between average areas for" + Compound_Name

- The second text field shows the calculated value:

  =Avg(AreaAggregator1(Compound_Name)) - Avg(AreaAggregator2(Compound_Name))

2 Select the two fields and create a composite group.

3 Repeat the composite group on **Compound_Name**.

After a number of tables, the generated template will show the text fields for each single compound.

To create an Aggregator based on a condition

This examples describes how to sum up only those peak areas that are greater than a certain value. To sum up the areas per compound, a composite group is used that is repeated on **Compound_Name**.

1 Add the **Compound Results** table to the template.

2 Open the **Column Properties** dialog of the **Area** column, and save the value as a variable.

   a Under **Calculation Variables**, select **Aggregator**.

   b Under **Calculation Variable Name**, enter a name. For example, *AreaIf*.

   c Under **Condition**, double-click **Expression...**.

   d In the **Expression Editor**, enter the following expression: *=Peak_Area > 3*

   e Save your settings.

3 Underneath the table, add a text field that shows the sum of all areas that meet the condition. Use the following condition: *=Sum(AreaIf)*

4 Add another text field that contains the *Clear* function: *=Clear(AreaIf)*

5 Clear the **Visibility** check box for the text field with the *Clear* function.

6 Select the table and both text fields, and create a composite group.

7 Repeat the composite group on **Compound_Name**.

For each compound, the generated template will show a table with all injections, and a textbox with the sum of peak areas. The sum is based on all peak areas greater than 3.

To use a Custom Extractor

The following example describes how to access the diagnostic data provided by a ChemStation system.

To create a custom extractor:

1 Add a text field to the template.

2 Enter the expression **=Injection_DiagnosticData** as a value.

3 In the Expression Editor, click **Save Expression Result As...**.

The **Save Expression Result As** dialog opens.

4 Make sure that the **CustomExtractor** option is selected, and enter a **Calculation CustomExtractor Name**, for example *MyDiagnosticData*.

NOTE No special characters are allowed in the variable name.

5 Save your settings.

6 Set the text field to invisible.

To use a Custom Extractor

1 Add a text field to the template, and place it underneath the text field created before.

2 Enter the following expression to access the start pressure of an injection: *=MyDiagnosticData(GetValue("StartPressure"))*. You can also select the variable and the function in the Expression Editor in the lower panels.

NOTE In this example, you access the start pressure with the key *StartPressure*. See "Keys in Diagnostic Data" on page 173 or "To find out the available keys for a complex custom field" on page 141 for information on other available keys.

To find out the available keys for a complex custom field

If you are not sure which keys are available in a complex custom field, you can use the following procedure to view the entire XML structure. The keys are given as *Name* attributes of the *CustomField* tags.

1 Add the complex custom field (for example, the field **DiagnosticData** in the **Injection** category) to the template.

The **CustomExtractor Info** dialog opens and asks you for a key name.

2 Leave the input field empty and click **Cancel**.

RTE adds the field to the template. The label shows the name of the field (for example, **Injection_DiagnosticData**), and the value shows the XML content.

3 Adjust the width of the field to the template width.

4 Generate a report preview to see the entire XML content.

5 Find the *Name* attributes. The values of these attributes are the keys that you can use for this complex custom field.

For example: *Name="StartPressure"*

15
Report Template Audit Trail

About the Report Template Audit Trail

The Report Template Audit Trail provides a detailed list of all modifications of a template. The list includes the following information:

- **Template Version**: Each time you save the template, the template version increases by one.
- **User Name**: Name of the user who modified the template. The name is provided by the operating system.
- **Machine Name**: Name of the PC on which the template was modified.
- **Date Time**: Date and time when the template version was saved.
- **Audit Entry**: Description of the modification.

The modifications are written to the Report Template Audit Trail when you save the report template. Thus, the Report Template Audit Trail shows all changes up to the last saving date.

16
Report Parameters

About Report Parameters

With report parameters, you can make your report templates more dynamic. There are two basic types of parameters:

- *Interactive report parameters (default):*

  You need to provide these parameters each time before the report is generated. An additional report parameter pane is shown at the top of the report preview area, where you can enter the required values. When you click **View Report**, the report is generated using the given parameters.

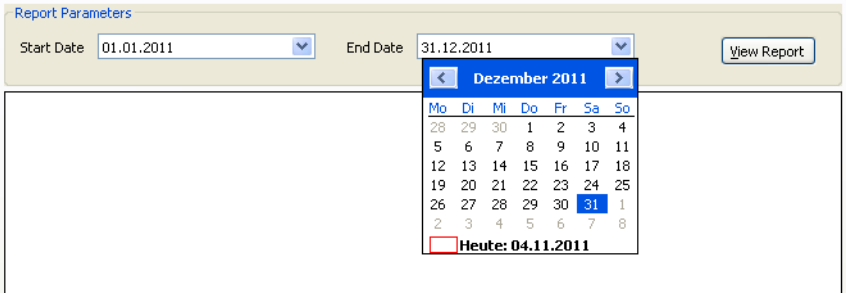


Figure 17 Report parameters example

  Interactive parameters can be, for example:

  - Start date
  - End date
  - Year
  - Compound name

- *Internal report parameters:*

  There is no input field for these parameters in the report preview. You set the parameter to a fixed value when you develop the template. You can then use this value in any expression in the entire template. The report is automatically generated using the given values.

  Examples for internal parameters are:

  - Correction factors that you use in several expressions
  - Amount values that you use in conditional formatting

Using Report Parameters

To create a single report parameter

This procedure explains how to create a simple report parameter with only one single value.

1 Click  to open the report properties.

2 In **Report Properties**, select the **Report Parameters** page.

3 Click **Add**.

A new parameter is created and added to the list.

4 Adjust the parameter name. For example, enter *Correction Factor*.

5 Adjust the data type. For example, select **Integer**

6 In the field **Prompt name**, provide a label for the report parameter. For example, enter *Correction Factor:*.

This text will be shown in the report parameter pane at the top of the preview area, where users provide the required values for the report parameters.

7 If required, select the **Internal** check box.

- To create an *interactive* report parameter: Ensure that the check box is *cleared*.

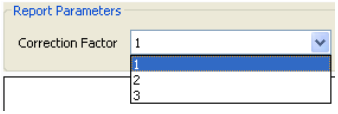
  When you preview the report, you will have to provide a value before you can generate the report.

- To create an *internal* report parameter: *Select* the check box.

  For internal report parameters, no input field will be shown in the report preview. The report is automatically generated using the default value.

8 Optional: Provide several labels and values under **Available Values**. To simplify matters, use the same entries for **Label** and **Value**.

If you provide several available values, their labels will be shown as a drop-down list where only one single value can be selected.



9 Provide a default value for the report parameter.

For interactive report parameters, the default parameter will be shown as a suggested value in the report preview. For internal report parameters, and also if the template is used in the context of an automated sequence run, the system will automatically access this default value.

To create a multi-value report parameter

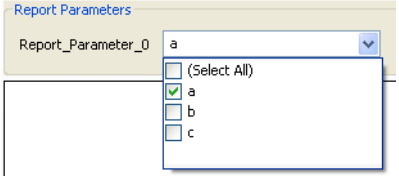
1 Create a new report parameter, and provide the information for **Parameter name**, **Data type** and **Prompt name**.

2 Under **Available Values**, enter the values that you want to offer to the user.

The labels will be shown in the user interface, the values will be used by the report when you calculate with the report parameter.

3 Select the **Multi-Value** check box.

The available values will be shown as list of check boxes in the report preview.



4 Enter one or more default values.

The default value must correspond to one of the available values. You can provide multiple default values. In this case, multiple check boxes will be selected by default.

To calculate with a report parameter

Single-value report parameter

For example, your report contains a table with peak results. You want to offer the possibility to multiply the results by correction factor.

In the **Report Parameters** dialog, you create a report parameter named *CorrectionFactor* with the data type **Integer** and the default value *1*.

In the table, you enter the following expression in the **Value** field for the column:

*=Compound_Amount * CorrectionFactor*

This syntax is valid as long as the **Multi-Value** check box is cleared. Even if you enter several values under **Available Values**, the user can only select one of these values, and the expression is unambiguous.

Multi-Value report parameter

If you have selected the **Multi-Value** check box, all selected values will be stored in a collection. Therefore, you must add an index to the parameter name to refer to a specific value.

- *=Report_Parameter(0)* to refer to the *first selected* value
- *=Report_Parameter(1)* to refer to the *second selected* value
- ... etc.

To filter for a multi-value report parameter

If you use multi-value report parameters, you may want to filter for multiple values at the same time. For example, you have create the report parameter *STypes* for sample types, and provide the following available values:

Label	Value
Calibration	1
Sample	3
Control	4

If the user selects multiple values, you want to show a table for all selected values. To achieve this, you can use the following filter expression for the table:

Expression	Operation	Value
=Join(STypes, " ").Contains(Sample_Type)	=	true

The *Join* function returns a string, created by concatenating the elements of an array.In this example, the array is the multi-value report parameter *STypes*. The second parameter of the Join function (in this example, a space " ") is the delimiter to be used when creating the string.

The *Contains* function returns *true*, if the preceding string contains the characters given as a parameter to the Contains function.

17
Document Map

About Document Map

The document map offers you a list of bookmarks in the report preview. With these bookmarks, you can easily jump to the page in the report that contains the corresponding information. For example, the report contains a sequence with 20 samples. Each sample has been injected several times, and for each injection there is a results table. With the bookmarks in the document map, you can directly jump to each specific injection.

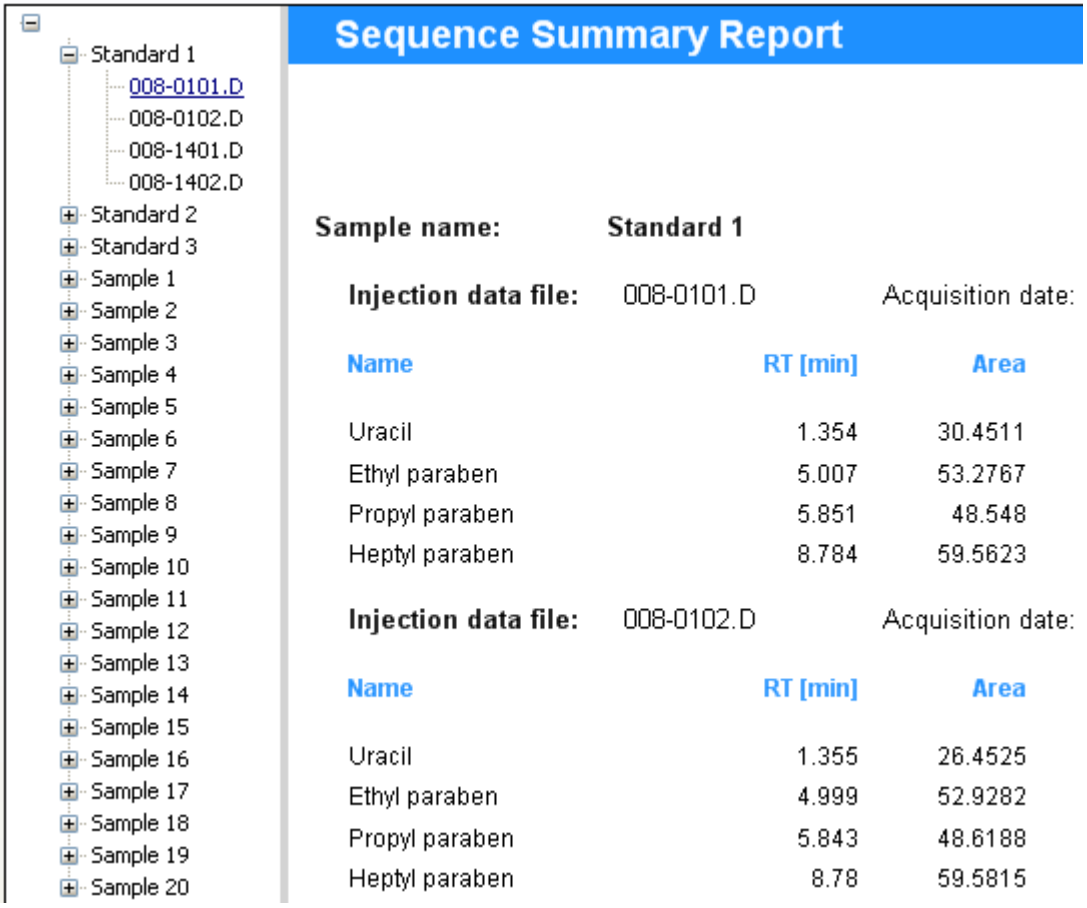


Figure 18 Example of a report preview with document map

You can create bookmarks for repeated tables or matrices: With these report items, the document map expression is always the same as the repeat-on expression.

In addition, you can specify bookmarks for other report items, such as text fields or data fields, inside a repeated composite group. In most cases the bookmark will reflect the value that you used to repeat the composite group. However, you can also customize this expression according to your requirements.

When you export a report to PDF that contains a document map, the bookmarks will be available in PDF as well.

Using Document Map

This example describes a sequence with several samples. Each sample has been injected several times. The document map shows a bookmark for each injection.

1. Create a new **Single Sequence Summary** template.
2. Add the following report items to your template and place them under each other:
   a. The **Sample_Name** data field
   b. The **Injection_DataFileName** data field
   c. The **Compound Results** table
3. Select the **Compound Results** table and the **Injection_DataFileName** field, and click  to create a composite group containing these two items.
4. Repeat the group on *=Injection_ID*.
5. Select the composite group and the **Sample_Name** data field, and click  to create another, superordinate composite group.
6. Repeat the superordinate composite group on *=Sample_Name*.
7. Set the document map expression for the **Sample_Name** data field to *=Sample_Name*.
8. Set the document map expression for the **Injection_DataFileName** field to *=Injection_DataFileName*.
9. In the report preview, click on the Plus icon  to expand the document map.

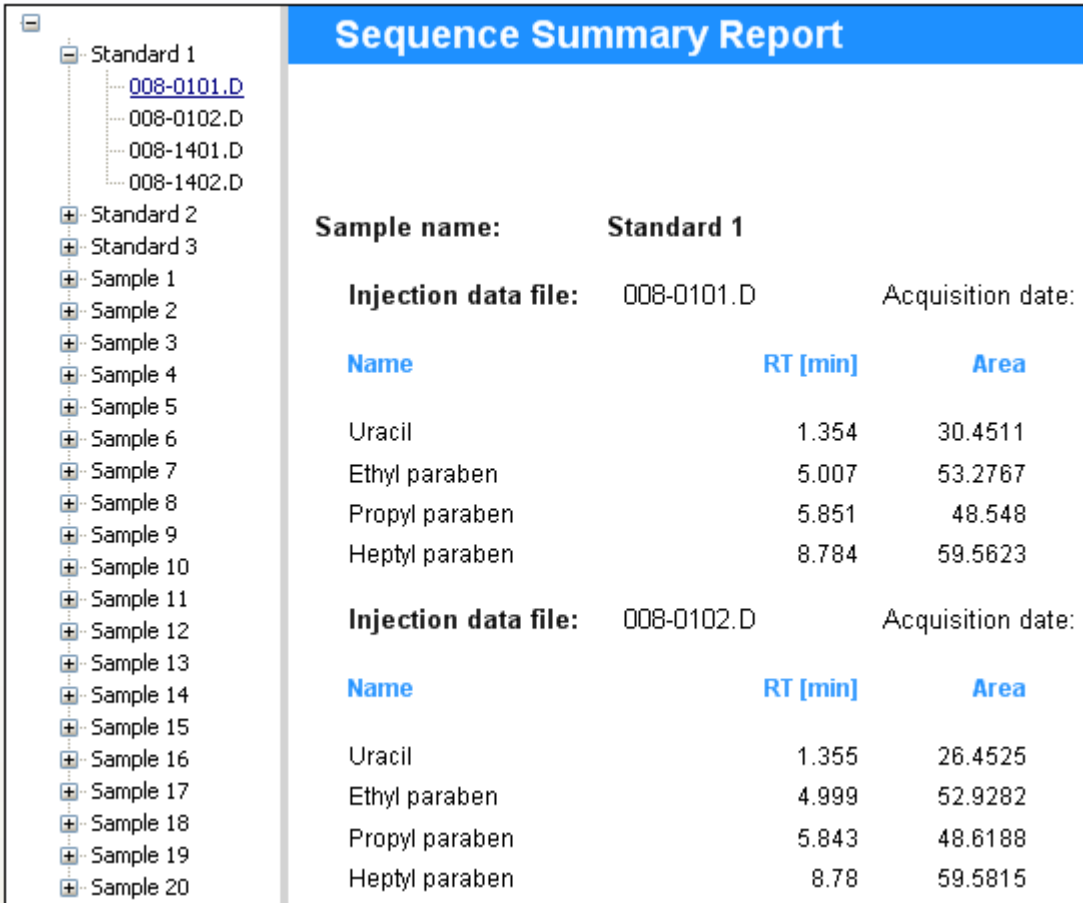


Figure 19 Example of a report preview with document map

18
Locked/Unlocked Report Items

About locked/unlocked report items

NOTE You can only lock or unlock items if you have the **Lock/unlock report item** privilege in Agilent OpenLAB Shared Services.

You can lock either single report items or composite groups containing multiple report items. A locked item is protected against any modification.

What is possible with a locked item:

- View properties.
- Move the item inside the template.

What is impossible with a locked item:

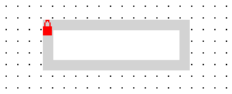
- Modify properties.
- Remove the item from the template.

For example, you can lock a composite group containing complex calculations that have been validated and approved. With the lock, you make sure that the items are not changed by accident.

To lock or unlock report items

1 Select the report item.

If the item is locked, a small red lock icon is shown in the top left corner of the selection border.



2 To unlock a locked item: Right-click the item and select **Unlock** from the context menu. Alternatively, you can click the **Unlock Report Item** icon in the toolbar: .

3 To lock an item: Right-click the item and select **Lock** from the context menu.

Alternatively, you can click the **Lock Report Item** icon in the toolbar:

NOTE The **Lock** and **Unlock** commands are only available if you have the required privilege in Agilent OpenLAB Shared Services.

18 Locked/Unlocked Report Items

To lock or unlock report items

19 Appendix

This chapter contains a list of all operators and functions available in the Expression Editor.

Enumerations

Some data fields contain specific numbers that stand for certain values. These so-called enumerations typically represent all data that is shown in a drop-down list in your chromatography data system.

Display enumerations

If you display these data fields in a data field, table column or matrix column, the RTE automatically selects the text value that corresponds to the stored number.

Filter for enumerations

If you want to filter for a specific value of an enumeration, you must enter the correct number in the **Value** field. The following sections you find the text list values and corresponding numbers of all enumerations.

BaselineModel enumeration

Number	Description
0	Unknown
1	Linear
2	Exponential
3	ExtendedExponential

BracketingMode enumeration

Number	Description
0	None
1	Standard
2	StandardClearCalibration
3	StandardOverlap
4	OverallSequence
5	SequenceBackCalculation

BracketingType enumeration

Number	Description
0	Undefined
1	Open
2	Close
3	Intermediate

CalibPeakRole enumeration

Number	Description
0	None
1	Main
2	Qualifier
3	Ignore
4	NewMain

Number	Description
5	NewIgnore
6	DetectorMain

CalibrationCurveOrigin enumeration

Number	Description
0	Undefined
1	Include
2	Force
3	Connect

CalibrationCurveType enumeration

Number	Description
0	Undefined
1	Linear
2	Quadratic
3	Cubic
4	Exponential
5	Logarithmic
6	Power
7	AverageRF
8	Piecewise
9	Custom

CompoundQuantitationType enumeration

Number	Description
0	Undefined
1	Area
2	Height
3	Count

CompoundType enumeration

Number	Description
0	Unknown
1	Expected
2	UncalibratedExpected
3	PeakSum
4	Group
5	NotIdentifiedExpected

InjectionSource enumeration

Number	Description
0	Undefined
1	StandardInjection
2	NoInjection
3	ManualInjection
4	InjectorProgram

InjectorPosition enumeration

Number	Description
0	Undefined
1	Front
2	Back

InstrumentTechnique enumeration

Number	Description
0	Undefined
1	LiquidChromatography
2	GasChromatography
3	MassSpectrometry
4	CapillaryElectrophoresis
5	UVVis
6	MicroFluidics

PackagingMode enumeration

Number	Description
0	Undefined
1	Classic
2	FullResultSet
3	ResultSetWithTemplates
4	ResultSetWithMethods
5	SimpleResultSet

PeakType enumeration

Number	Description
0	Unknown
1	Tangent
2	Solvent
3	AreaSum
4	FrontShoulderDropLine
5	FrontShoulderTangent
6	Manual
7	ManualNegative
8	ManualNegativeShoulderDropLine
9	ManualNegativeShoulderTangent
10	ManualShoulderDropLine
11	ManualShoulderTangent
12	ManualTangentSkimExpo
13	ManualTangentSkimNewExpo
14	ManualTangentSkimNormal
15	Negative
16	NegativeShoulderDropLine
17	NegativeShoulderTangent
18	NormalPeak
19	RearShoulderDropLine
20	RearShoulderTangent
21	ReCalcSolventPeak
22	ShoulderDropLine
23	ShoulderTangent
24	TangentSkimExpo

Number	Description
25	TangentSkimNewExpo
26	TangentSkimNormal

QuantificationMethod enumeration

Name	Description
0	Undefined
1	Area%
2	ESTD
3	ESTD%
4	Height%
5	ISTD
6	ISTD%
7	Norm%

ResponseFactorCalcMode enumeration

Number	Description
0	Undefined
1	AmountPerResponse
2	ResponsePerAmount

ResponseFactorUpdate enumeration

Number	Description
0	Undefined
1	NoUpdate
2	Replace
3	Average
4	Bracketing
5	DeltaPercent

RetentionTimeUpdate enumeration

Number	Description
0	Undefined
1	NoUpdate
2	Replace
3	Average
4	Bracketing

RunType enumeration

Number	Description
0	Undefined
1	ClearAllCalibration
2	ClearCalibrationAtLevel
3	PrintCalibrationReport
4	AverageReplicates

Number	Description
5	ClearReplicates
6	BeginLoop
7	EndLoop
8	Shutdown
9	PrintAdditionalReports
10	BeginSystemSuitability
11	SystemSuitablityStandard
12	EndSystemSuitability
13	BeginSummary
14	SummaryRun
15	EndSummary
16	VialSummary
17	QCCheckStandard
18	Unspiked
19	Spiked
20	Spike1Of2
21	Spike2Of2
22	Duplicate
23	BeginCalibration
24	EndCalibration
25	BaselineCheck
26	BaselineFile

SampleContextIntegrity enumeration

Number	Description
0	Undefined
1	Complete
2	Partial

SampleContextSource enumeration

Number	Description
0	Undefined
1	Acquisition
2	Reprocessed
3	Virtual

SampleContextType enumeration

Number	Description
0	Undefined
1	SingleSample
2	Sequence

SampleType enumeration

Number	Description
0	Unspecified
1	Calibration
2	Checkout
3	Sample
4	Control
5	Blank
6	Ladder
7	SystemSuitability

SeparationMediumPosition enumeration

Number	Description
0	Unknown
1	Front
2	Left
3	Rear
4	Right

Keys in Diagnostic Data

Keys in the Injection_DiagnosticData field

The keys used in the **Injection_DiagnosticData** field depend on the generator that created the data. They may include Early Maintenance Feedback (EMF) counters such as the number of hours of the detector lamp.

The following table shows the most common keys according to the generator used.

NOTE If you are not sure about the correct keys, see "To find out the available keys for a complex custom field" on page 141.

ChemStation	ChemStore
DAD1UVOnTime	n/a
DAD1UVBurnTime	n/a
DADVisOnTime	n/a
DAD1VisBurnTime	n/a
StartPressure	BegPumpPres
StopPressure	EndPumpPres
StartFlow	BegPumpFlow
StopFlow	EndPumpFlow
PumpType	n/a
StartLeftTemp	BegLTemp
StopLeftTemp	EndLTemp
StartRightTemp	BegRTemp
StopRightTemp	EndRTemp
AirTemp	n/a

ChemStation	ChemStore
InjVolume	n/a
ActInjVolume	n/a
InjVolumeText	n/a
ActInjVolumeText	n/a

Index

E

F

H

I

K

L

M

N

P

Q

R

S

T

U

V

W

X

Y

In This Book

This guide contains information for template developers. It describes the concepts and advanced features of the Report Template Editor (RTE).

19 Appendix

In This Book

www.agilent.com

Printed in Germany
01/2013

G4635-90014

Agilent Technologies