Chem2XL Workflow – Quick Reference Guide
How to Create Excel Reports

Agilent ChemStation® B.02.01 SR1 and higher

INTRODUCTION

Chem2XL is designed to easily create Microsoft Excel® reports from your ChemStation results. This guide explains the steps involved in creating single and multi-sample reports.

Preparing your ChemStation for Chem2XL sequence reporting:

ChemStation (B.02.01 SR1 and higher) has a data analysis workflow that Chem2XL utilizes to create reports faster. In order to create reports efficiently, you need to setup the ChemStation preferences to help load the correct method with your sequence of data files. Locate the ChemStation preferences dialog (from the ChemStation menu View and then Preferences, there is also a Preferences button on the top toolbar). Selecting the Sequence method (see figure 1) will auto load the sequence method when a sequence of data is loaded in the ChemStation explorer. Having the sequence method specified will ensure that the same method is used when you create Chem2XL reports. Once the Chem2XL report template is saved to the sequence method, all subsequent samples will be reported through the same Chem2XL report template.

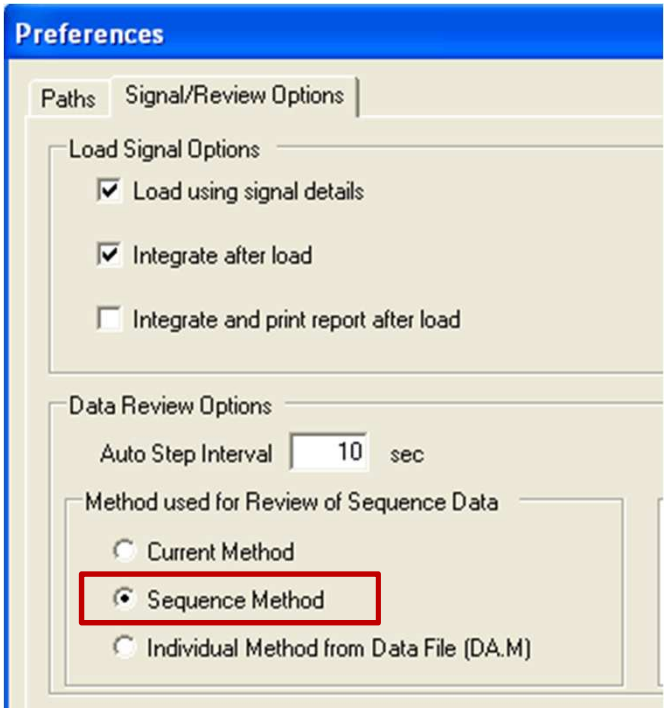


Figure 1 – ChemStation Preferences – Sequence Method

Steps to Create Chem2XL reports

1. Load the ChemStation Sequence (or data file) from the ChemStation Explorer.
   Double click on the sequence (data file) you want to load. (See figure 2)
   Note: Items that have 3 small vials to the left of the name are Sequences

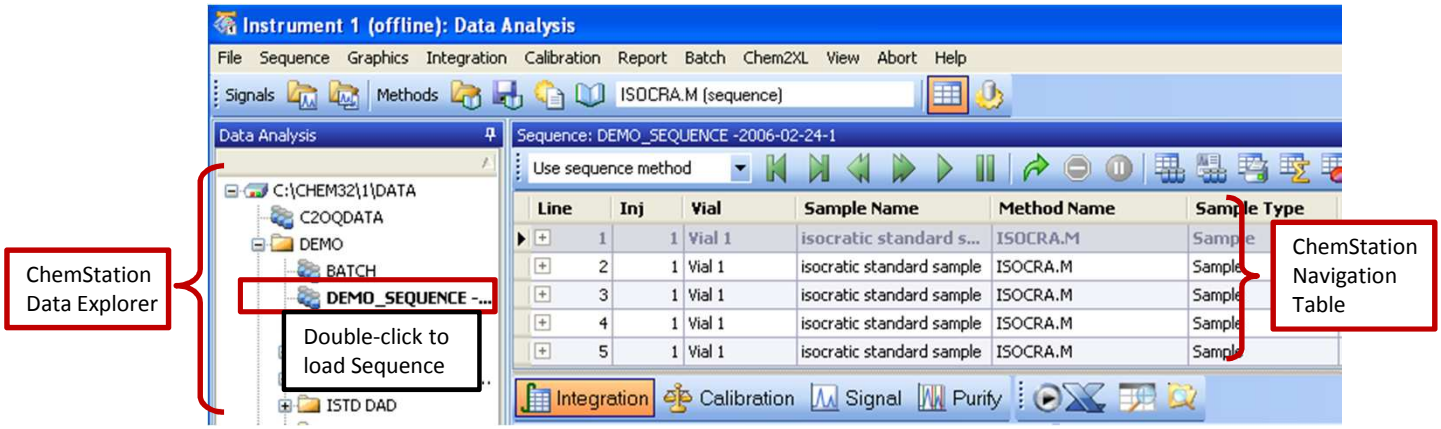


Figure 2 – Load a sequence from the ChemStation Explorer

2. Specify Chem2XL Template - Once the sequence data is loaded in the ChemStation, specify a Chem2XL report template in the ChemStation report styles. The report style setting can be saved as part of the ChemStation method and will be used as the default report style whenever that method is loaded. After you have changed the report style remember to save the ChemStation method.

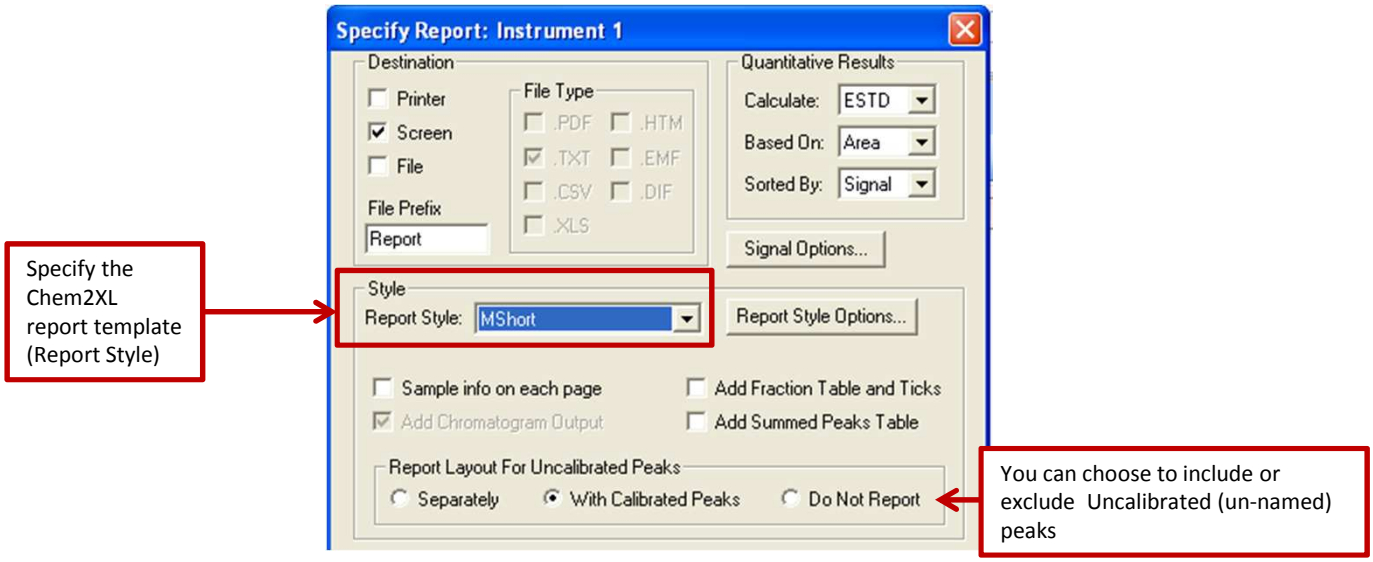


Figure 3 – Specify Chem2XL Report Style

Note: you can save the Chem2XL report template in the ChemStations master method as the default report style. All subsequent sequences that utilize this method will use the specified Chem2XL report template.
Example location of master methods: C:\Chem32\1\Methods\...

3. <u>*Generate the Chem2XL Reports*</u> *- There are 2 basic ways to generate Chem2XL reports, Interactively or Sequence Reprocess.*

   a. ***Interactively*** *(one by one, sample by sample) by pressing the "Create Chem2XL Report" Menu item or clicking the Create Chem2XL button. Loading a data file and pressing the create Chem2XL report will add one new line in a Multi-Sample (figure 5) report or create one complete Single-Sample report (figure 6).*

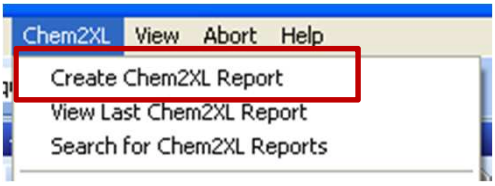


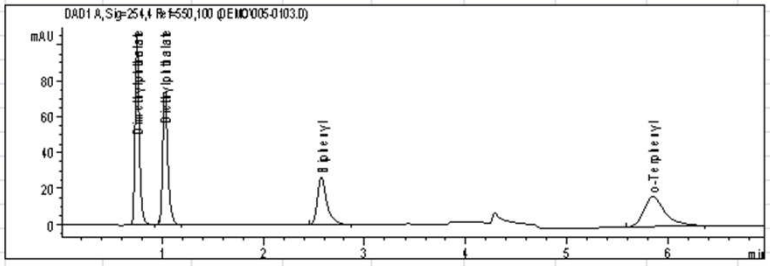
Figure 4a – Create Chem2XL Report Menu item

Figure 4b – Create Chem2XL Report button

	A	B	C	D	E	F	G	H	I	J	K	L
1			Dimethylphthalate			Diethylphthalate			Biphenyl			
2	Sample Name	Vial Loc.	RT	Area	Amount	RT	Area	Amount	RT	Area	Amount	RT
3	Isocratic Std. 1	Vial 5	0.748	296.782	0.090	1.023	264.747	0.089	2.570	176.501	0.006	5.8
4	Isocratic Std. 2	Vial 6	0.747	458.275	0.139	1.024	406.529	0.136	2.571	452.497	0.015	5.8
5												
6												

Figure 5 – Create a Chem2XL Multi-Sample

Sample Name Isocratic Std. 1
Data File C:\CHEM32\1\DATA\DEMO\005-0103.D
Method DEMO.M
Vial Location Vial 5



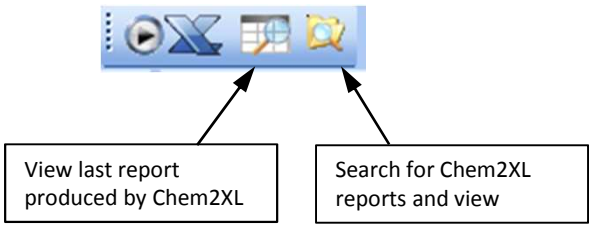
Signal Description: DAD1 A, Sig=254,4 Ref=550,100

Item	Detector	RT	Area	Amount	Peak Name
1	DAD1 A	0.75	296.78	0.090	Dimethylphthalate
2	DAD1 A	1.02	264.75	0.089	Diethylphthalate
3	DAD1 A	2.57	176.50	0.006	Biphenyl
4	DAD1 A	5.85	253.07	0.018	o-Terphenyl

Figure 6 – Create a Chem2XL Single-Sample

b. Sequence Reprocess - To create a Multi-Sample (summary) or Single-Sample report for the entire sequence, press the "Start Sequence Reprocessing" button. If you are asked to save the method say yes if you have just changed the Chem2XL report style.

Figure 7 - Create Chem2XL Multi-Sample or Single-Sample Reports using Sequence Reprocess



Running a sequence with a Multi-Sample Chem2XL template selected can produce reports similar to the one below.

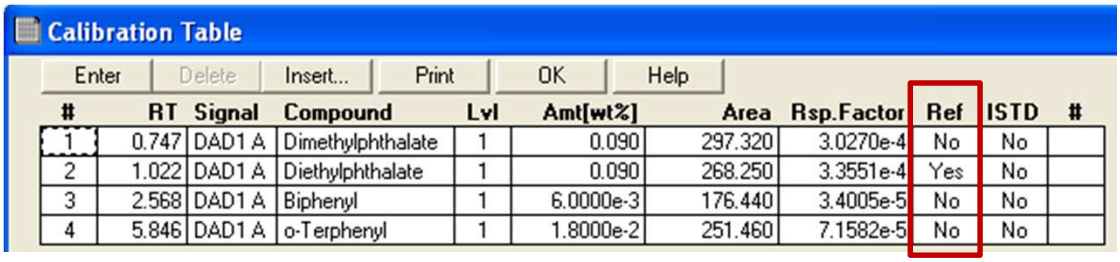
	A	B	C	D	E	F	G	H					
1			Dimethylphthalate			Diethylphthalate							
2	Sample Name	Vial	RT	Area	Area %	RT	Area	Area %	RT	Area	Area %	RT	Area
3	Std. 1 inj 1	Vial 5	0.747	294.5	30.0	1.021	260.3	26.5	2.565	176.1	17.9	5.837	250.7
4	Std. 1 inj 2	Vial 6	0.747	458.3	26.8	1.024	406.5	23.8	2.571	452.5	26.5	5.855	393.2
5	Std. 1 inj 3	Vial 7	0.748	644.9	29.8	1.025	577.2	26.7	2.580	387.3	17.9	5.875	556.0
6													
7		Average	0.747	465.896	28.859	1.023	414.672	25.646	2.572	338.649	20.761	5.856	399.953
8		Std Dev	0.000	175.325	1.793	0.002	158.624	1.628	0.007	144.480	4.931	0.019	152.724
9		RSD	0.06	37.63	6.21	0.18	38.25	6.35	0.29	42.66	23.75	0.33	38.19
10													

Figure 8 -Example Chem2XL Multi-Sample Report after Sequence Reprocess

Appendix:

Relative Retention Time (RRT)

To output RRT on Chem2XL reports you must specify one time reference peak in the ChemStation calibration table. To specify which compound is to be used as the RRT divisor peak select Yes in the "Ref" column of the calibration table.

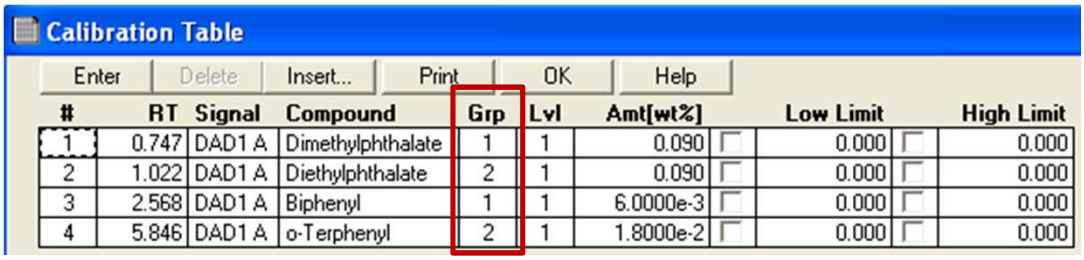


#	RT	Signal	Compound	Lvl	Amt[wt%]	Area	Rsp.Factor	Ref	ISTD	#
1	0.747	DAD1 A	Dimethylphthalate	1	0.090	297.320	3.0270e-4	No	No	
2	1.022	DAD1 A	Diethylphthalate	1	0.090	268.250	3.3551e-4	Yes	No	
3	2.568	DAD1 A	Biphenyl	1	6.0000e-3	176.440	3.4005e-5	No	No	
4	5.846	DAD1 A	o-Terphenyl	1	1.8000e-2	251.460	7.1582e-5	No	No	

Figure 9 - ChemStation calibration table overview – selecting the RRT peak

Compound (Peak) Grouping

To output compound grouping on Chem2XL reports you must group compounds in the ChemStation calibration table (Compound Details view in the calibration table).



#	RT	Signal	Compound	Grp	Lvl	Amt[wt%]		Low Limit		High Limit
1	0.747	DAD1 A	Dimethylphthalate	1	1	0.090		0.000		0.000
2	1.022	DAD1 A	Diethylphthalate	2	1	0.090		0.000		0.000
3	2.568	DAD1 A	Biphenyl	1	1	6.0000e-3		0.000		0.000
4	5.846	DAD1 A	o-Terphenyl	2	1	1.8000e-2		0.000		0.000

Figure 10 - ChemStation calibration table (Compound Details) – selecting compound groups.

A Single-Sample template is included during installation named SDemoCalc.xlt that demonstrates how to group compounds.

Removing Templates from ChemStation report styles

To remove Chem2XL report styles from the ChemStation report styles, click the Chem2XL menu item and choose "Remove Template from Styles". A dialog box will appear that will allow you to remove an individual report style or select "Remove All Chem2XL Report Styles" to remove all report styles.