

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

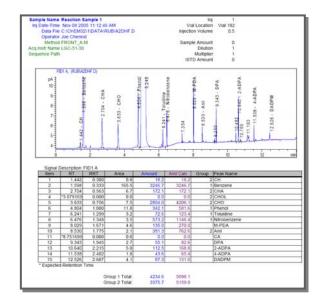
Automating custom reporting for the Agilent ChemStation with the power of Excel®

application note

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.

Chem2XL®

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note	1. Start the Agilent ChemStation (revision A.10.02, B.01.01 or ne	wer)
5	2. Go to data analysis within the Agilent ChemStation	
	3. Select the Chem2XL menu "Create Chem2XL Template" (see Fi	gure 1)
application	Signals Compared Analysis Analysis Sequence: BATCH.M (sequence) Create Che View Last Compared Analysis Create Che Che Che Che Che Che Che Che Che Ch	EXL Log 12XL IBATCH.M ew, select "Single Sample Report". Selecting ropriate options for a single sample report.
QD	File Report Help Report Type Include Chromatagraph C Multi-Sample Report (Summary Report) Include Chromatagraph Single Sample Report Autosize Column Widths Unnamed Peaks (Uncal)	Include chromatogram and desired tabular data (named / un peaks) included in template.
	Excel Report Header: My Report Title	Insert title (optional).
	Sample Information Sample Name Inj Inj Date-Time Operator Data File Method Data File Method Sample Info Sequence Path Vial Location Acq Instr Name	Select individual items that will appear on the template header section.
sample of change	Area Sum Symmetry Signal/Noise Ratio Height Slope Detector Height Percent Intercept Peak Name Height Sum Corr. Coefficient Inter Number Inter Width Compound Group Intercept	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
	kPrime USP Tailing Selectivity Statistical Moment 0 Plates Half Width Width Half Height Resolution Half Width Statistical Moment 1 Plates Tangent Width Tangent Resolution Tangent Statistical Moment 2 Plates 5 Sigma Width 5 Sigma Resolution 5 Sigma Statistical Moment 3 Plates Statistical Width 7 Sigma Resolution 5 Sigma Statistical Moment 4	reports to fit on one page. The auto-sizing feature reduces the report scaling for wide reports; however this make the fonts smaller.
	Table/Columns Estimator Approximate Number of characters in the Data 72 Keep the total characters under 100 if possible. More may exceed Excel page width. Number Of Peaks 5 Approximate Number of characters in the Data 72 Keep the total characters under 100 if possible. More may exceed Excel page width.	This section is information only and estimates how wide the Chem2XL table will be.
	Quit Open Template Create Template Close Template Close Template	When finished select "Create Template". The Wizard will now build a framework on a
	Figure 2: Customizing the Setup Wizard	Microsoft Excel spreadsheet.

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.

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Figure 3: Chem2XL Template Layout Designer

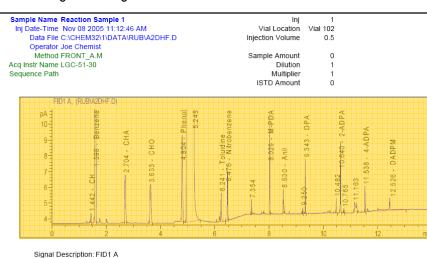
6. Sample information items can be customized by changing the font type, size, color, etc. To change basic formatting, right click on the selected sample item cells (name and value cells) and select "Format Cells". Items may also be moved around to different positions on the report screen. Note: be sure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

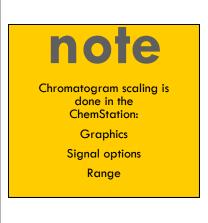
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Figure 4: Right click to Format Cells

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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.





Item	RT	RRT	Area	Amount	Amt Calc	Group	Peak Name
1	1.442	0.300	0.8	18.2	18.2	2	СН
2	1.598	0.333	165.5	3246.7	3246.7	1	Benzene
3	2.704	0.563	6.7	172.1	172.1	2	CHA
4	*3.079169	0.000	0.0	0.0	0.0	2	CHOL
5	3.633	0.756	7.5	2804.0	4206.1	2	СНО
6	4.804	1.000	11.8	342.1	581.6	1	Phenol
7	6.241	1.299	3.2	72.6	123.4	1	Toluidine
8	6.476	1.348	3.5	573.2	1146.4	1	Nitrobenzene
9	8.029	1.671	4.6	135.0	270.0		M-PDA
10	8.530	1.775	2.1	381.3	762.6	2	Anil
11	*8.751699	0.000	0.0	0.0	0.0		CA
12	9.343	1.945	2.7	55.1	82.6		DPA
13	10.640	2.215	5.0	112.5	168.8		2-ADPA
14	11.538	2.402	1.8	43.6	65.4		4-ADPA
15	12.526	2.607	4.1	87.3	131.0		DADPM
Expecte	d Retention	Time					
		~	roup 1 Total:	4234.6	5098.1		
		G	roup 1 Total:	4234.6	0098.1		

Figure 6: Chromatogram location on the report

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.

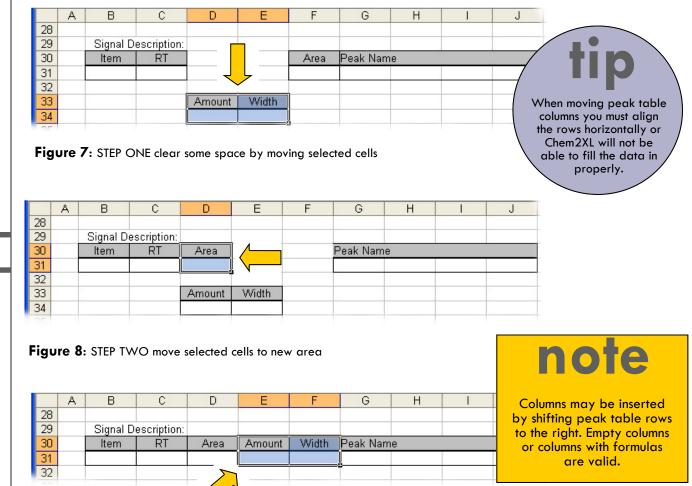


Figure 9: STEP THREE align cells horizontally with columns

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.

Chem2XL	×
Save This	Exit Back
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Figure 10: Saving the Chem2XL Template

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).

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Figure 11: Add Chem2XL template to ChemStation report styles.

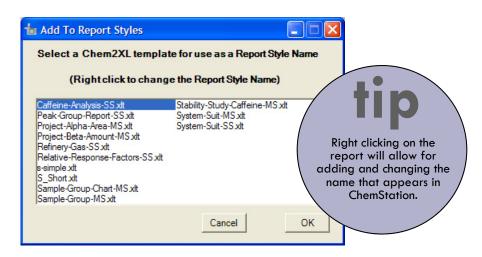


Figure 12: Add To Report Styles

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

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

Specify Report: Instrument 1	
Destination	Quantitative Results
☑ Printer ☑ Screen	
File Type	Based On: Are
	Sorted By: Sig To enable printing of
Report .XLS .HTM	Signal Options Chem2XL reports Click Destination "Printer"
Style Report Style: Caffeine-Analysis-SS	Report Style Options
	Add Fraction Table and Ticks Add Summed Peaks Table
Report Layout For Uncalibrated Peaks C Separately C With Calibrated Pe	eaks 💿 Do Not Report
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OK Cancel	Help

Figure 13: Chem2XL template specification



(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

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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.