Compound Discoverer 3.1 Reporting Quick Start

This quick start guide shows you how to open a result file, create a new report template, modify an existing report template, and print a report. You can perform these tasks without an active Thermo Compound Discoverer™ software license.

Contents

Selecting the Data

To select the data that you want to include in a report, open a result file. Review, filter, and sort the data. Save the result file to keep the sort order. For more information about filtering and sorting the data, refer to the Compound Discoverer tutorials, the *Compound Discoverer User Guide*, or the Help.

❖ To open a result file

Do one of the following:

- From the Compound Discoverer menu bar, choose **File > Open Result**.
- On the Start Page, click the result file name in blue hypertext. If the Start Page is closed, choose **View > Start Page** from the Compound Discoverer menu bar.
- On the Job Queue page, double-click a completed run.

–or–

- On the Analysis Results page of a study, double-click a completed run or select a completed run and click **Open Result** in the Analysis Results command bar.

❖ To select the data for the report

Select the main table of interest and apply the appropriate filters so that the report only uses the rows displayed.

> **IMPORTANT** Some tables, such the Expected Compounds per File, Expected Compounds, and Compounds tables can contain thousands of rows. Because report generation is limited to 2000 pages and for practical reasons, reduce the number of rows to only the rows of interest by applying the appropriate filters.

Generating a Report

You can use one of the following templates or one of your own custom report templates to generate reports that display the items of interest in a result file.

These eight report templates (.cdReportTemplate) come with the application:

- Expected Compounds with Structures with Graphs A4
- Expected Compounds with Structures No Graphs A4
- Expected Compounds with Graphs A4
- Expected Compounds No Graphs A4
- Expected Compounds per File with Graphs A4
- Expected Compounds per File No Graphs A4
- Compounds with Graphs A4
- Compounds No Graphs A4

❖ To preview and print a report by opening an existing report template

1. Open a result file.

   The reporting menu commands and the reporting toolbar icons become available.

2. Determine which main table you want to include in the report and filter the data in this table.

3. To select an existing report template, choose **Reporting > Create Report** from the menu bar or click the **Create Report** icon, .

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

   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.

4. Select the appropriate report template and click **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.

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If the template contains ReportInfo items, the application does not display the rendered pages until it has rendered all of the report pages.

5. 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 "To change the print width, paper size, or page orientation" on page 6).
6. On the report resolution page, click the **Print** button, , in the toolbar to print the report.

   The Print dialog box opens.
7. 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.

8. As appropriate, change the paper type for your printer.
9. Click **OK** to print the report.

Creating 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.

❖ To create a new report template

1. Open a result file.
2. From the application menu bar, choose **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. Select the information that you want to include in the report as follows:
   - Under Columns, select the check boxes 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 check boxes for the graphs that you want to include in the report.
   - Under Related Tables, select the check boxes for the related tables and the columns in these tables that you want to include in the report.
5. Customize the appearance of the report as follows:
   - To draw a separator line above the column headers for the main table and the selected related tables, make sure that the **Draw Lines** check box is selected (Default: Draw Lines).
   - To indent a related table, select the check box for the related table in the data item list, select the table name to highlight it in blue, and type 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** check box.

   > **Tip** For each table that you want to transpose, select the table name to highlight it in blue, and then select the **Transpose Data** check box.

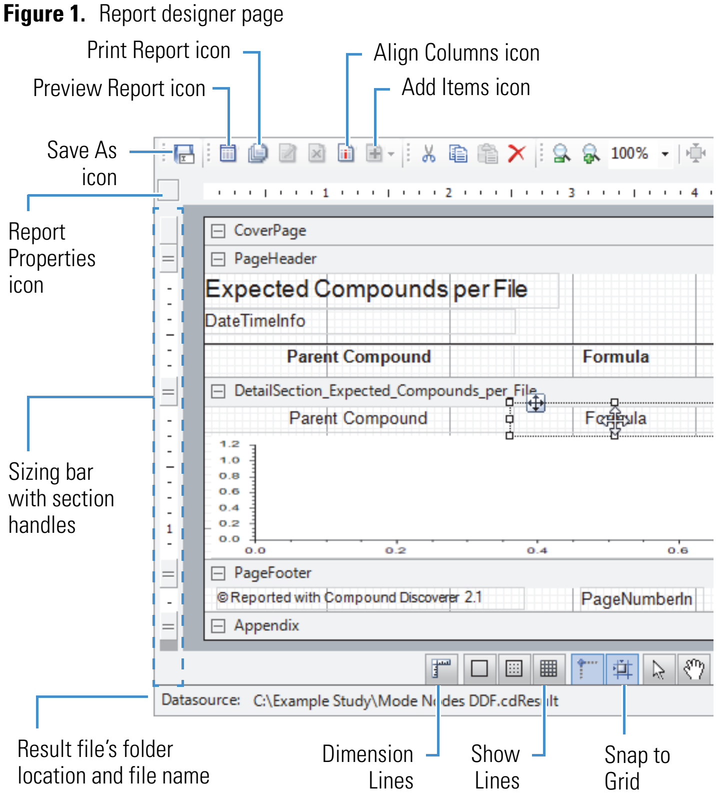
   - To apply a color scheme to a table, select the table listing, and then select a color scheme from the Color scheme list.
6. In the General Settings area, do the following:
   - To modify the paper size, type the first letter of the paper size in the Paper Kind list or make a selection from the list. 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, click the browse button to the right of the Logo Image and browse to the image file of interest.
7. Click **OK** to apply the settings.

   The report designer page opens.
8. Click the **Preview Report** icon, , to preview the report.

   The Report Preview dialog box opens.
9. Do one of the following:
   - To continue editing the template, close the Report Preview dialog box and follow the instructions in "Editing a Report Template" on page 3.
   - To save the report template, see "To save the report template with a different name" on page 6.
   - To export or print the report, see "Exporting or Printing a Report" on page 6.

Figure 1 shows the workspace sections, sizing bar, and toolbars.

Figure 1. Report designer page



Editing a Report Template

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

Follow these procedures as needed:

- To open an existing report template
- To change the logo image
- To change the date-and-time stamp format
- To add a data graph for a main table
- To edit a design item by using the mouse and keyboard
- To modify a design item’s properties
- To align a column heading to its associated data field
- To transpose the data fields from columns to rows or from rows to columns
- To resize a workspace section vertically
- To add a non-data item
- To add a column from a related table to the template
- To edit the properties of subreport columns
- To move a subreport column up to the set of main table columns
- To modify the cover page section
- To change the print width, paper size, or page orientation
- To save the report template with a different name

❖ To open an existing report template

1. Choose **Reporting > Edit Report Template** from the menu bar or click the **Edit Report Template** icon, , in the Toolbar.

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

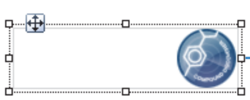
2. Select a report template and click **Open**.

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

   Existing Report Template Name

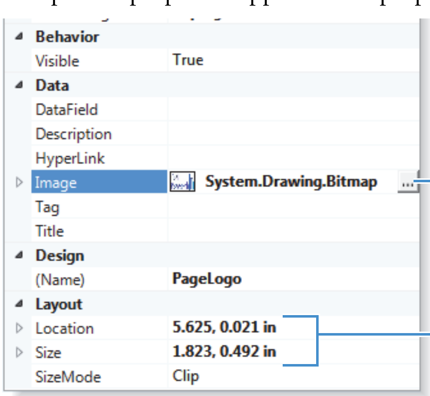
❖ To change the logo image

1. Select the logo image (picture container).



Selected picture container showing the container’s handle points

The picture properties appear in the properties pane.



Click to open the Open dialog box where you can select a different image.

Size and location of the picture container

2. In the Data area, click the browse icon, , to the right of the Image property. You might have to click 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 click **Open**.

   The selected image appears in the container.

4. Modify the Layout properties as appropriate.

❖ To change the date-and-time stamp format

1. In the PageHeader section, select the **DateTimeInfo** TextBox design item.

   The TextBox properties appear in the Properties pane.

2. In the OutPutFormat box, click the browse icon, .

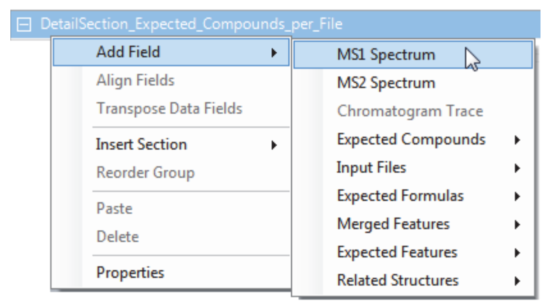
   The OutPutFormat dialog box opens.

3. Select an appropriate data-and-time stamp and click **OK**.

❖ To add a data graph for a main table

Do one of the following:

- Right-click the **DetailSection_*Main_Table_Name*** bar and choose **Add Field > *Data Graph***.



–or–

a. Click the **DetailSection_*Main_Table_Name*** bar.

b. In the toolbar, click the **Add Items** icon, , to open a list of data graphs and related table selections.

c. 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.

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.

❖ To edit a design item by using the mouse and keyboard

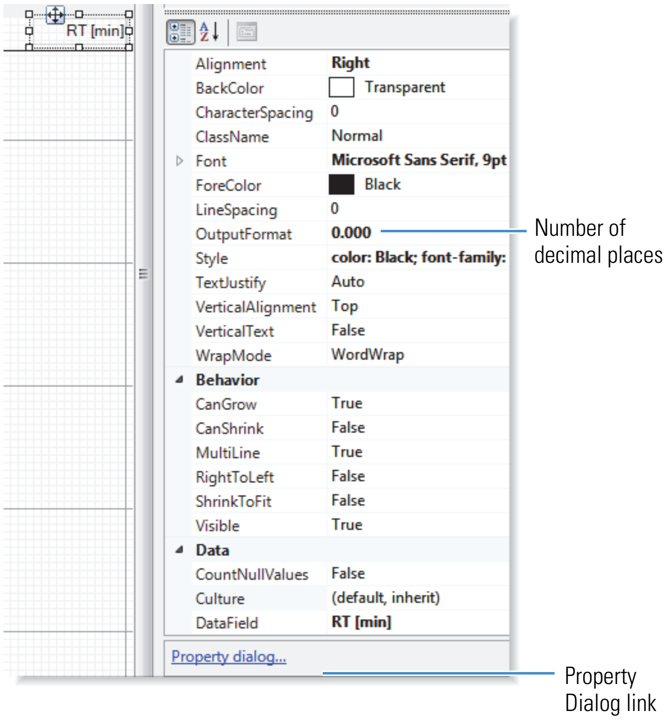
Select the design item on the report designer page, and then modify the item as follows:

- 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.

❖ To modify a design item's properties

1. Select the design item on the report designer page.

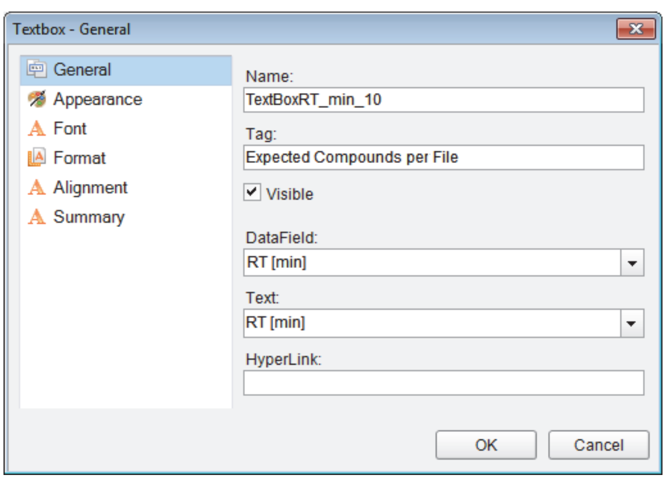
   The properties for the selected design item appear in the properties pane, at the bottom right of the report designer page. This figure shows the properties pane for the RT [min] data field.



2. In the properties pane, modify the properties of interest, including the size and location of the selected design item and the number of decimal places for a numeric data field.

   –or–

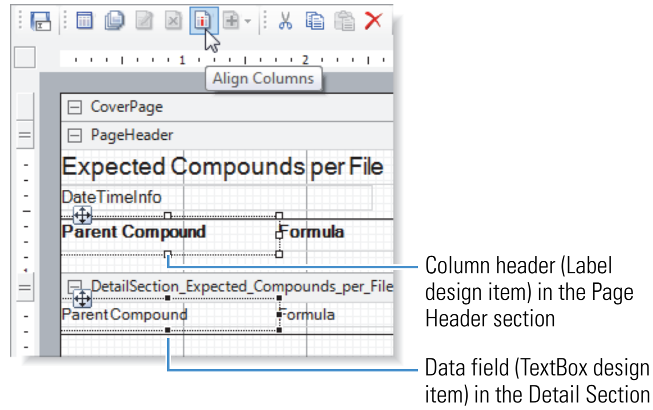
   Double-click the **Property Dialog** link to open a dialog box where you can modify the properties.



❖ To align a column heading to its associated data field

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 (Figure 1 on page 2).



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

❖ To transpose the data fields from columns to rows or from rows to columns

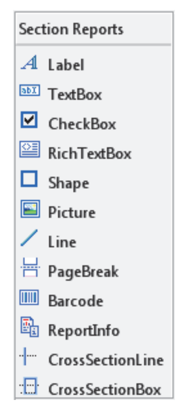
1. Right-click a column heading (Label) or a column data field (TextBox) and choose **Transpose Data Fields**.
2. To undo the change, if necessary, right-click a column heading (Label) or a column data field (TextBox) and choose **Transpose Data Fields**.

❖ To resize a workspace section vertically

To enlarge a workspace section, in the sizing bar (Figure 1 on page 2), 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.

❖ To add a non-data item

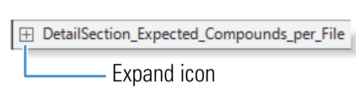


1. In the Section Reports pane to the right of the workspace area, select a design item and drag it to the appropriate location in a workspace section; for example, add **PageBreak** to break the section to the next page.
2. In the properties pane, edit the item's properties.

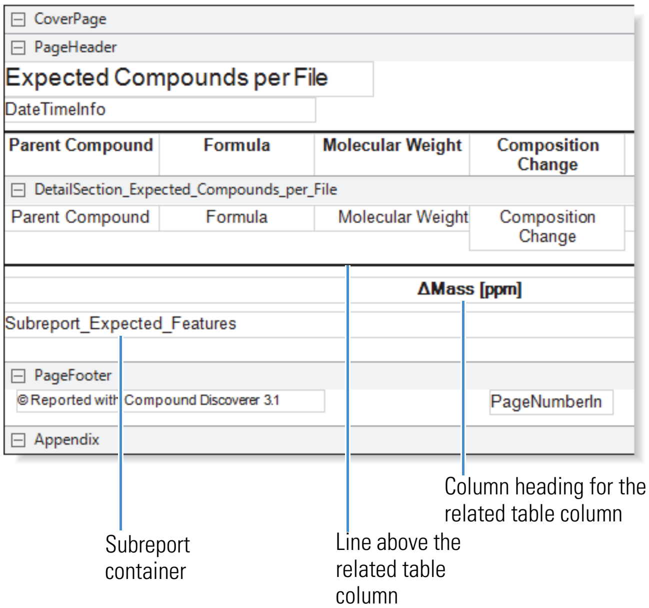
❖ To add a column from a related table to the template

1. Select the **DetailSection_*Main_Table_Name*** bar.
2. In the report designer toolbar, click the **Add Items** icon, , 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. Choose an available related table from the list, and then choose a table column.
4. If the Detail Section is collapsed, click the expand icon to open the section.



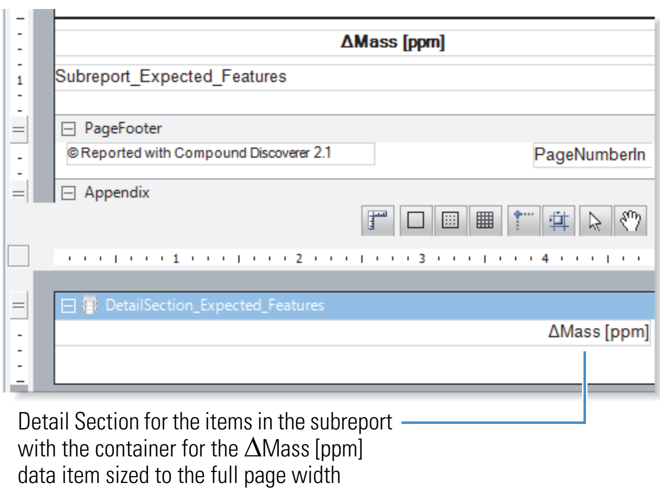
The added table column appears at the bottom of the Detail Section (data area). The application automatically adds a line above the column heading.



❖ To edit the properties of subreport columns

1. To open the subreport editor area, double-click the **Subreport_*Related_Table_Name*** container.

   The TextBox design item for the related table column appears in a separate section. The item's container is sized to the full page width.



2. To change the properties of the TextBox design item in the Detail Section for the subreport, select the design item.

   The properties for the selected design 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.

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

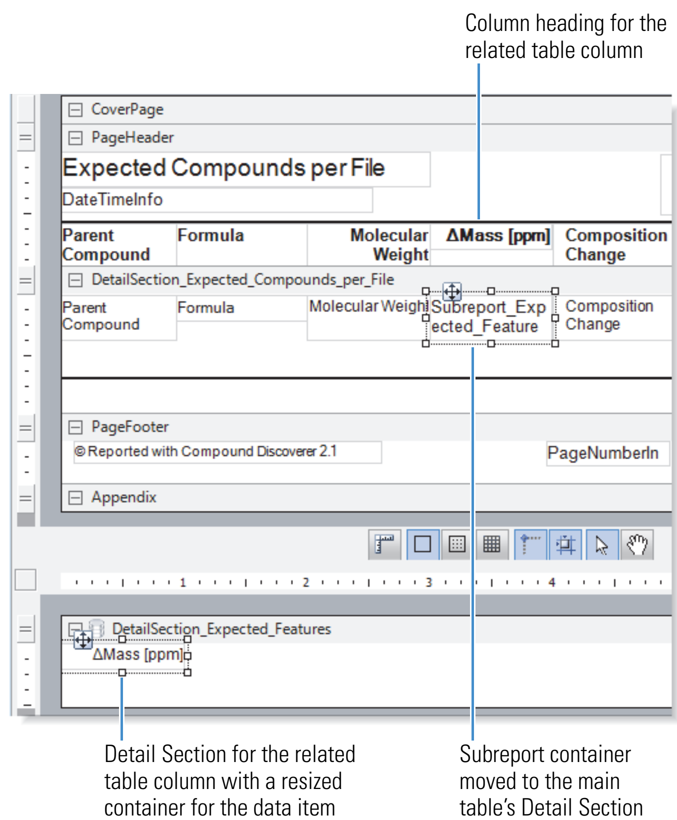
❖ To move a subreport column up to the set of main table columns

1. Resize the column heading container for the subreport column. Then, move it to an appropriate location in the set of main table columns.

2. Resize the **Subreport_*Related_Table_Name*** container. Then, move it to the appropriate location in the DetailSection.

3. In the related table's Detail Section, resize the data item's container.

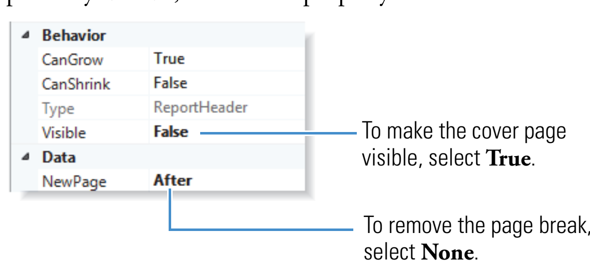
   This figure shows a report template for the Expected Compounds per File table with an additional column from the related Expected Features table.



❖ To modify the cover page section

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.



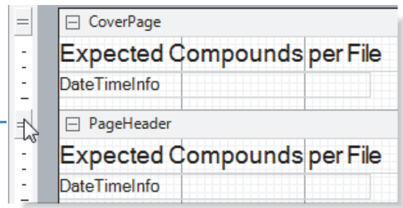
2. Under Behavior, select **True** for Visible.

3. To preview the report, click the **Preview Report** icon, .

   By default, the cover page appears as the first page of the report.

4. (Optional) Under Data, select **None** for NewPage to remove the page break between the cover page and the report items.

5. 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).



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

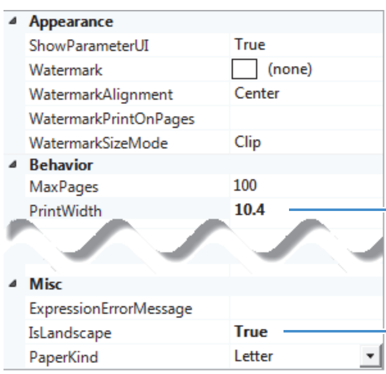
IMPORTANT To add textual information, such as an explanation about the purpose of the report, use the RichTextBox item. Do not use the TextBox item on the cover page.

❖ To change the print width, paper size, or page orientation

1. Click the **Report Properties** icon (square in the upper left corner, below the toolbar) (Figure 1 on page 2).

   The report properties appear in the properties pane (Figure 2).

Figure 2. Report properties



2. To change the print width, type an appropriate numeric value for the PrintWidth parameter.
3. To change the page orientation, under Misc, in the IsLandscape list, select **True** for Landscape or **False** for Portrait.
4. 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.

❖ To save the report template with a different name

1. In the report designer toolbar, click the **Save As** icon, .

   The Save Report Template As dialog box opens.

2. Select a directory folder where you want to store the report template and name the report template.
3. Click **Save**.

Previewing a Resolved Report

You can preview a completely resolved report on the report resolution page (see "Generating a Report" on page 1) 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 (Figure 2) is too large for the selected paper size.

❖ To preview the report in the Report Preview dialog box

In the toolbar on the report designer page, click the **Preview Report** icon, .

The Report Preview dialog box opens, resolves the current result file with the current template, and displays up to five pages.

❖ To preview the report in the Report Print dialog box

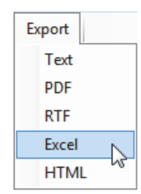
In the report designer toolbar, click the **Print Report** icon, .

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 (2/18) provides a page count estimate.

Exporting or Printing a Report

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

❖ To export a report to a file



1. In the toolbar, click **Export** and choose 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 click **Save**.

❖ To print a report

1. In the toolbar, click the **Print** icon, , to open the Print dialog box.
2. Select a printer and the page range that you want to print.
3. Click **OK** to print the report.

Trademarks

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