

Compound Discoverer 3.5 Reporting Quick Start Guide

The Reporting Quick Start Guide provides instructions on how to perform reporting tasks using the Thermo Scientific™ Compound Discoverer™ software. See the following topics for details on how to perform the tasks for reporting:

- [Open a result file and select the data for the report.](#)
- [Generate a report.](#)
- [Edit a Report Template](#)
- [Preview a Resolved Report](#)
- [Export or Print a Report](#)

NOTE: These tasks can be performed even without an active software license for Compound Discoverer application.

Open a result file and select the data for the report

The Compound Discoverer application enables you to open a result file and select the data as per study requirement. You can also review, filter, and sort the data that you want to include in a report. For more information about filtering and sorting the data, refer to the Compound Discoverer tutorials, the Help.

Procedure

1. Do any one of the following to open a result file:
 - From the Compound Discoverer menu bar select **File > Open Result**.
 - On the Start Page, select the result file name in blue hypertext. If the Start Page is closed, select **View > Start Page** from the Compound Discoverer menu bar.
 - On the Job Queue page, double-click a completed run.
 - On the Analysis Results page of a study, double-click a completed run or select a completed run and then, select **Open Result** in the Analysis Results command bar. The reporting menu commands and the reporting toolbar icons become available. See [Reporting menu commands](#).
2. Select the main table of interest and apply the appropriate filters, as the report only uses the rows displayed.

NOTE: The report only uses the rows displayed.

3. Select **View > Result Filters** view to reduce the number of rows (or compounds) for the report.

IMPORTANT: The compounds tables can contain thousands of rows. Because report generation is limited to 2,000 pages, and for practical reasons, reduce the number of rows to only the rows of interest by applying the appropriate filters.

4. Save the result file to keep the sort order and filter settings.

Reporting menu commands

The following table describes the reporting menu commands.



Create a report document from the active result file.



Create a new report template.



Edit an existing report template.

Generate a report

You can do either of the following to generate reports that display the items of interest in a result file:

- Use any one of the 14 reporting templates (.CDReportTemplate) available in the application by default. See [Preview and print a report from an existing report template](#).
 - Compounds No Graphs A4
 - Compounds with Graphs A4
 - Compounds with Graphs and mzCloud Mirror Plot A4
 - Expected Compounds No Graphs A4
 - Expected Compounds with Graphs A4
 - Expected Compounds per File No Graphs A4
 - Expected Compounds per File with Graphs A4
 - Expected Compounds with Structures No Graphs A4
 - Expected Compounds with Structures with Graphs A4
 - GC-EI Compounds with Structure
 - GC-EI Compounds with Structure, Chrom and Spectra
 - GC PCI Compounds Structures 3 Graphs Predicted Comp Rel Page Break
 - GC PCI Compounds with Structure, Chrom and MS1 and MS2 Spectra
 - GC PCI Compounds with Structure
- You can create one of your own custom report templates. See [Create a New Report Template](#).

Preview and print a report from an existing report template

You can preview and print a report by opening an existing report template.

Procedure

1. [Open a result file and select the data for the report](#).

2. Do any one of the following to select an existing report template:

- Select **Reporting > Create Report** from the menu bar.
- Select the **Create Report** .

The Open Report Design Template dialog box opens to the Report Templates folder.

NOTE: To select an appropriate report template, you must know what data the report template is designed to resolve. Typically, a report template resolves the filtered data from one of the main tables and one or more of the graphs associated with the table. A report template can also resolve data from one or more related tables.

3. Select the appropriate report template and select **Open**.

The report resolution page opens with the thumbnail pane on the left and a report preview on the right.

The tab format for the report resolution page is as follows:

 *Report Template Name*


As the application resolves the data with the report template, you see a progress icon.



When the data is resolved, the progress icon disappears, and the application begins rendering the report pages. The current page/estimated pages box lists the progress. If the template contains ReportInfo items, the application does not display the rendered pages until it has rendered all of the report pages.

4. Review the contents of the report.

- If the report still contains too many pages, consider applying one or more additional filters to the main table and any reported related tables.
- If a red line appears in the right page margin, check the report's print width. See [Change the print width, paper size, or page orientation](#).

5. On the report resolution page, select **Print**  in the toolbar to print the report. The Print dialog box opens.

6. Select the appropriate printer and the page range that you want to print.

IMPORTANT: The report templates that come with the application print on A4 paper. If you are not printing on A4 paper, change the printer setting to avoid printing errors.

7. As appropriate, change the paper type for your printer.

8. Select **OK** to print the report.

Create a New Report Template

A report template contains the layout for the data items that you want to extract from a result file. A report can contain the data in a selected main table and its related tables and graphical results that are associated with the main table and related tables.

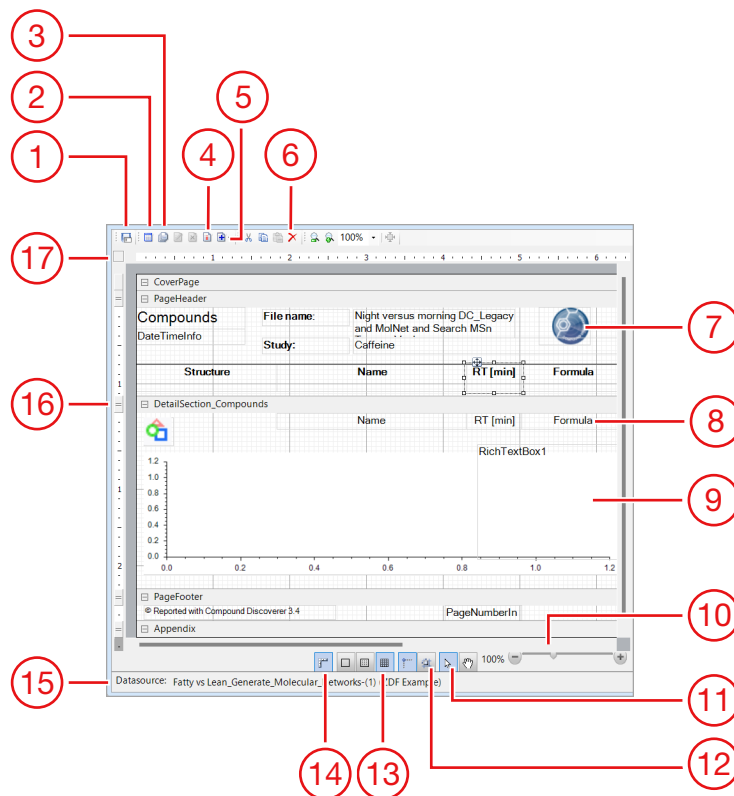
Procedure

1. Open a result file.
2. From the application menu bar, select **Reporting > Create Report Template**.
The Customize Report dialog box opens with the name of the current table displayed in the Reported Table list.
3. To create a report for a different table, select the table in the list.
4. Do the following to select the information that you want to include in the report:
 - Under Columns, select the checkboxes for the columns that you want to include in the report. Clear the check boxes for the columns that you do not want to include.
 - Under Graphs, select the checkboxes for the graphs that you want to include in the report.
 - Under Related Tables, select the checkboxes for the related tables and the columns in these tables that you want to include in the report.
5. Do the following to customize the report:
 - To draw a separator line above the column headers for the main table and the selected related tables, make sure that the Draw Lines checkbox is selected (Default: Draw Lines).
 - To indent a related table, select the checkbox for the related table in the data item list, select the table name to highlight it in blue, and enter a value in the Indenting box.
 - To transform a table's columns from a horizontal layout to a vertical layout, select the table in the data item list, and then select the **Transpose Data** checkbox.


TIP: For each table that you want to transpose, select the table name to highlight it in blue, and then select the **Transpose Data** checkbox.

6. To apply a color scheme to a table, select the table listing, and then select a color scheme from the Color scheme list.
7. Do the following in the General settings area:
 - To modify the paper size, type the first letter of the paper size in the Paper Kind list or make a selection from the list. For example, when you type L, the application selects Letter.
 - To modify the orientation, select **Portrait** or **Landscape** from the Orientation list.
 - To add a custom logo, select the browse button to the right of the Logo Image and browse to the image file of interest.
8. Select **OK** to apply the settings.
The report designer page opens.

Figure 1 Report designer page



No.	Description	No.	Description
1	Save As	10	Zoom
2	Preview Report	11	Selection Mode
3	Print Preview	12	Snap to Grid
4	Align Columns	13	Show Lines
5	Add Items	14	Dimension Lines
6	Delete	15	Result file's folder location and file name
7	Logo image	16	Sizing bar with section handles
8	Textbox with object name selected	17	Report Properties
9	Image container for selected graph		

9. Select **Preview Report**  to preview the report.
The Report Preview dialog box opens.
10. Do any one of the following:
 - To continue editing the template, close the Report Preview dialog box and follow the instructions in [Change the logo image](#).
 - To save the report template, see [Save the report template with a different name](#).
 - To export or print the report, see [Export or Print a Report](#).

Edit a Report Template


The report designer page shows the items that you selected in the Customize Report dialog box or the items in the selected report template. Some of the items appear in a container where you can add text, images, or data graphs.

Follow these procedures as needed:

- [Open an existing report template](#)
- [Change the logo image](#)
- [Change the date-and-time stamp format](#)
- [Add a data graph for a main table](#)
- [Add an mzCloud mirror plot](#)
- [Edit an item by using the mouse and keyboard](#)
- [Modify the properties of an item](#)
- [Align a column heading to its associated data field](#)
- [Transpose the data fields from columns to rows or from rows to columns](#)
- [Resize a workspace section vertically](#)
- [Add a non-data item](#)
- [Add a page break between the compounds in the main result table](#)
- [Add a column from a related table to the template](#)
- [Edit the properties of subreport columns](#)
- [Move a subreport column up to the set of main table columns](#)
- [Modify the cover page section](#)
- [Change the print width, paper size, or page orientation](#)
- [Save the report template with a different name](#)

Open an existing report template

Procedure

1. Do any one of the following:
 - Select **Reporting > Edit Report Template** from the menu bar.
 - Select the **Edit Report Template**  icon in the Toolbar.

The Open Report Design Template dialog box opens to the Report Templates folder.

2. Select a report template and select **Open**.

The report designer page opens as a tabbed document. The tab format is as follows:

 *Existing Report Template Name.*

Change the logo image

Procedure

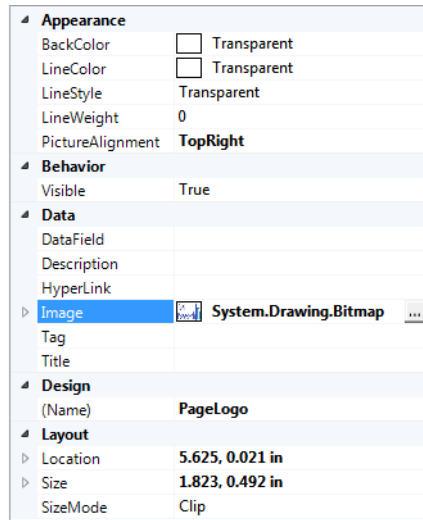
1. Select the logo image (picture container).


Figure 2 Selected picture container showing the container's handle points



The picture properties appear in the properties pane.

Figure 3 Picture properties



2. In the Data area, select **Browse**  to the right of the Image property. You might have to select the row to make the browse icon appear.

The Open dialog box opens with a setting of All image files for the file type.


3. Browse to the folder where you stored the logo of interest, select the logo, and select **Open**.

The selected image appears in the container.

4. Modify the Layout properties as appropriate.

Change the date-and-time stamp format

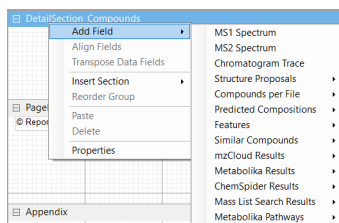
Procedure


1. In the PageHeader section, select the **DateTimeInfo** text box item.
The text box properties appear in the Properties pane.
2. In the **OutPutFormat** text box, select browse  icon.
The OutPutFormat dialog box opens.
3. Select an appropriate data-and-time stamp and select **OK**.

Add a data graph for a main table

Procedure

1. Do any one of the following:
 - Right-click the *DetailSection_Main_Table_Name* bar and then select **Add Field > Data Graph**.




- Select the `DetailSection_Main_Table_Name` bar.
- In the toolbar, select **Add Items**  to open a list of data graphs and related table selections.
 - Select an available data graph from the list.
The items in the Add Items list or Add Field menu include the data graphs and related tables for the current main table.

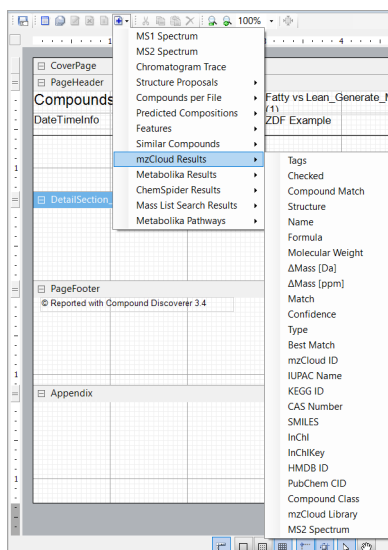
NOTE: When the table columns are positioned from left to right, the data graph appears below the table columns and to the right of any existing data graphs.

Add an mzCloud mirror plot

You can add an mzCloud mirror plot to a Compounds table, GC CI Compounds table, or GC EI Compounds table.

Procedure

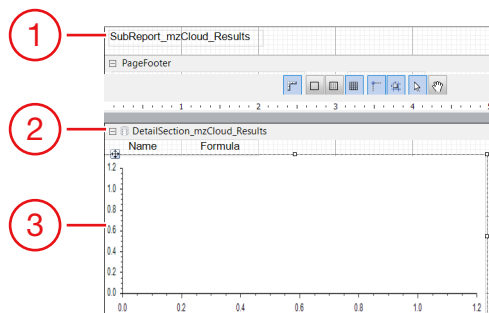
- Add a sub report for the mzCloud results table to the details section as follows:
 - Select the `DetailSection_Main_Table_Name` bar.
 - In the toolbar, select the **Add Items**  and select **mzCloud Results > Name** (or any table columns that you want to report).



The `SubReport_mzCloud_Results` report appears in the `DetailSection` area.

- Double-click **SubReport_mzCloud_Results**.
The `DetailSection_mzCloud_Results` area appears below the bottom toolbar.

- Right-click DetailSection_mzCloud_Results and select **Add Field > MS2 Spectrum**. The MS Spectrum data field appears in the detail section for the related mzCloud Results table.



No.	Description	No.	Description
1	Sub Report	3	MS2 Spectrum added
2	Details section for the mzCloud Results		

Edit an item by using the mouse and keyboard

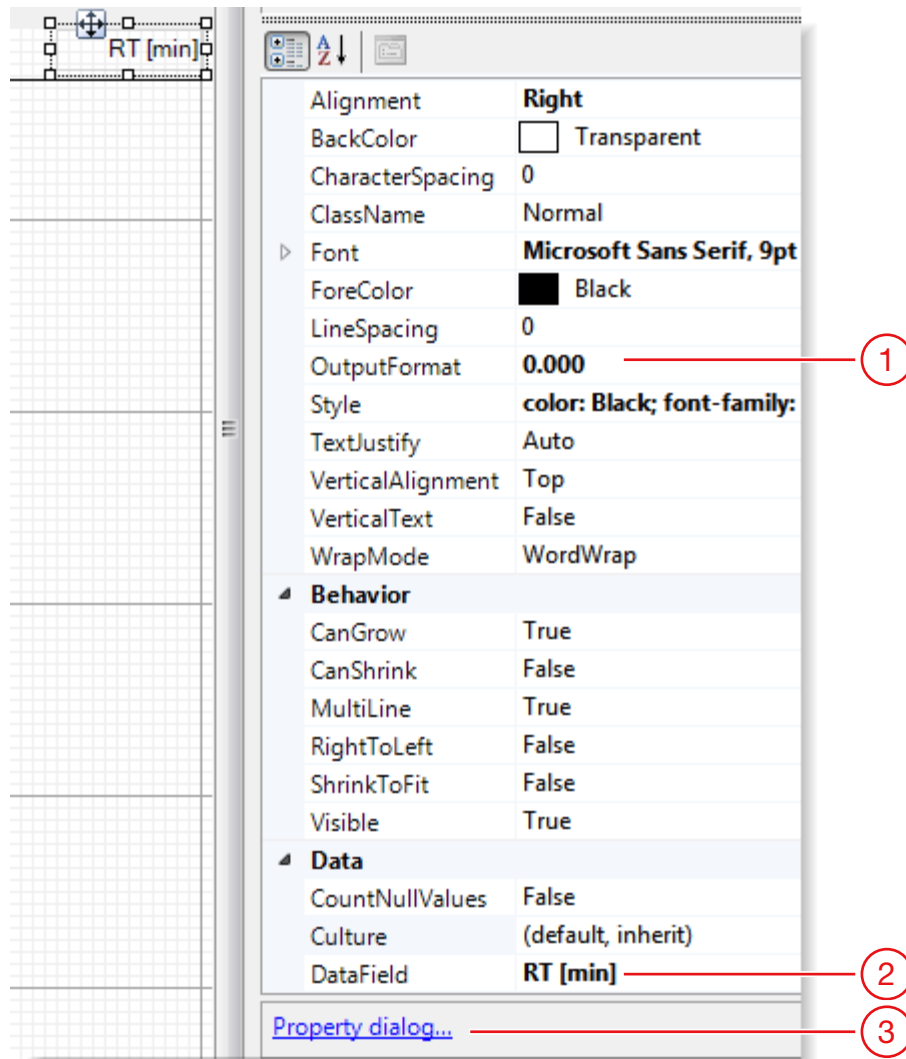
Procedure

- Select the item on the report designer page, and then modify the item as follows:
 - Move the item by dragging it to a different location or by using the arrow keys on the keyboard.
 - Resize the item by dragging the container's handle points.

Modify the properties of an item

Procedure

- Select the item on the report designer page. The properties for the selected item appear in the properties pane, at the bottom right of the report designer page. The figure below shows the properties pane for the RT [min] data field.

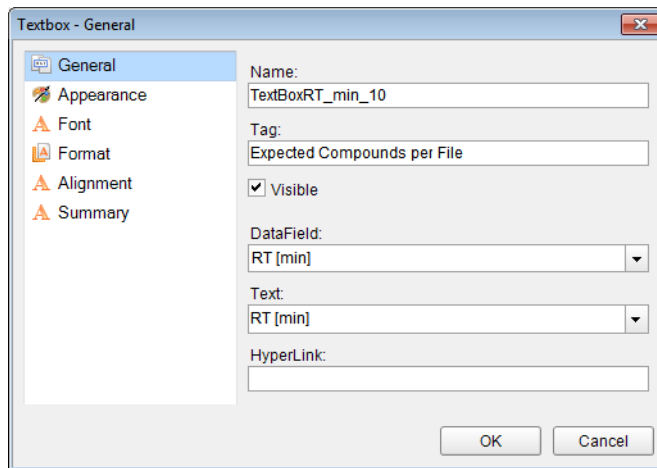


No.	Description	No.	Description
1	Number of decimal places	3	Property Dialog link
2	Data field set (RT selected)		

2. Do any one of the following:

- In the properties pane, modify the properties of interest, including the size and location of the selected item and the number of decimal places for a numeric data field.
- Double-click the Property Dialog link to open a dialog box where you can modify the properties.

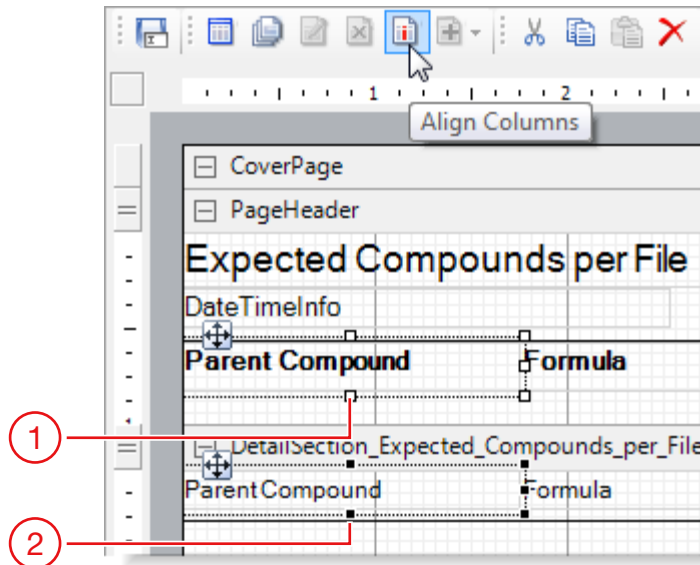
Align a column heading to its associated data field




Procedure

1. In the Page Header section, select the column heading that you want to align with its associated data field in the Detail Section.

The Align Columns icon becomes available.



No.	Description	No.	Description
1	Column header (Label item) in the Page Header section	2	Data field (TextBox item) in the DetailSection

2. In the report designer page toolbar, select **Align Columns**  .

Procedure

1. Right-click a column heading (Label) or a column data field (TextBox) and select **Transpose Data Fields**.
2. To undo the change, if necessary, right-click a column heading (Label) or a column data field (TextBox) and select **Transpose Data Fields**.

Transpose the data fields from columns to rows or from rows to columns

Resize a workspace section vertically

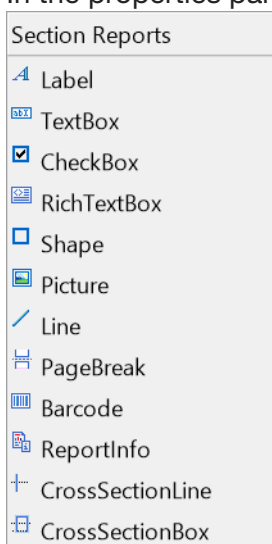
Procedure

1. Do any of the following:
 - To enlarge a workspace section, in the sizing bar drag down the handle that is aligned with the header of the subsequent section.
 - To reduce a section, drag the handle up.
 - To enlarge the Appendix section, drag it down by its bottom edge.
 - To reduce this workspace section, drag the bottom edge up.

Add a non-data item

Procedure

1. In the Section Reports pane to the right of the workspace area, select an item and drag it to the appropriate location in a workspace section; for example, add **PageBreak** to break the section to the next page.
2. In the properties pane, edit the properties of the item to add a non-data item.




Add a page break between the compounds in the main result table

Drag the PageBreak item from the Section Reports pane to the bottom of the Detail Section of the report template to add a page break between the compounds in the main result table.

No.	Description	No.	Description
1	Page break in the Detail Section	2	Page break properties

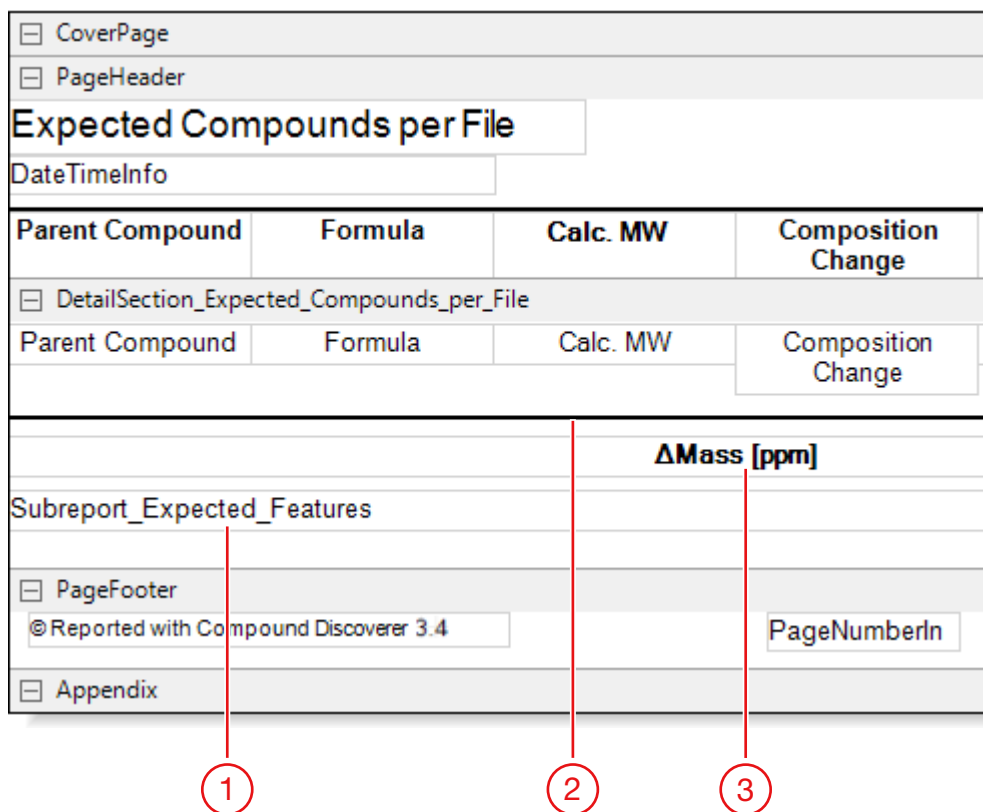
Add a column from a related table to the template

Procedure

1. Select the *DetailSection_Main_Table_Name* bar.
2. In the report designer toolbar, select **Add Items**  to open a list of data graphs and related table selections.

The available items in the list include the data graphs associated with the current main table and the related tables for the current main table.

3. Select an available related table from the list, and then select a table column.
 4. If the Detail Section is collapsed, select the expand icon to open the section.
- The added table column appears at the bottom of the Detail Section (data area). The application automatically adds a line above the column heading.



No.	Description	No.	Description
1	Subreport container	3	Column heading for the related table column
2	Line above the related table column		

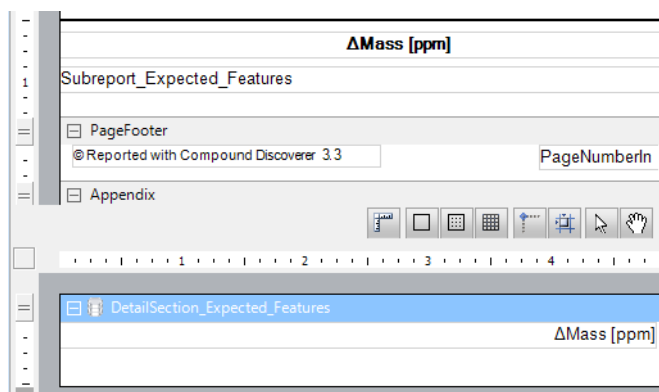
Edit the properties of subreport columns

Procedure

1. Double-click the *Subreport_Related_Table_Name* container to open the subreport editor area.
The TextBox item for the related table column appears in a separate section. The container for the item is sized to the full page width.
2. To change the properties of the TextBox item in the Detail Section for the subreport, select the item.
The properties for the selected item appear in the properties pane to the right of the workspace.
3. Make changes as necessary in the properties pane or double-click the Property Dialog link below the properties pane to open the TextBox dialog box where you can make similar changes.

- To close the subreport section, select the **Close Sub-Report** icon in the report designer toolbar.

Figure 4 Detail Section for the items in the subreport with the container for the Δ Mass [ppm] data item sized to the full page width

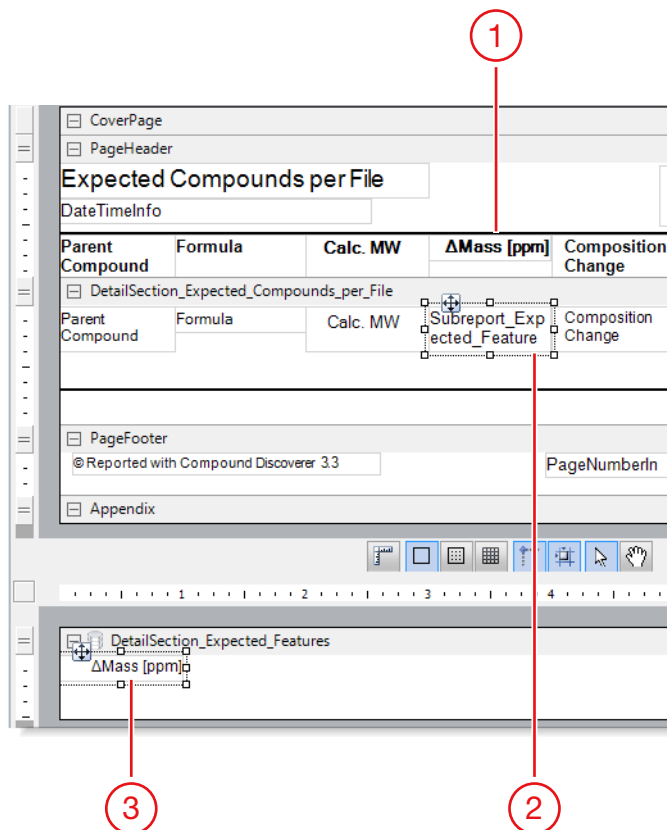


Move a subreport column up to the set of main table columns

Procedure

- Resize the column heading container for the subreport column. Then, move it to an appropriate location in the set of main table columns.
- Resize the *Subreport_Related_Table_Name* container. Then, move it to the appropriate location in the DetailSection.
- In the related table's Detail Section, resize the container for the data item. The figure below shows a report template for the Expected Compounds per File table with an additional column from the related Expected Features table.

Figure 5 Column from a related table added to the reported columns

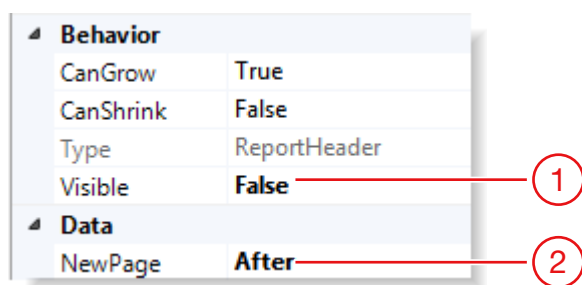


No.	Description	No.	Description
1	Column heading for the related table column	3	Detail Section for the related table column with a resized container for the data item
2	Subreport container moved to the main table's Detail Section		


Modify the cover page section

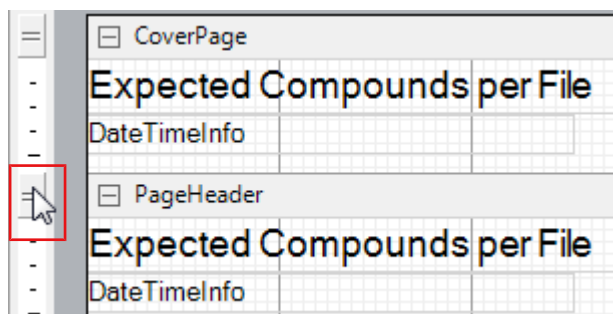
Procedure

1. In the report template designer, select the **Cover Page** section. The properties for the Cover Page section appear in the properties pane. By default, the Visible property is set to False.



No.	Description	No.	Description
1	To make the cover page visible, select True.	2	To remove the page break, select None.

- Under Behavior, select **True** for Visible property.
- To preview the report, select **Preview Report** .
- By default, the cover page appears as the first page of the report.
- (Optional) Under Data, select **None** for NewPage to remove the page break between the cover page and the report items.
- To add more information to the cover page, expand the Cover Page section by dragging down the sizing bar handle (to the left of the Page Header section).



- To add non-data text or images to the cover page, select an item in the Section Reports area and drag it to the cover page section.

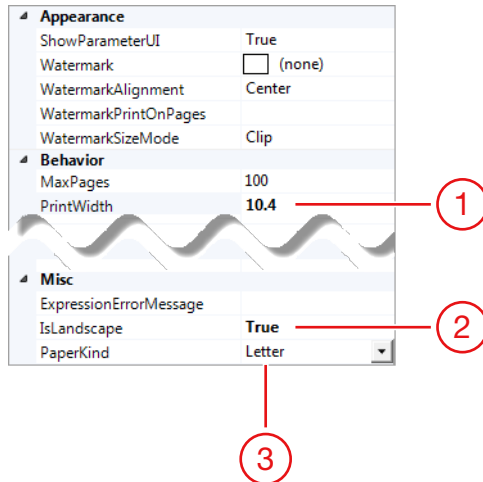
IMPORTANT: To add a text description, such as an explanation about the purpose of the report, use the RichTextBox item. Do not use the TextBox item on the cover page.

Change the print width, paper size, or page orientation

Procedure

- Select the Report Properties icon (square in the upper left corner, below the toolbar). The report properties appear in the properties pane.

Figure 6 Report properties




No.	Description	No.	Description
1	For landscape orientation, 10.4 inches is too wide for letter-size paper.	3	Select the appropriate paper size for the printer.
2	Select True for landscape. Select False for potrait.		

- To change the print width, type an appropriate numeric value for the PrintWidth parameter.
- To change the page orientation, under Misc, in the IsLandscape list, select **True** for Landscape or **False** for Portrait.
- To change the paper size for the printer, under Misc, in the PaperKind list, select the appropriate paper size.
- To open the list to the paper size of interest, type the first letter or first few letters of the paper-size name; for example, type **L** for Letter.

Save the report template with a different name



Procedure

- In the report designer toolbar, select the **Save As** . The Save Report Template As dialog box opens.
- Select a directory folder where you want to store the report template and name the report template.
- Select **Save**.

Preview a Resolved Report

You can preview a completely resolved report on the report resolution page (see [Generate a report](#)) or in the Report Print dialog box. You can preview up to five resolved pages in the Report Preview dialog box. A red line in the right page margin indicates that the print width is too large for the selected paper size.

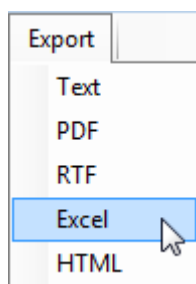
Procedure


1. Do the following to preview the report in the Report Preview dialog box:
 - a. In the toolbar on the report designer page, select **Preview Report** .
The Report Preview dialog box opens, resolves the current result file with the current template, and displays up to five pages.
2. Do the following to preview the report in the Report Print dialog box:
 - a. In the report designer toolbar, select **Print Report** .
The Report Preview dialog box opens and resolves the current result file with the current template. The page thumbnails pane displays all of the report pages, and the current page box provides a page count estimate.

You can export or print a report either from the Report Print dialog box or the Report Resolution page.

Procedure

1. Do the following to export a report to a file:
 - a. In the toolbar, select **Export** and select a file type from the dropdown list.
The Save As dialog box opens.



2. Select a directory folder, type a name in the file name box, and then select **Save**.
3. Do the following to print a report:
 - a. In the toolbar, select **Print**  to open the Print dialog box.
 - b. Select a printer and the page range that you want to print.
 - c. Select **OK** to print the report.

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**Revision
history**

Pub. No	Revision	Date	Description	Software version
B51007956	A	October 2025	Initial release	CD 3.5