Chem2**XL**®

Creating a single sample report template in Chem2XL for use with the Agilent ChemStation®

*Automating custom reporting for the Agilent ChemStation with the power of Excel®*

INTRODUCTION

Chem2XL is designed to enhance automated reporting with powerful customization capabilities saving valuable time and laboratory resources.

This application note explains the process of creating a single sample Chem2XL template. This template can then be used to automate ChemStation custom reporting. The reports can be sent to a printer or to Microsoft Excel file. Chem2XL eliminates manually entering data for calculations and reporting. Chem2XL can save time making your lab more productive and efficient.
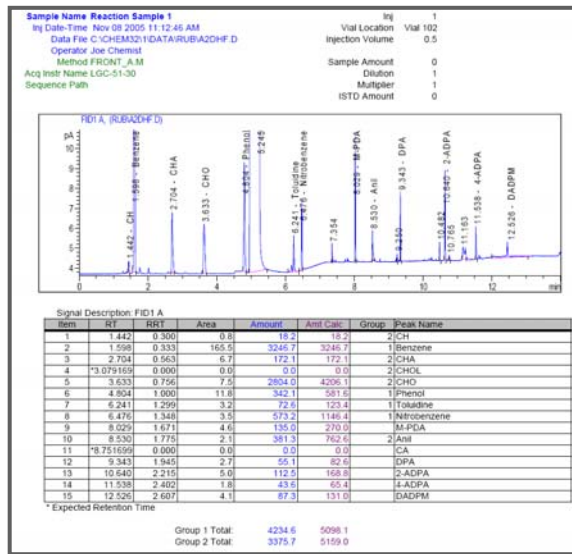
PROCEDURE

To create a Chem2XL report, a template must first be generated. This template is used by Chem2XL to create a customized report. Creating a custom single sample report is a simple process with Chem2XL. This application note will enable the user to create a single sample Chem2XL report template. The new Chem2XL template is selected as the report style in the ChemStation method. Once the Chem2XL report template is assigned to a method it is ready for automatic printing and report generation. Report generation can be automated after each run in a sequence or interactively in data analysis. Finally Chem2XL saves the report as an MS Excel document along with the data for easy use and archiving.

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Template Creation using Chem2XL Setup Wizard

application note

1. Start the Agilent ChemStation (revision A.10.02, B.01.01 or newer)

2. Go to data analysis within the Agilent ChemStation

3. Select the Chem2XL menu "Create Chem2XL Template" (see Figure 1)
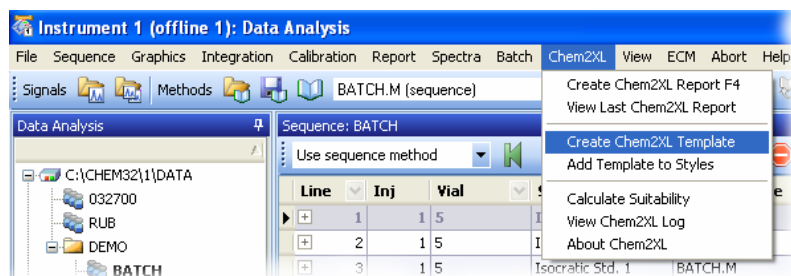

Figure 1: Create Chem2XL template menu

4. With the Chem2XL Setup Wizard as seen in Figure 2 now in view, select "Single Sample Report". Selecting Single Sample Report allows the setup wizard to have the appropriate options for a single sample report. (For multiple samples see Application Note for Multi Sample Reporting). Follow Figure 2 settings below.

	Include chromatogram and desired tabular data (named / un peaks) included in template.
	Insert title (optional).
	Select individual items that will appear on the template header section.
	Information from this section will appear in the peak data table. Select only the peak details and peak performance (suitability) items that are needed. **Note:** Selecting too many peak table items results in report not fitting on one page. Chem2XL is designed to auto-size wide reports to fit on one page. The auto-sizing feature reduces the report scaling for wide reports; however this make the fonts smaller.
	This section is information only and estimates how wide the Chem2XL table will be.
	When finished select "Create Template". The Wizard will now build a framework on a Microsoft Excel spreadsheet.

tip

Right clicking on any sample or peak item will change the name that appears in the report

Figure 2: Customizing the Setup Wizard

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5. After the Wizard creates the customized template, further customization may be done to the layout by changing formatting, adding borders, changing column and row sizes. Moving items around in the template is also possible. Note: Changing the order of the columns in the peak table is easily done by following a few simple rules laid out in Step 8.
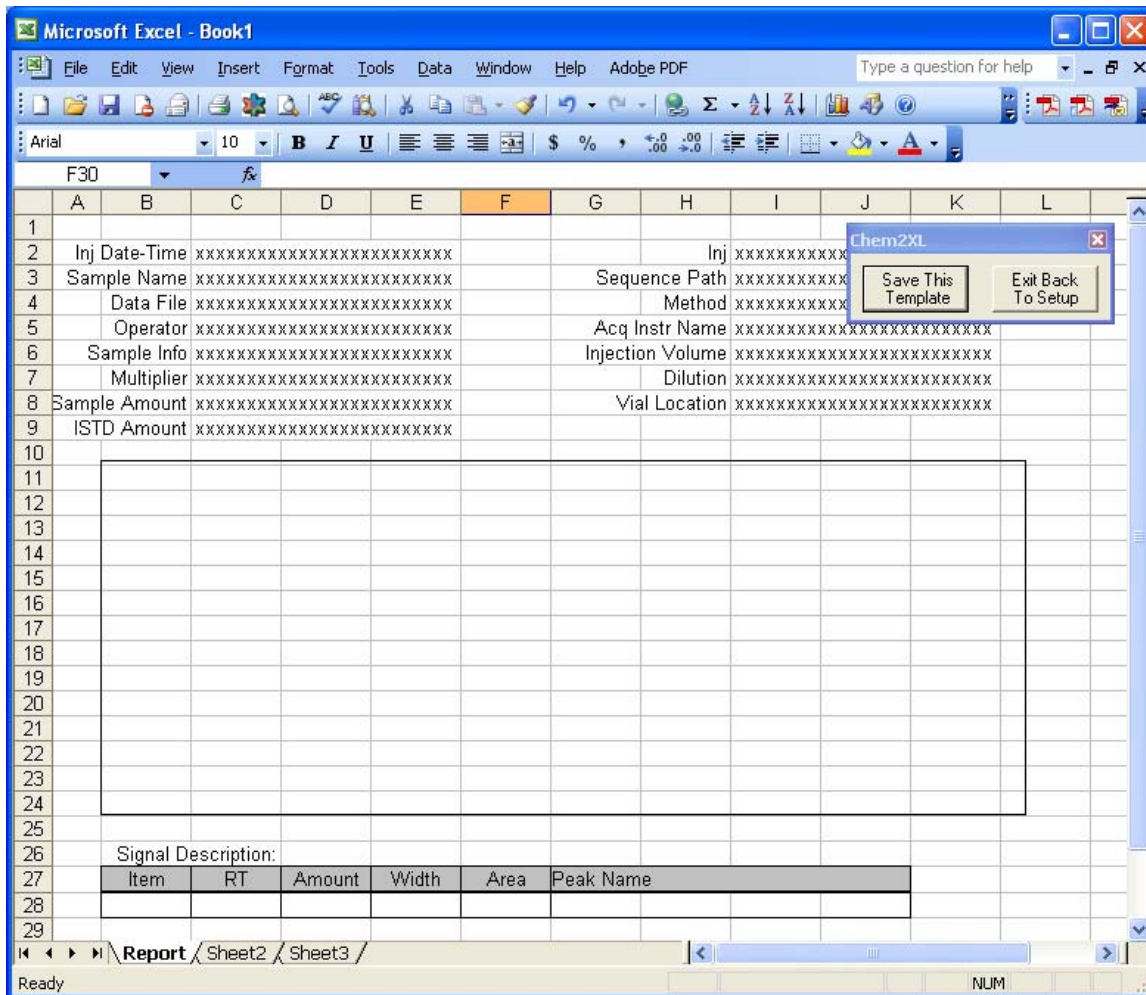

Figure 3: Chem2XL Template Layout Designer

6. Sample information items can be customized by changing the font type, size, color, etc. To change basic formatting, right click on the selected sample item cells (name and value cells) and select "Format Cells". Items may also be moved around to different positions on the report screen. Note: be sure to select the name and value cells and move them together.
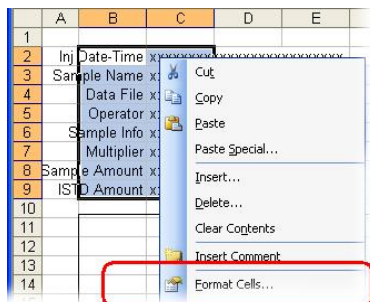

Figure 4: Right click to Format Cells
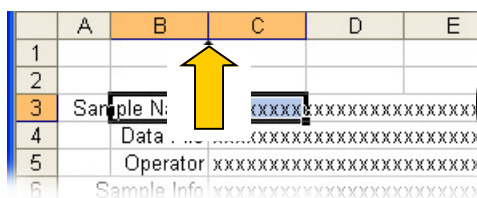

Figure 5: Moving Sample Information cells

tip

It is important when moving sample items around to select two adjacent cells: the label and value cells. For example select B3 "Sample Name" and C3 the value cell to the right.

application note

7. The empty rectangle is where the chromatogram will be located (see an example report Chromatogram in Figure 6). To move the chromatogram box around in the template, click and drag the box to the desired location. The chromatogram rectangle may also be resized to desired size by clicking and dragging the rectangle. See Figure 6 below.
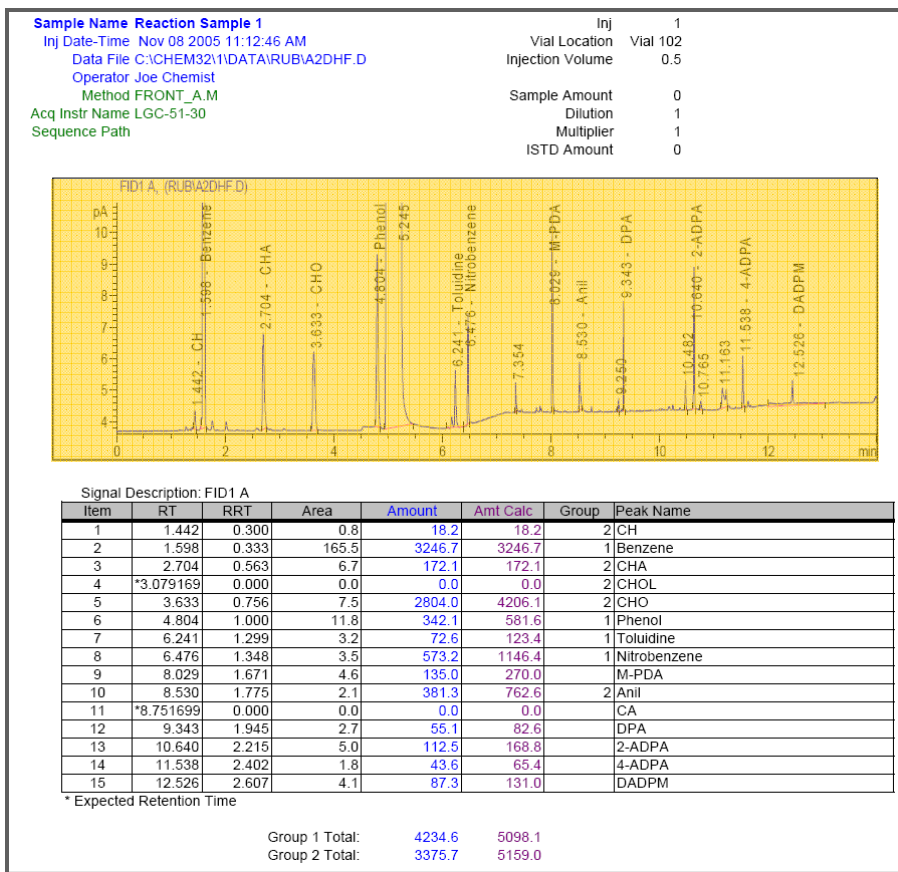
note

Chromatogram scaling is done in the ChemStation:

Graphics

Signal options

Range

Figure 6: Chromatogram location on the report

application note

8. When moving the order of the columns in the peak table cells around, the column heading and the cell directly below need to be moved together. Figures 7, 8 and 9 show the basic concept of moving cells correctly.

Figure 7: STEP ONE clear some space by moving selected cells

tip

When moving peak table columns you must align the rows horizontally or Chem2XL will not be able to fill the data in properly.

Figure 8: STEP TWO move selected cells to new area

note

Columns may be inserted by shifting peak table rows to the right. Empty columns or columns with formulas are valid.

Figure 9: STEP THREE align cells horizontally with columns

9. After editing the template is complete, save the template. To do this, press the Chem2XL "Save This Template" button (see Figure 10). By pressing this button, the template will be properly saved in the template directory. Saving to the Excel file/save will not allow Chem2XL to use the template properly. After editing is complete, save the template by clicking "Exit Back to Setup" which will save and close the template (see Figure 10). "Quit" the Chem2XL Setup Wizard.
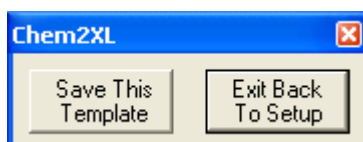

Figure 10: Saving the Chem2XL Template

application note

10. To print a Chem2XL report it is necessary to add the template to the ChemStation report styles. After creating a template and saving it (see steps 1-9), select Chem2XL from drop down menu, then click on "Add Template to Styles" (see Figure 11).
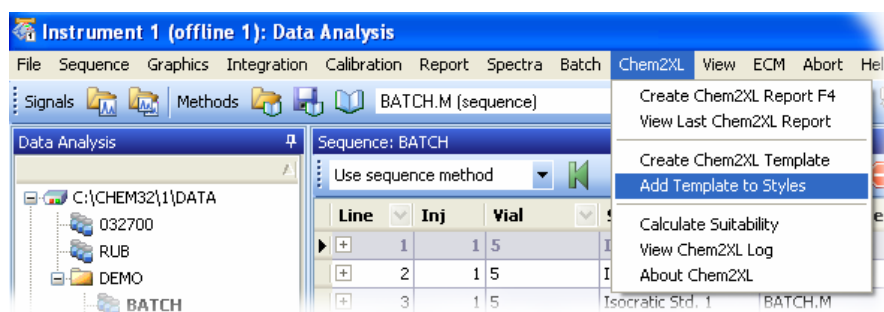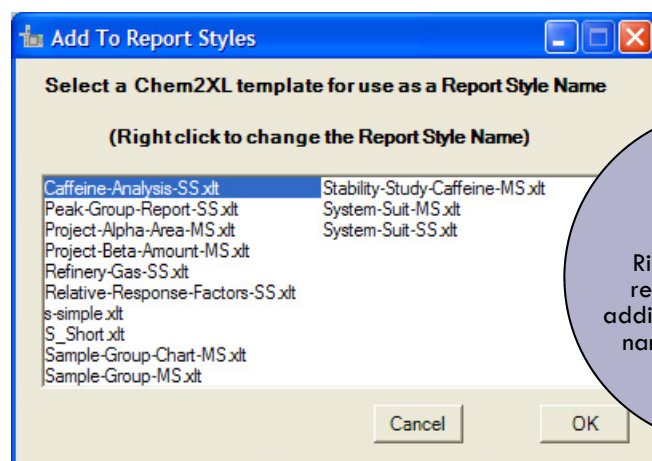

Figure 11: Add Chem2XL template to ChemStation report styles.

tip

Right clicking on the report will allow for adding and changing the name that appears in ChemStation.

Figure 12: Add To Report Styles

application note

11. Select the desired report style to be used for the ChemStation method. Chem2XL allows different reporting templates for each ChemStation method. Select the new report template style in ChemStation by going to the "Reports" menu and selecting "Specify Reports". Scroll down in the Style list to select the new report template (see Figure 13).

note

"Report Layout For Uncalibrated Peaks" determines whether a Chem2XL report prints only named and unnamed peaks on a Chem2XL report.
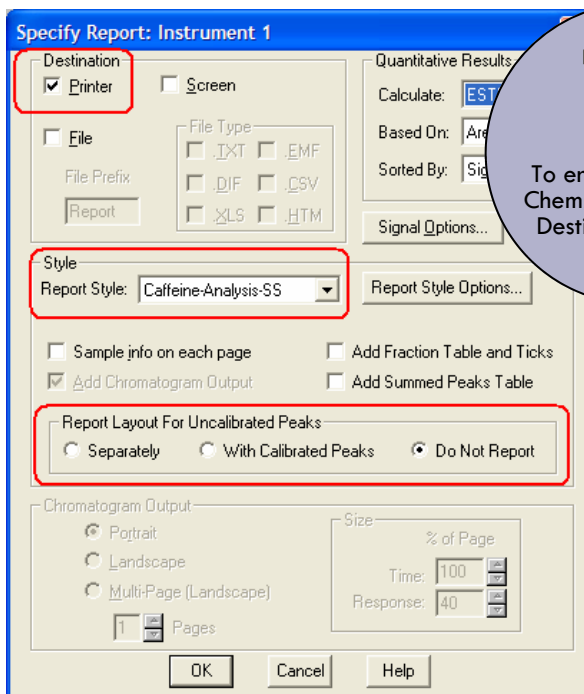

tip

To enable printing of Chem2XL reports Click Destination "Printer"

Figure 13: Chem2XL template specification

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application note

12. There are two options for generating Chem2XL reports:
1) reports are automatically produced after each run in the sequence
2) interactively in Data Analysis. In data analysis with a data file loaded and a Chem2XL template selected load a data file
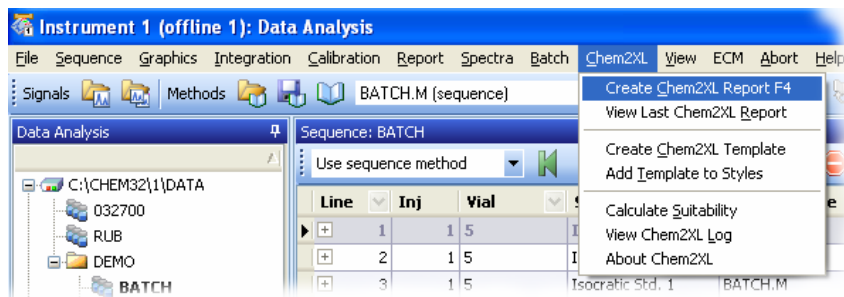

Figure 14: Interactively create Chem2XL Reports

CONCLUSION

Chem2XL is an integrated add-on for the Agilent ChemStation designed to increase productivity by automating specialized reports and calculations. Once a template is developed, the template can be used with single methods or multiple methods. Chem2XL templates offer the power of Microsoft Excel within the Agilent ChemStation.