

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 multi-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 saves time making labs more productive and efficient which ultimately reduces operating costs.

Sample Name	Injection Date-Time	Injection Volume	Vial Location	Caffeine		
				RT	Area	Amount
caff Std .005	9/12/2005 10:21:06 PM	2	Vial 1	5.824	59.359	0.005
caff Std .025	9/12/2005 10:36:14 PM	2	Vial 2	5.825	291.098	0.024
caff Std .125	9/12/2005 10:51:24 PM	2	Vial 3	5.813	1505.118	0.127
caff Std .250	9/12/2005 11:06:35 PM	2	Vial 4	5.810	2937.001	0.249
Coke	9/12/2005 11:36:52 PM	2	Vial 22	5.809	1120.160	0.095
Pepsi	9/12/2005 11:52:01 PM	2	Vial 23	5.804	1253.992	0.106
Diet Pepsi	9/13/2005 12:07:15 AM	2	Vial 24	5.802	1139.361	0.096
Mountain Dew	9/13/2005 12:22:34 AM	2	Vial 25	5.799	1809.786	0.153
Surge	9/13/2005 12:37:54 AM	2	Vial 26	5.796	1666.863	0.141
caff Std .005	9/13/2005 12:53:03 AM	2	Vial 1	5.801	59.532	0.005
caff Std .025	9/13/2005 1:08:12 AM	2	Vial 2	5.798	294.141	0.025
caff Std .125	9/13/2005 1:23:22 AM	2	Vial 3	5.795	1476.750	0.125
caff Std .250	9/13/2005 1:38:34 AM	2	Vial 4	5.792	2959.280	0.251
				StDev	0.0105	
				Avg	5.805	

Multi-Sample Report Example

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 multi-sample report is a simple process with Chem2XL. This application note will enable the user to create a multi-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. Multi-sample templates create a single Excel file for each ChemStation sequence of samples. For example a sequence of 30 injections will include 30 rows of data in the excel spreadsheet, one row for each sample (see above).

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)

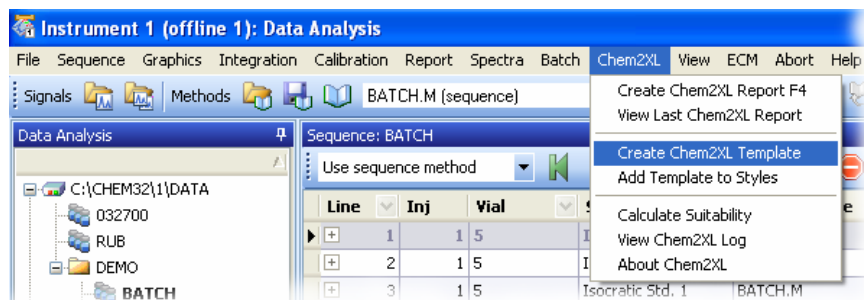


Figure 1: Create Chem2XL template menu

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

Chem2XL Setup Wizard		Select Multi-Sample Report and desired tabular data (named and/or un peaks) to be included in the template. (note Chromatograms cannot be included in a multi-sample report)
Report Type <input checked="" type="radio"/> Multi-Sample Report (Summary Report) <input type="radio"/> Single Sample Report	<input checked="" type="checkbox"/> Include Chromatograph Picture <input checked="" type="checkbox"/> Autosize Column Widths	
Excel Report Header:		Insert title (optional).
Sample Information Sample Name <input checked="" type="checkbox"/> Inj <input type="checkbox"/> Sample Amount <input type="checkbox"/> Signal Description <input type="checkbox"/> Inj Date-Time <input checked="" type="checkbox"/> Operator <input type="checkbox"/> Multiplier <input type="checkbox"/> Template Name <input type="checkbox"/> Data File <input checked="" type="checkbox"/> Method <input type="checkbox"/> Dilution <input type="checkbox"/> Template Create Date <input type="checkbox"/> Sample Info <input type="checkbox"/> Sequence Path <input type="checkbox"/> Internal Std Amount <input type="checkbox"/> Vial Location <input type="checkbox"/> Acq Instr Name <input type="checkbox"/> Injection Volume <input type="checkbox"/>		Select individual items that will appear on the template sample identification section.
<input checked="" type="checkbox"/> RT <input type="checkbox"/> Area Sum <input type="checkbox"/> Symmetry <input type="checkbox"/> Signal/Noise Ratio <input type="checkbox"/> <input checked="" type="checkbox"/> Height <input type="checkbox"/> Slope <input type="checkbox"/> Detector <input type="checkbox"/> <input checked="" type="checkbox"/> Height Percent <input type="checkbox"/> Intercept <input type="checkbox"/> Peak Name <input type="checkbox"/> <input checked="" type="checkbox"/> Height Sum <input type="checkbox"/> Corr. Coefficient <input type="checkbox"/> Item Number <input type="checkbox"/> <input type="checkbox"/> Width <input type="checkbox"/> Compound Group <input type="checkbox"/>		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 in combination with “Number Of Expected Peaks Per Sample” results in the report exceeding 256 columns. Items that exceed 256 columns will be truncated. (Note, use the estimator below for Multi-Sample reports so that they will not exceed 256 columns)
Table/Columns Estimator Number Of Peaks Expected Per Sample: 5 Total Number Of Excel Columns: 18 Note: Excel is limited to 256 columns. Do not exceed this amount.		This section estimates the number of columns in the Chem2XL Multi-Sample report
<input type="button" value="Quit"/> <input type="button" value="Open Template"/> <input type="button" value="Create Template"/> <input type="button" value="Close Template"/>		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 allows changes to the name that appears in the report.

Figure 2: Customizing the Setup Wizard

- When moving the order of the columns in the table, the column heading and the cell directly below need to be moved together. Figures 5, 6 and 7 show the basic concept of moving cells correctly.

	A	B	C	E	F	G	H
1				Compound Name			
2	Sample Name	Inj Date-Time	Data File	RT	Area		
3	XXXXXXXXXXXXXXXXXXXXXXXXXXXX	XXXXXXXXXXXXXXXXXXXXXXXXXXXX	XXXXXXXXXXXXXXXXXXXXXXXXXXXX	0.000		0.000	
5					Amount		
6					0.000		
7							
8							
9							

Figure 5: STEP ONE clear some space by moving selected cells down

	A	B	C	E	F	G	H
1				Compound Name			
2	Sample Name	Inj Date-Time	Data File	RT	Area		
3	XXXXXXXXXXXXXXXXXXXXXXXXXXXX	XXXXXXXXXXXXXXXXXXXXXXXXXXXX	XXXXXXXXXXXXXXXXXXXXXXXXXXXX	0.000	0.000		
5					Amount		
6					0.000		
7							
8							
9							

Figure 6: STEP TWO move selected cells to new area

	A	B	C	E	F	G	H
1				Compound Name			
2	Sample Name	Inj Date-Time	Data File	RT	Area	Amount	
3	XXXXXXXXXXXXXXXXXXXXXXXXXXXX	XXXXXXXXXXXXXXXXXXXXXXXXXXXX	XXXXXXXXXXXXXXXXXXXXXXXXXXXX	0.000	0.000	0.000	
5							
6							
7							
8							
9							

Figure 7: STEP THREE move cells to align rows horizontally (yellow and red rows must align)

- After editing the template, save and name the template. To do this, press the Chem2XL “Save This Template” button (see Figure 8). By pressing this button, the template will be properly saved in the template directory. (Note: Saving using Excels file/save will not allow Chem2XL to use the template properly.) After saving is complete, exit the template by clicking “Exit Back To Setup” which will close the template (see Figure 8). Finally, “Quit” the Chem2XL Setup Wizard.

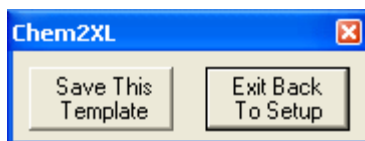


Figure 8: Saving the Chem2XL Template

9. 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 1-8), select Chem2XL from drop down menu in ChemStation, then click on “Add Template to Styles” (see Figure 9). When the Add to Report Styles dialog box appears, (see Figure 10) select the newly created template and click OK. This process adds the template the ChemStation's report style selection list.

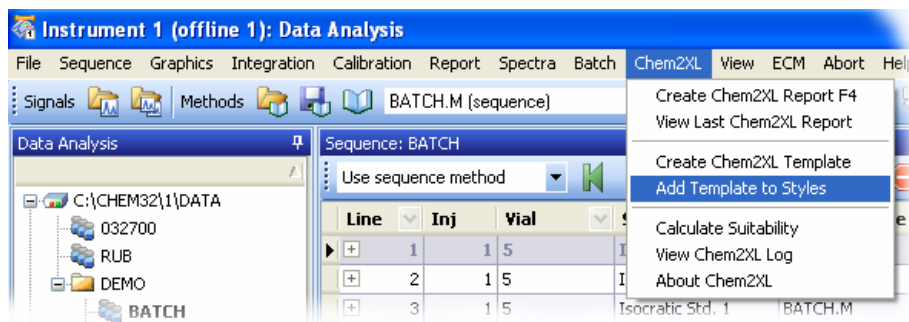
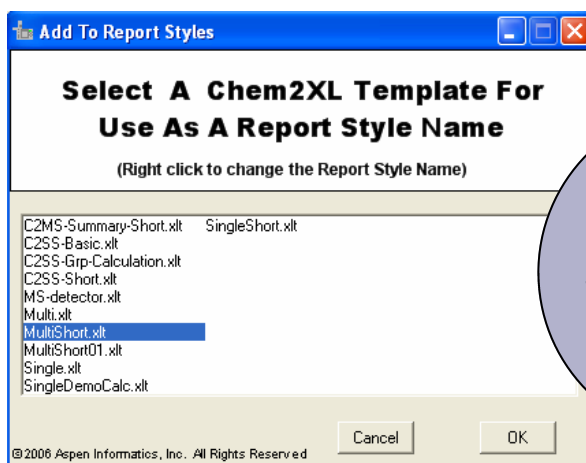


Figure 9: Add Chem2XL template to ChemStation report styles.



tip

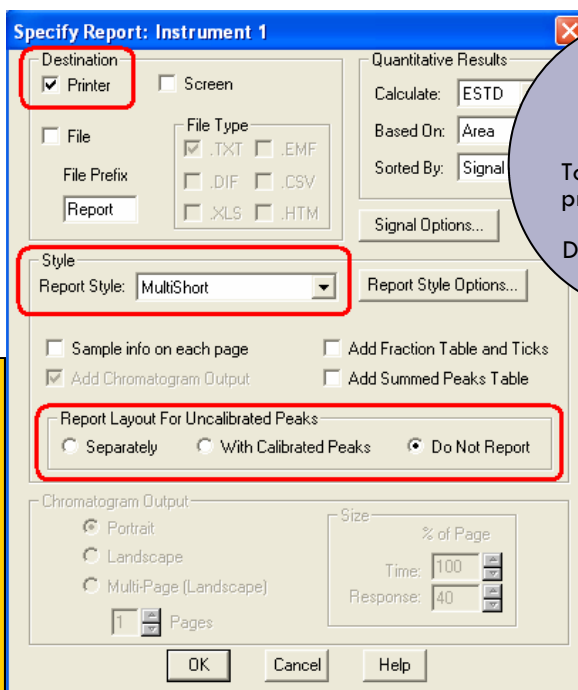
Right clicking on the template name enables the user to change the text that appears in ChemStation specify report.

Figure 10: Add To Report Styles

10. 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 11). After the report style is selected, save the ChemStation method to make the change permanent.

note

“Report Layout For Uncalibrated Peaks” determines whether the Chem2XL reporting engine prints only named (Do Not Report) or prints named and unnamed peaks on a Chem2XL report.



tip

To enable automatic printing of Chem2XL reports Click Destination “Printer”

Figure 11: Chem2XL template specification

11. There are two options for generating Chem2XL reports:
- 1) reports can be automatically produced after each run in the sequence
 - 2) reports can be interactively produced in Data Analysis (note: to produce a report in data analysis, first select a data file, select a Chem2XL report template, pull down the Chem2XL menu and select "Create Chem2XL report" (see Figure 12)

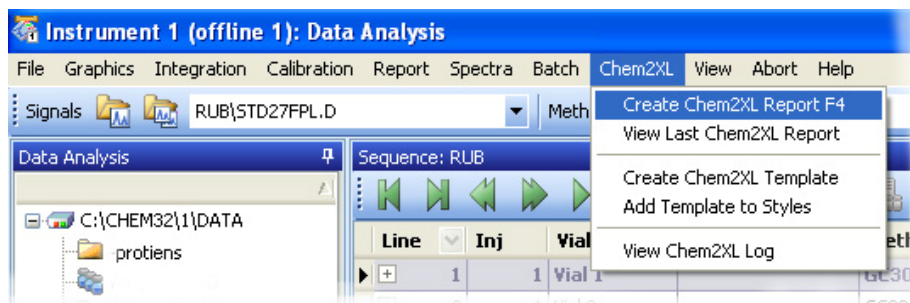


Figure 12: Interactively create Chem2XL Reports

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 saved to one or more methods. Chem2XL templates use the power of Microsoft Excel within the Agilent ChemStation.