Chem2XL User Guide

Overview

Chem2XL is an add-on software reporting tool developed for Agilent Technologies'® ChemStation®. Chem2XL supports ChemStation 32 bit versions B.02.01 through B.04.xx. Chem2XL automates the reporting process of the ChemStation by sending data results from the ChemStation into Microsoft® Excel® spreadsheets. Chem2XL is integrated directly into the ChemStation menu allowing the user to set up and use report templates with the click of a mouse. Templates automate the reporting process and can be set-up to handle sophisticated reporting calculations. The generated reports are then saved for future use, or can be printed, or saved as PDF (with pdf generation software). Two types of templates can be created with Chem2XL, a single sample template (one sample per page) or a summary template (multiple samples per page). Chem2XL was created to allow for the flexibility to generate reports automatically after each sample injection, or summary reports after an entire sequence. For qualification purposes, Chem2XL offers an add-on Installation Qualification and Operational Qualification feature (IQ/OQ) which is an automated set of programs that qualifies the installation and operation of Chem2XL.

For additional support assistance, e-mail support@chem2xl.com or visit our website at www.chem2XL.com

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Verify

Chem2XL installation requires Chem2XL files to be saved to the target Agilent ChemStation. To ensure proper installation and operation of Chem2XL, a number of applications must be loaded prior to initial installation.

Verify the following prior to installing Chem2XL:

1. Computer meets or exceeds the minimum hardware specifications for Agilent ChemStation B.02.01 through B.04.xx (see your ChemStation documentation for details). Chem2XL supports 32 and 64 bit versions of Windows 7 & Windows 8 operating systems.

2. ChemStation has all necessary applications loaded:
   - ChemStation B.02.01 through B.04.xx supported
   - MS Excel 2007 or higher

3. Install a printer in Microsoft Windows.

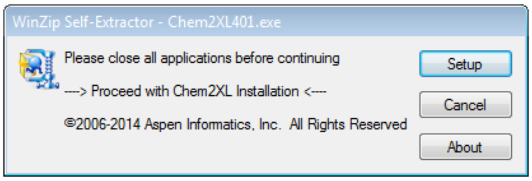
ChemStation B.02.01 through B.04.xx 32 bit versions are recommended for optimal performance of Chem2XL

Install

Before installing Chem2XL, close all programs (including ChemStation) and log on as Administrator

1. Important: before installing Chem2XL, close all applications (including the Agilent ChemStation) and login as the Windows Administrator.

2. Chem2XL may be installed from CD or downloaded. Contact sales@chem2xl.com. To install the downloaded version, run the Chem2XLnnn.exe (where nnn stands for the version number) program and then click Setup.



For the CD Install, insert the Chem2XL CD then locate and execute the program C2Install.exe.

3. Press the Install button to start installation. (see Figure 1.1)

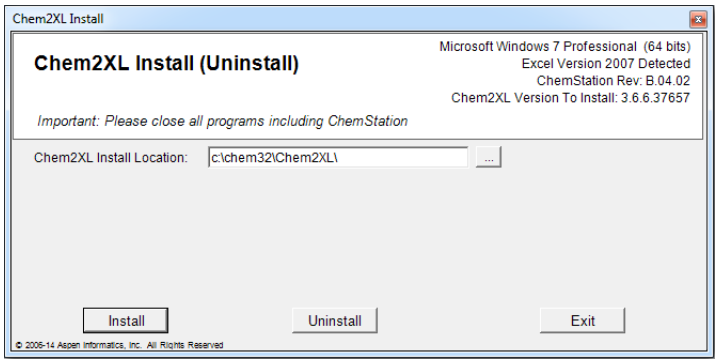


Figure 1.1 Chem2XL installation screen

4. Enter a valid Chem2XL Product License Key for each ChemStation. (see Figure 1.2) Enter the product license key that was sent with the download link or located inside the CD cover. The Chem2XL product license code is 4 groups of 4 characters.

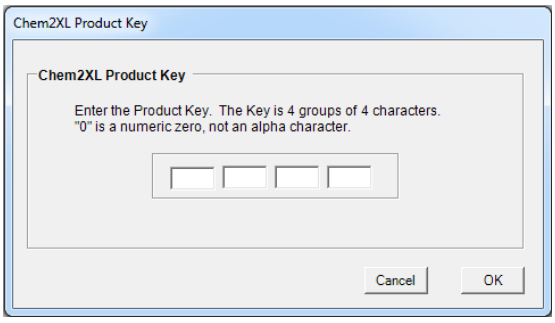


Figure 1.2 Chem2XL Product key validation screen

Install

5. Acceptance of the Chem2XL License Agreement is necessary to proceed with the installation. Select the accept checkbox and click Next if you agree to the license (see Figure 1.3). If you do not agree to the license press Cancel to exit.

If Microsoft Excel version 2003 or older is found on the PC, Chem2XL Installer will look for Microsoft Excel Viewer 2003. If it is found, this viewer will become the default "viewing" program for the Excel reports. This does not apply if newer versions of Microsoft Excel (2007 or higher) are found.

If a PDF viewer is not found on the PC, a dialog box will indicate this. After Chem2XL Installer has completed, a link is provided to download Adobe Viewer. All popular PDF viewers will work. PDF documents are used for Chem2XL User Guide etc.

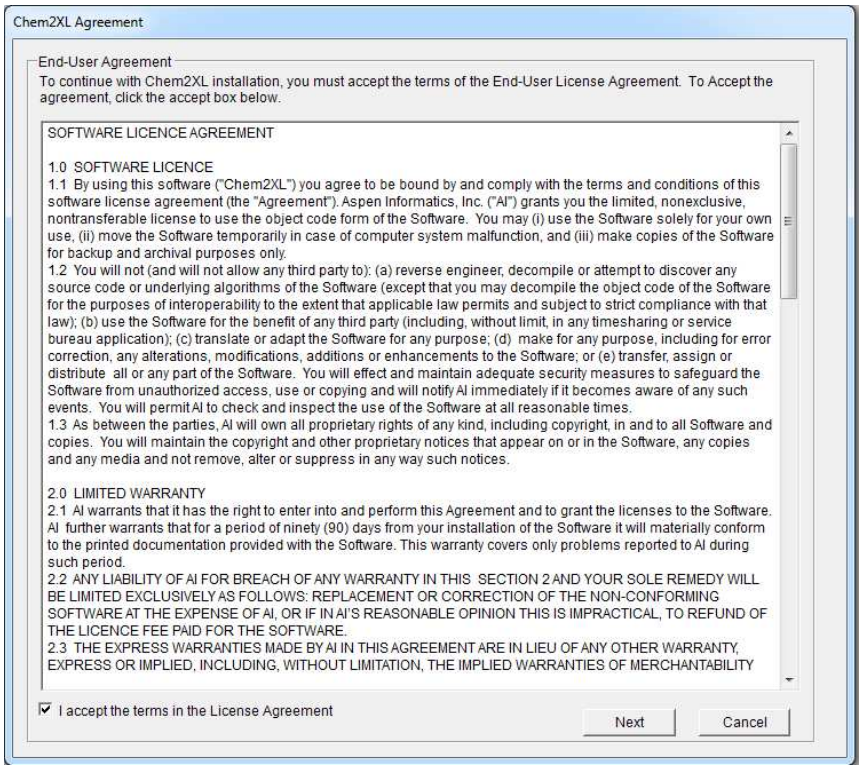


Figure 1.3 Chem2XL license agreement acceptance

Template Creation Workflow

Template Creation allows you to create custom Chem2XL reports. Figure 2.1 shows the basic workflow steps needed to create templates.

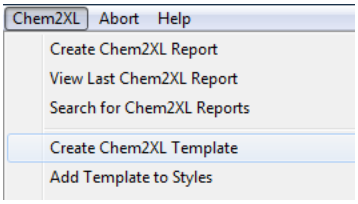
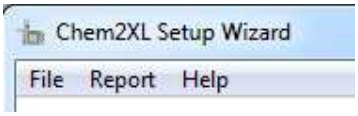
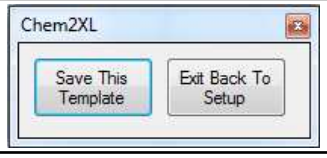
Template Creation Workflow			
STEP	**ACTION**	**Page # FOR MORE INFORMATION**	**CORRESPONDING GRAPHIC**
1	Click the Chem2XL Menu item then Select Create Chem2XL Template	Single-Sample Reports (SS) Pages 7-14 Multi-Sample Reports (MS) (Summary) Pages 15-21	
2	Template Setup Wizard appears Check desired items		
3	Click Create Template Template will be generated		Excel Spreadsheet (Template)
4	Edit Excel Template		Excel Spreadsheet (Template)
5	Save & Name Chem2XL Template	Pages 12 (SS) and 19 (MS)	

Figure 2.1 Basic template creation steps

Report Creation Workflow

Below are the steps to create a Chem2XL report from data and methods in the ChemStation. Figure 2.2 shows the basic workflow steps to produce a report.

Report Creation Workflow

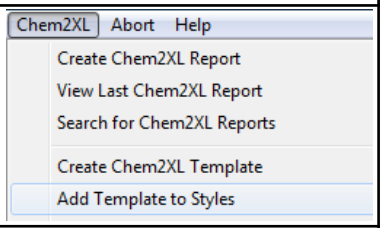
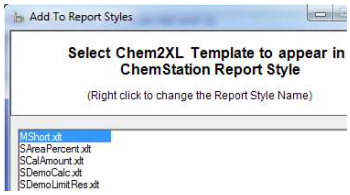
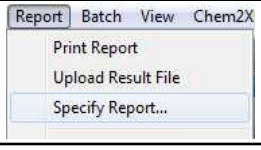
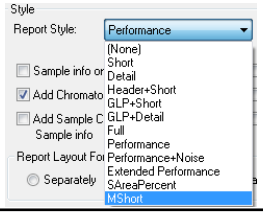
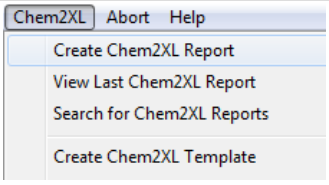
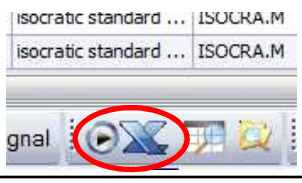
STEP	ACTION	Page # FOR MORE INFORMATION	CORRESPONDING GRAPHIC
1	Add Chem2XL Template to ChemStation Styles	See Page 12 for Single Sample (SS) or Page 19 for Multi-Sample (MS)	
2	Select a Template Style to add to the ChemStation Styles **Note:** Once the Chem2XL template is added to the ChemStation report menu it does not need to be added again		
3	In the Data Analysis mode, Load a ChemStation Data File and Method		
4	Select Specify Report… from ChemStation Report Menu	Pages 13 (SS) and 20 (MS)	
5	Select Chem2XL Template from Report Style: **Note:** the selected Chem2XL template can be saved with the ChemStation method - Save Method	See Pages 11 (SS) or 18 (MS) for information on editing templates	
6a	Select Create Chem2XL Report from menu …OR…		
6b	Select Create Chem2XL Report from Chem2XL icon **Note:** you can also reprocess a sequence to produce all reports in the sequence		

Figure 2.2 Basic steps to produce report

Overview

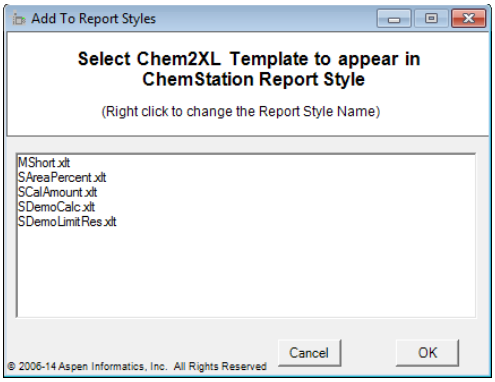


Figure 3.1 Chem2XL templates

To create a Chem2XL report, a template must first be generated (or you can use one of the built-in report templates). You have the option to create your own or use the standard templates included with Chem2XL. The included templates can be found in the Chem2XL pull down menu by clicking *Add Template to Styles.* (See Figure 3.1)

To create a custom single-sample, or multi-sample report, you will create a template using the Template Wizard. The Wizard allows you to define the options included in the report. Correct set up of the templates is very important to receive maximum results from Chem2XL. After the Template Wizard is complete, templates are named and selected as the report style for the ChemStation method. Once the Chem2XL report template is assigned to a method, it is ready for automatic report generation. Report generation can be automated after each run in a sequence or interactively in Data Analysis. Chem2XL saves the report as a Microsoft Excel Workbook for easy use and archiving.

Creating a Single-Sample Template

1. Start the Agilent ChemStation
2. Go to Data Analysis within the Agilent ChemStation
3. Select from the Chem2XL menu Create Chem2XL Template (see Figure 3.2).

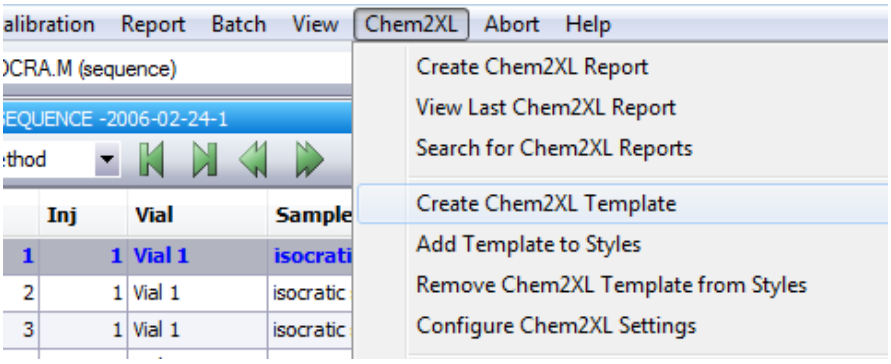


Figure 3.2 Create Chem2XL Template pull down menu

Template Setup Wizard

4. For Single Sample Report, click *Single Sample* and *Include Chromatogram Picture* if desired (see #4 on Figure 3.3).

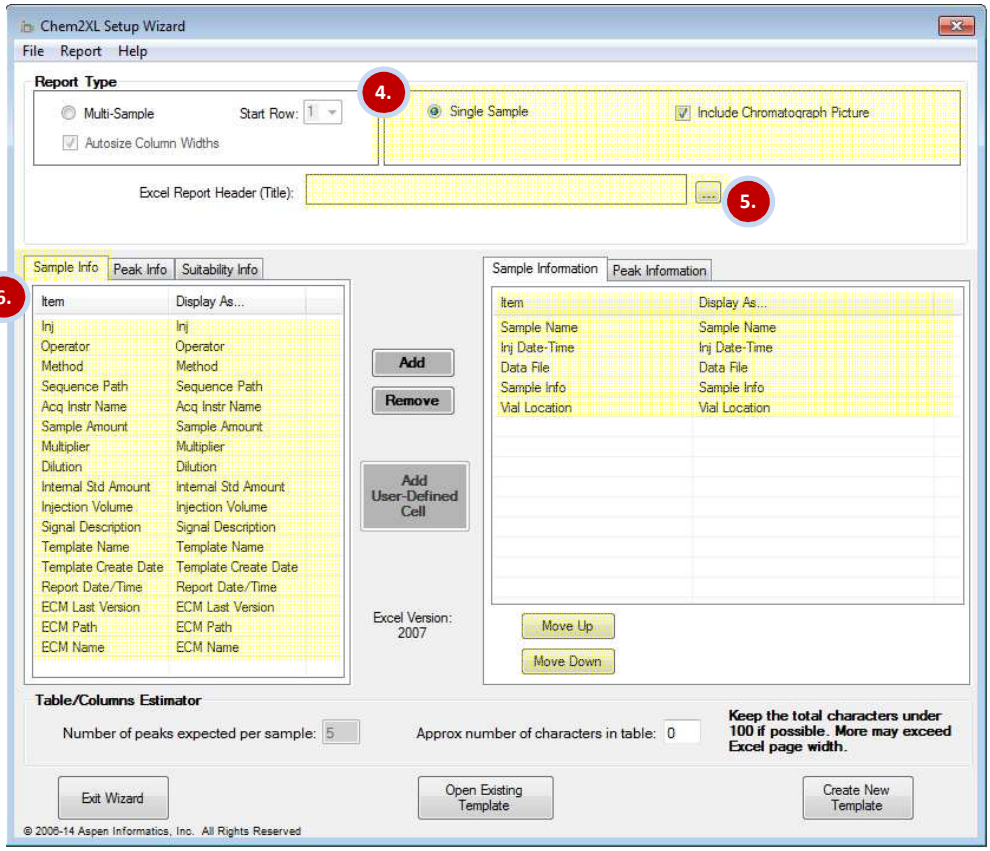


Figure 3.3 Template Setup Wizard

5. (optional) Enter the title that will appear at the top of the Excel Report. Click the [...] box to change the font/size for the Excel Header (see #5 on Figure 3.3)

6. From the Sample Info tab (see #6 on Figure 3.3), choose items to appear on Report Header Section. Click each item desired on the left then click Add (or simply double-click the item). The item will then appear in the Sample Information tab to the right and will now be utilized in the template. If an item is no longer desired, click on the item on the right and then click Remove (or double-click the item to remove it). Items in the Sample information and Peak Information sections will be placed onto the report template in the order of selection. The order of Items may be changed by selecting the item and choosing *Move Up* or *Move Down*. You may also choose *Add User Defined Cell* while the Peak Info tab is selected (see #8 on page 9 for more information

Template Setup Wizard

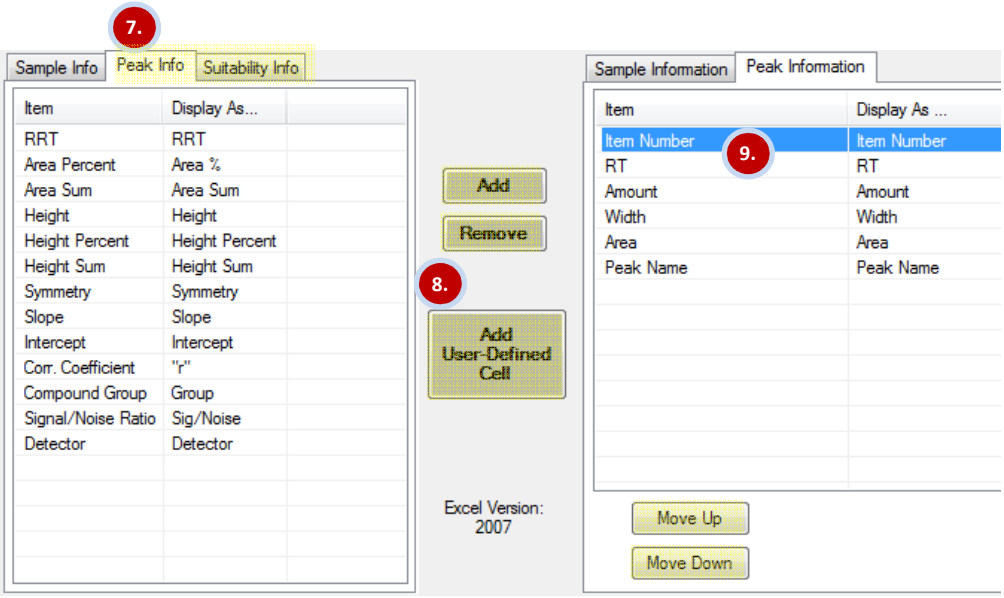


Figure 3.4 Template Setup Wizard continued

Selecting too many Peak Info or Suitability Info items may result in reports 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 makes the font size smaller.

7. Choose the Peak Info tab (see #7 Figure 3.4) and make choices from the left by clicking the choice and clicking Add (or double-clicking the item). Choices will then appear on the right. Items in the Sample Information and Peak Information sections will be placed onto the report template in the order they were selected. The order of Items may be changed by selecting the item and choosing Move Up or Move Down. If an item is no longer desired, click on the item on the right and then click Remove. Items chosen from Peak/Suitability Info sections will appear in the Peak Information Table of the Single-Sample report. Select only the peak items and peak performance (suitability) items that are necessary. See note.

8. (optional) Clicking Add User-Defined Cell (enabled only when the Peak Info or Suitability Info tabs are selected) will place a cell onto the spreadsheet that can then be "programmed" to any mathematical function that Microsoft Excel supports (after the Excel spreadsheet appears on the screen). (see #8 Figure 3.4)

9. Selecting then right clicking on any item name in Sample Information or Peak Information in the right column will allow you to change the text that appears on the report. (See #9 in Figure 3.4 and Figure 3.5)

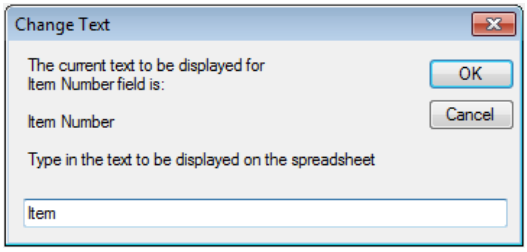


Figure 3.5 Renaming Sample and Peak Information

Template Setup Wizard

10. Table/Column Estimator - estimates the width of the spreadsheet.

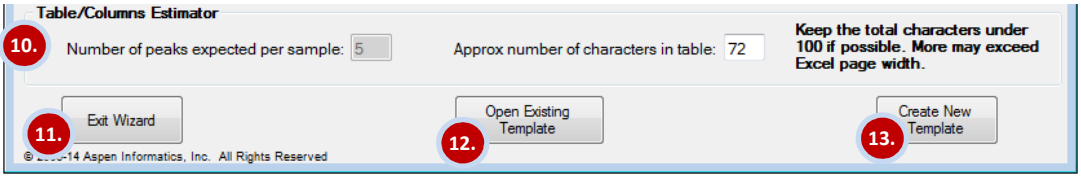


Figure 3.6 Template Setup Wizard continued

11. Choose *Exit Wizard* to discontinue the program.

12. Select *Open Existing Template* to edit a template that has previously been created.

13. Select *Create New Template* when you are satisfied with the choices made within the Setup Wizard. The Wizard will now build a Single-Sample template based on your choices.

14. The template now appears (See Figure 3.7). Further customization may be done to the layout to change formatting (see next page), add borders, change column and row sizes. Moving items around in the template is also possible (however it is best to use the Setup Wizard)

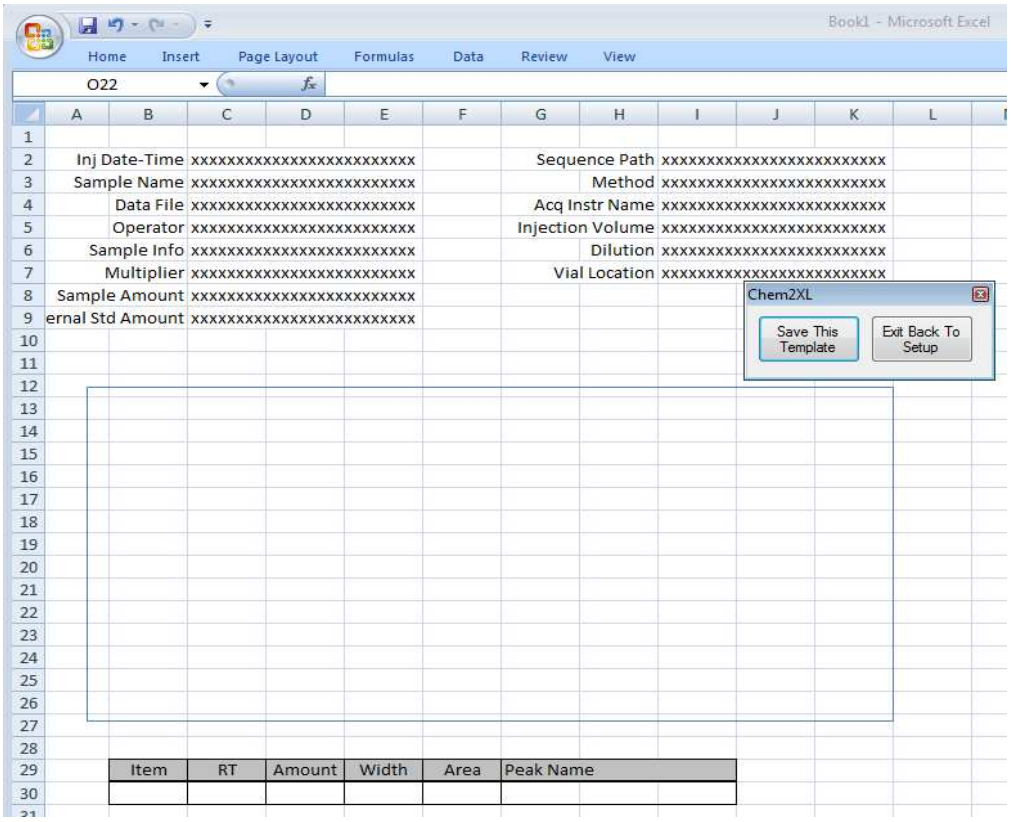


Figure 3.7 Template Setup Wizard continued

Template Customization

15. 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* (see Figure 3.8). Items may also be moved around to different positions on the report screen, (See Note and Figure 3.9).

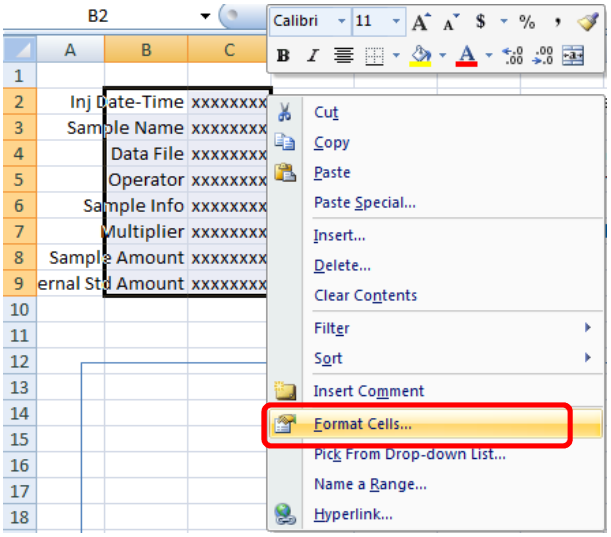


Figure 3.8 Right click to Format Cells

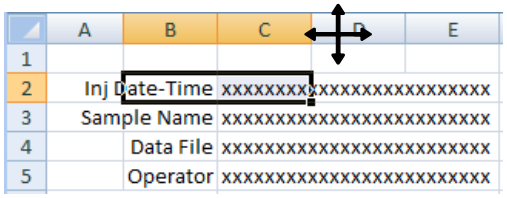


Figure 3.9 Moving Sample Information cells

Be sure to select the name and value cells and move them together.

It is important when moving Sample Information 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 (see Figure 3.9).

Chromatogram Location

16. The empty rectangle in the template is where the chromatogram will be located (see Figure 3.7 page 10). 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 by clicking and resizing the rectangle.

Save Template

17. After editing the template is complete, save the template. Click the Chem2XL *Save This Template* (see Figure 3.10). By pressing this button, the template will be properly saved to the Chem2XL Template Directory. ***Note: Using Excel's File/Save will not automatically save the template to the proper location.*** After saving the template, click *Exit Back to Setup* which will close the template (see Figure 3.10). Exit the Chem2XL Setup Wizard.

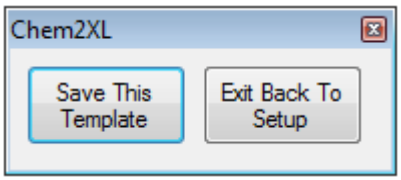


Figure 3.10 Save the template and return to Setup Wizard

Add Template to Styles

18. To create a Chem2XL report, it is necessary to add the template to the ChemStation report styles. After creating a template and saving it (steps 1-17), select Chem2XL drop-down menu, then click on *Add Template to Styles* (see Figure 3.11 & 3.12).

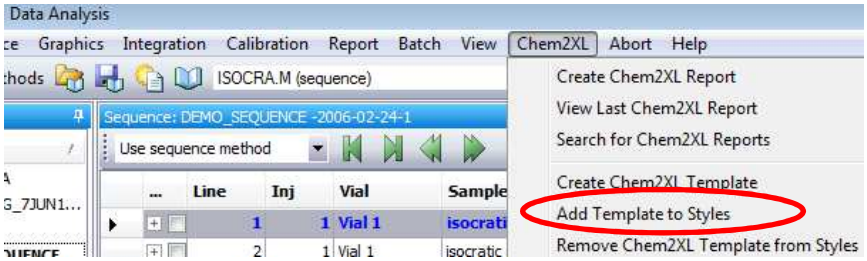


Figure 3.11 Add Chem2XL template to ChemStation Styles.

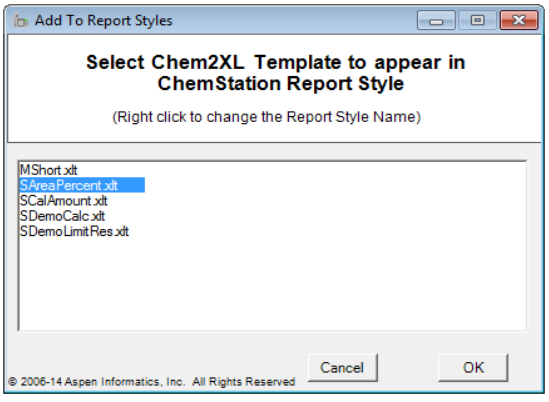


Figure 3.12 Add to Report Styles.

Specify Report

Peaks that are not defined in a Calibration Table will not be output to Excel unless "Report Layout For Uncalibrated Peaks" has been selected. Select either "Separately" or "With Calibrated Peaks" to insure those peaks are output to the Excel report.

When using Multi-Sample reports, it doesn't matter which option you choose, Uncalibrated peaks will be output as "Unnamed Peak". When using Single-Sample reports, it does make a difference. When "Separately" is selected, Uncalibrated peaks will be output to the Table after Calibrated peaks.

19. After a report style has been added, select the ChemStation Report menu item then click *Specify Report...* (see Figure 3.13) Select the desired report style (Chem2XL template) to be used with the ChemStation Method. Chem2XL allows different reporting templates for each ChemStation Method. Select the new report template style in ChemStation by scrolling through the Style list to select the new report template (see Figure 3.14).
Note: After the Chem2XL template is specified, save the ChemStation method and this template will always be used for reporting (until the Report Style is changed and the ChemStation method is resaved)

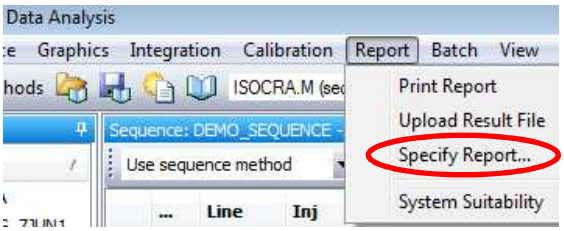


Figure 3.13 Specify Report Menu

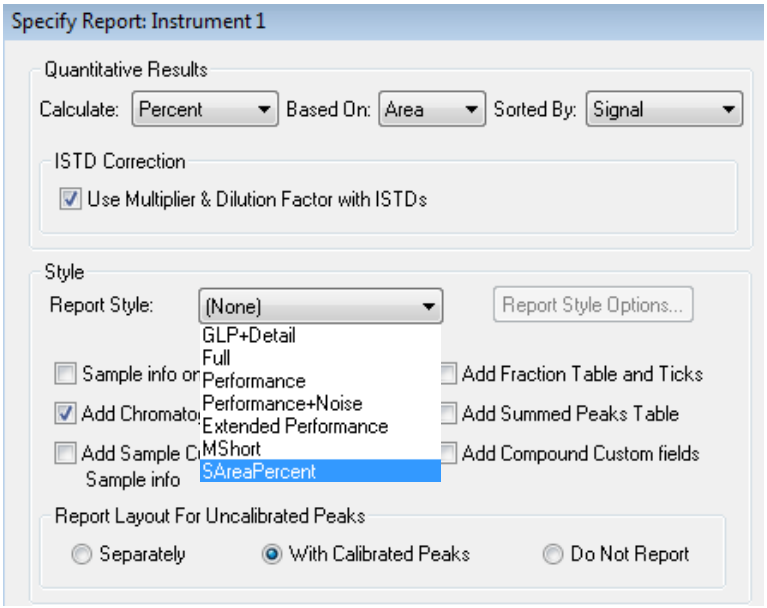


Figure 3.14 Chem2XL Template selection.

Creating Reports

20. Chem2XL will automatically generate output reports by following step 19. To stop automatically creating Chem2XL reports, return to the *ChemStation Report Menu, Specify Report…* and select any item that is not a Chem2XL report style template, for example "*Short Report*".

    Chem2XL will also manually create reports by selecting the Chem2XL pull-down menu and clicking *Create Chem2XL Report* (Figure 3.15) or by clicking the Chem2XL Icon (Figure 3.16).

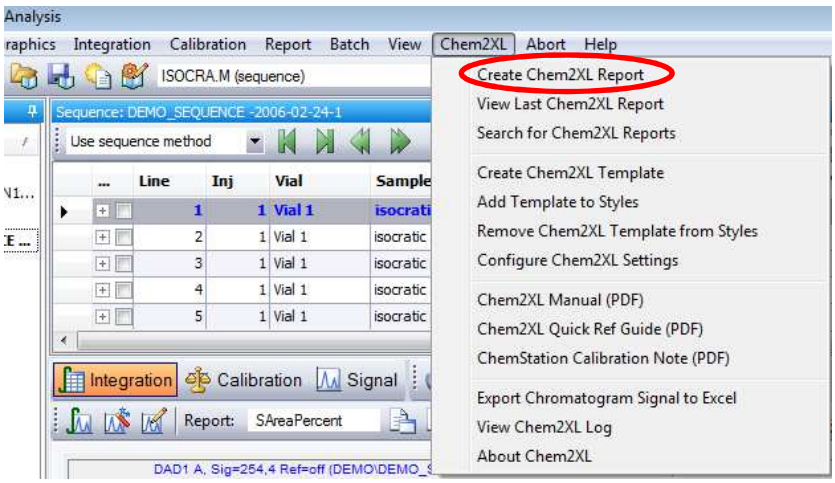


Figure 3.15 Manually Create Chem2XL Report

For ChemStation B.02.01 through B.04.xx, three icons are added to the ChemStation icon bar (Figure 3.16).
The three shortcut Chem2XL icons are:

1. Create Chem2XL Report
2. View Last Chem2XL Report
3. Search For Chem2XL Reports

Figure 3.16 Chem2XL Icons (ChemStation version B.02.01 through B.04.xx)

Overview

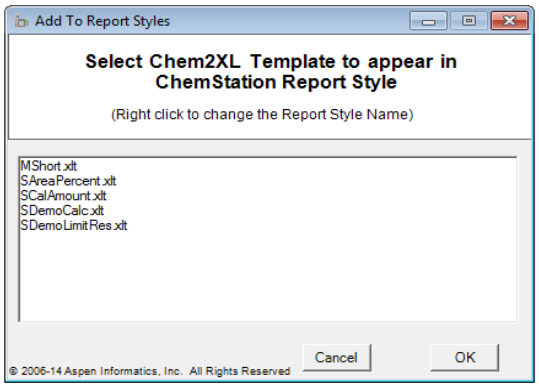


Figure 4.1 Chem2XL templates

To create a Chem2XL report, a template must first be generated. You have the option to create your own or use the standard templates included with Chem2XL. Included templates can be found in the Chem2XL pull down menu by clicking Add Template to Styles. (see Figure 4.1)

To create a custom single-sample, or multi-sample report, you will create a template using the Template Wizard. The Wizard allows you to define the options included in the report. Correct set up of the templates is very important to receive maximum results from Chem2XL. After the Template Wizard is complete, templates are named and selected as the report style for the ChemStation method. Once the Chem2XL report template is assigned to a method, it is ready for automatic report generation. Report generation can be automated after each run in a sequence or interactively in Data Analysis. Chem2XL saves the report as a Microsoft Excel Workbook for easy use and archiving.

Creating a Multi-Sample Template

1. Start the Agilent ChemStation
2. Go to Data Analysis within the Agilent ChemStation
3. Select the Chem2XL menu *Create Chem2XL Template.* (see Figure 4.2)

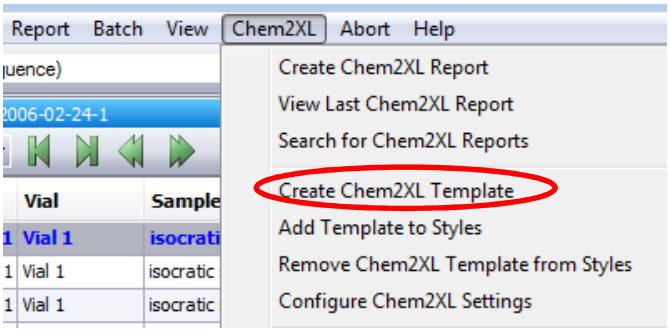


Figure 4.2 Create Chem2XL Template pull down menu

Template Setup Wizard

4. Click *Multi-Sample* (and *Auto Size Column Widths* if desired). Choose the row to start placing the data on the sheet. You can leave up to 9 rows empty at the top for things like company logos, etc. (see #4 on Figure 4.3).

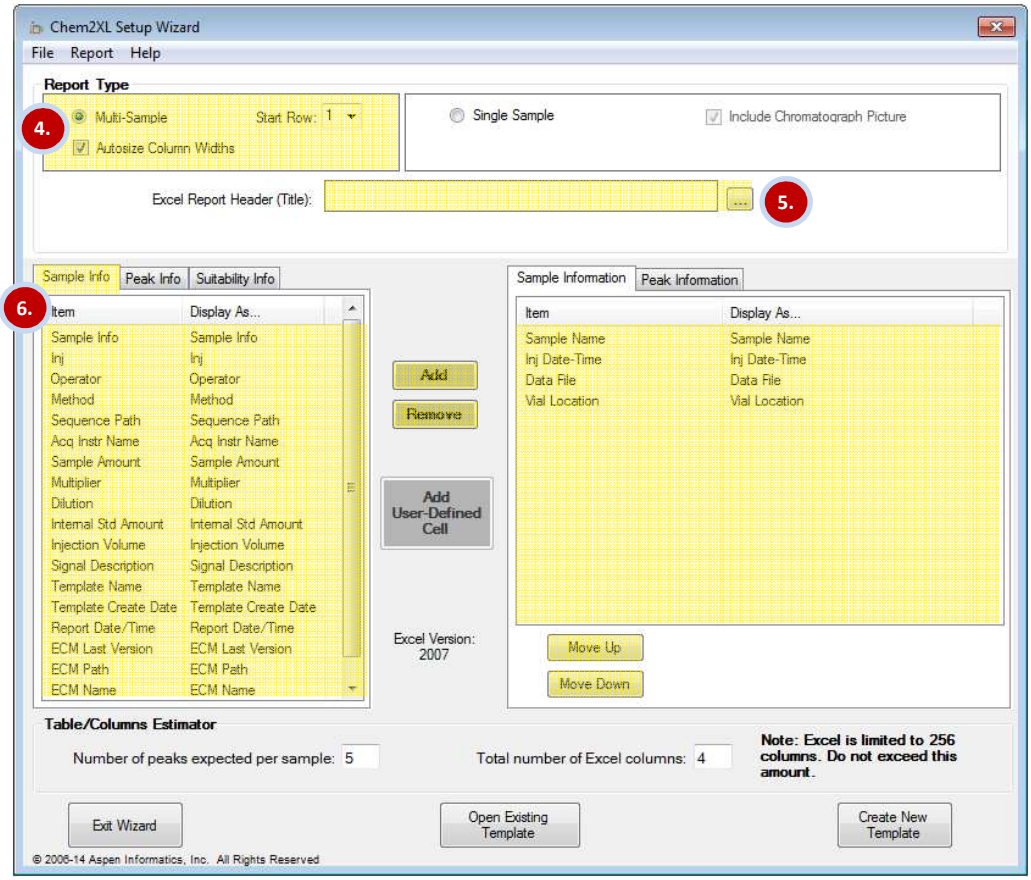


Figure 4.3 Template Setup Wizard

5. (optional) Enter the title that will appear at the top of the Excel Report. Click the [...] box to change the font/size for the Excel Header (see #5 Figure 4.3)

6. From the *Sample Info* tab (see #6 Figure 4.3), choose items to appear on Report Header Section. Click each item desired on the left and click *Add* (or double-click the item). The item will then appear in the Sample Information tab to the right and will now be utilized in the template. If an item is no longer desired, click on the item on the right and then click *Remove* (or double-click the item to remove it). Items in the Sample Information and Peak Information sections will be placed into the report template in the order of selection. The order of Items may be changed by selecting the item and choosing *Move Up* or *Move Down.*

Template Setup Wizard

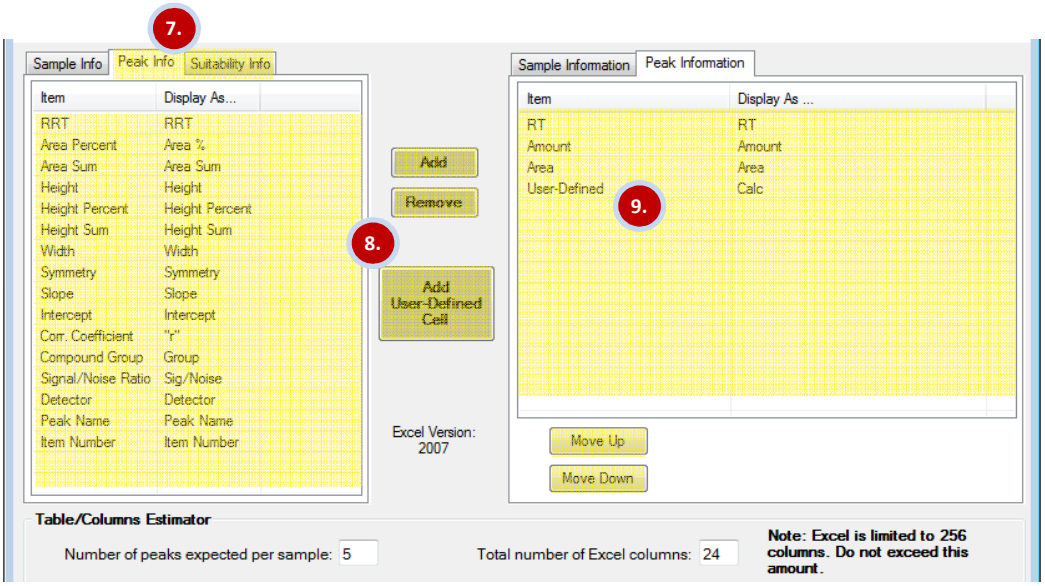


Figure 4.4 Template Setup Wizard continued

Column Estimator: The Compound/Peak Name for each peak detected will be placed onto the report. Under each of these Peak Names, the peak/suitability info will be placed. Column usage example: if 5 Peaks are detected and each Peak Name has 4 peak/suitability info items, 20 Excel columns will be utilized plus the number of Sample Info items selected.

The example in Figure 4.4 has 4 Sample Info items selected & 4 Peak Info items selected. If 5 peaks are detected, 24 Excel columns will be utilized. If 30 peaks are detected, 124 columns will be utilized.

7. Choose the *Peak Info* tab (see #7 on Figure 4.4) and make choices from the left by clicking the choice and choosing *Add* (or double-click the item). Choices will then appear on the right. Items in the Sample Information and Peak Information sections will be placed onto the report template in the order of selection. The order of Items may be changed by selecting the item and choosing *Move Up* or *Move Down*. To remove an item from the right column, click on the item and then click Remove. Items chosen from Peak/Suitability Info sections will appear under the Compound/Peak Name on the report. Select only the peak items and peak performance (suitability) items that are necessary. See Column Estimator note.

8. Clicking *Add User-Defined Cell* (enabled in the Peak & Suitability Info tabs only) will place a cell onto the spreadsheet that can then be "programmed" to any mathematical function that Microsoft Excel supports (after the Excel spreadsheet appears on the screen). (see #8 on Figure 4.4)

9. Right clicking on any item name in Sample Information or Peak Information in the right column will allow you to change the text that appears on the report. (see #9 in Figure 4.4 and 4.5)

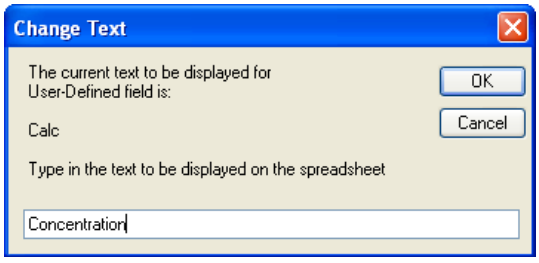


Figure 4.5 Renaming Sample and Peak Information

Template Setup Wizard

10. Select *Create New Template* to create an Excel Template using the choices you have made in steps 1 through 9.

11. The template now appears (see Figure 4.6).

12. Figure 4.6 also shows an example of a formula in cell I3: =G3/25)*10 entered into a *User Defined cell* with a title of "Concentration".

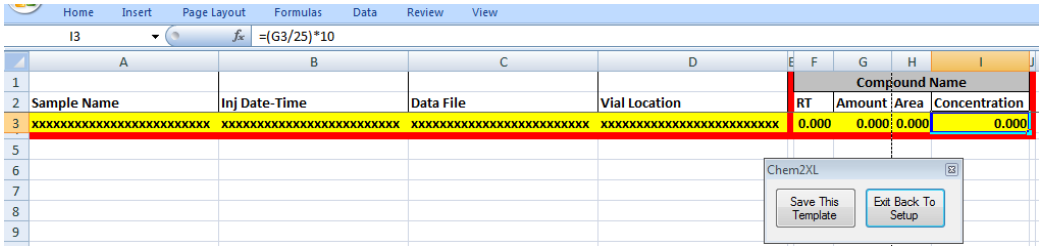


Figure 4.6 Multi-Sample Template example

In Figure 4.6, is a sample of the newly created Multi-Sample Template. The row & columns that are colored red will be removed the first time the template is used to create a report. The yellow color in the cells will be removed.

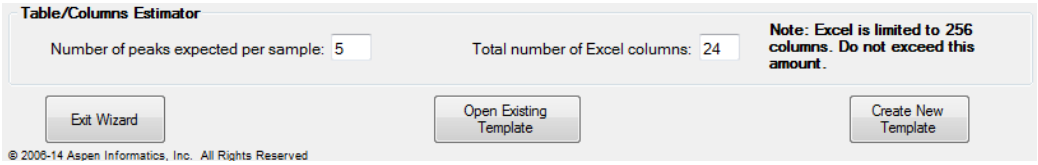


Figure 4.7 Shows the following:

Table/Column Estimator: This will calculate the number of columns to be used on the spreadsheet.

Exit Wizard will exit the Setup Wizard.

Open Existing Template to open/edit a template that has previously been created.

Save Template

13. After editing the template is complete, save the template. Click the Chem2XL *Save This Template.* (see Figure 4.8) By clicking this button, the template will now be properly saved into the Chem2XL Template directory. **Note: saving using the Excel file/save menu will not automatically save the template to the proper location.** After saving the template, click *Exit Back to Setup* which will then close the template (see Figure 4.8) and return to Setup. Quit the Chem2XL Setup Wizard.

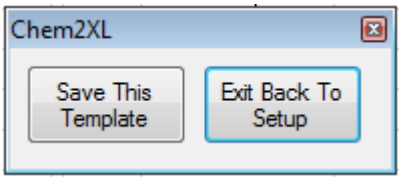


Figure 4.8 Save the template and return to Setup

Add Template to Styles

14. In order for Chem2XL to output reports, it is necessary to add the template to the ChemStation report styles. After creating a template and saving it (steps 1-13), select Chem2XL from the drop down menu and click on *Add Template to Styles.* (see Figure 4.9 and 4.10)

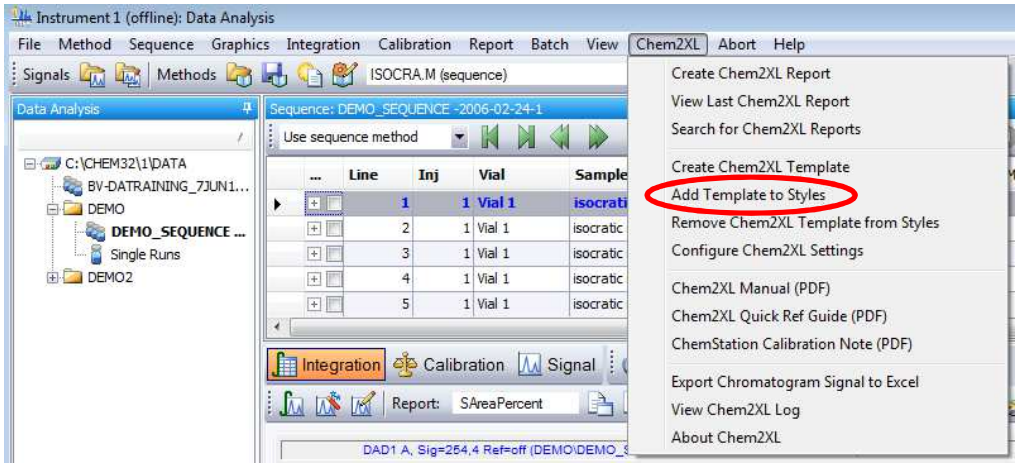


Figure 4.9 Add Chem2XL template to ChemStation Styles.

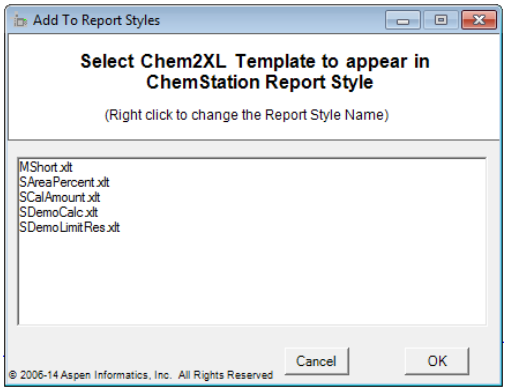


Figure 4.10 Add to Report Styles.

Specify Report

15. After a report style has been added, select the ChemStation Report menu item then click *Specify Report...* (see Figure 4.11)

Select the desired report style (Chem2XL template) to be used with the ChemStation Method. Chem2XL allows different reporting templates for each ChemStation Method. Select the new report template style in ChemStation by scrolling through the Style list to select the new report template (see Figure 4.12).

Note: After the Chem2XL template is specified, save the ChemStation method and this template will always be used for reporting (until the Report Style is changed and the ChemStation method is resaved)

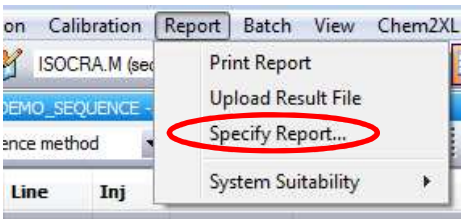


Figure 4.11 Specify Report Menu

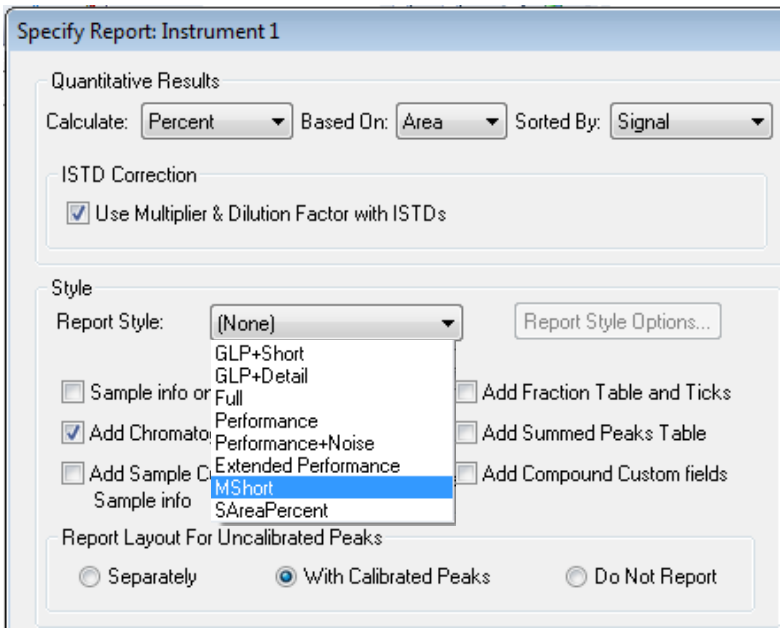


Figure 4.12 Chem2XL template(Style) selection

Creating Reports

16. Chem2XL will automatically generate output reports by following step 15. To stop automatically creating Chem2XL reports, return to the *ChemStation Report Menu, Specify Report…* and select any item that is not a Chem2XL report style template, for example "*Extended Performance*".

    Chem2XL will also manually create reports by selecting the Chem2XL pull-down menu and clicking *Create Chem2XL Report* (Figure 4.13) or by clicking the Chem2XL Icon. (Figure 4.14)

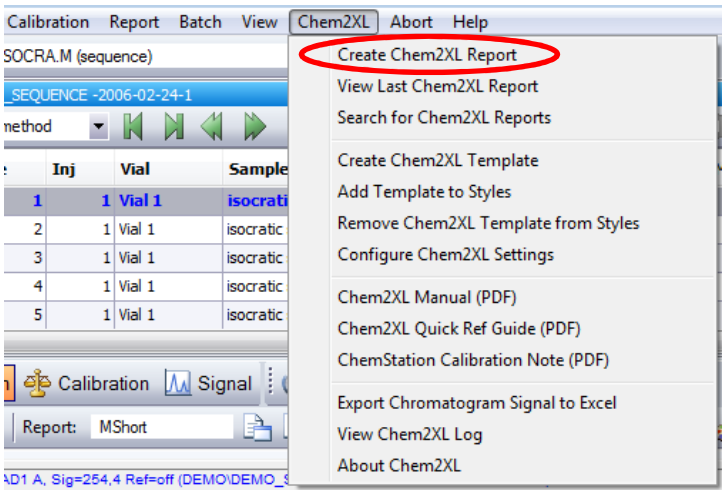


Figure 4.13 Specify Report Menu

For ChemStation B.02.01 through B.04.xx, three icons are added to the ChemStation icon bar (Figure 4.14).
The three shortcut Chem2XL icons are:

1. Create Chem2XL Report
2. View Last Chem2XL Report
3. Search For Chem2XL Reports

Figure 4.14 Chem2XL Icons (ChemStation version B.02.01 through B.04.xx)

Overview

The Chem2XL Configuration Utility determines the following choices:

- Location for saving the output report files
- Naming report files
- Viewing output report files
- Chromatogram export configurations
- Date-Time format
- Miscellaneous Options

Chem2XL Default Report Location

During the installation of Chem2XL, the default directory (or folder) of the ChemStation data files is determined (the ".D "directories). This will be the default location of Chem2XL Single-Sample reports. Select the Chem2XL Configuration menu item. (see Figure 5.1) Shown in Figure 5.2 is the Chem2XL configuration screen with the default locations and names selected.

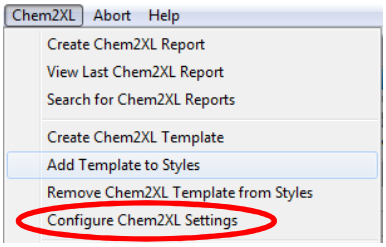


Figure 5.1 Configure Chem2XL Settings

By default, Single-Sample reports will be stored in the ChemStation data file directories. For example, a directory named Demo, the "Parent" directory of the ".D" directories, has multiple data directories beneath it: c:\chem32\1\data\Demo\005-0101.D and c:\chem32\1\data\Demo\005-0102.D. Chem2XL will store reports for 005-0101.D in the 005.0101.D directory and will store reports for 005-0102.D in the 005-0102.D directory. (see Figure 5.2)

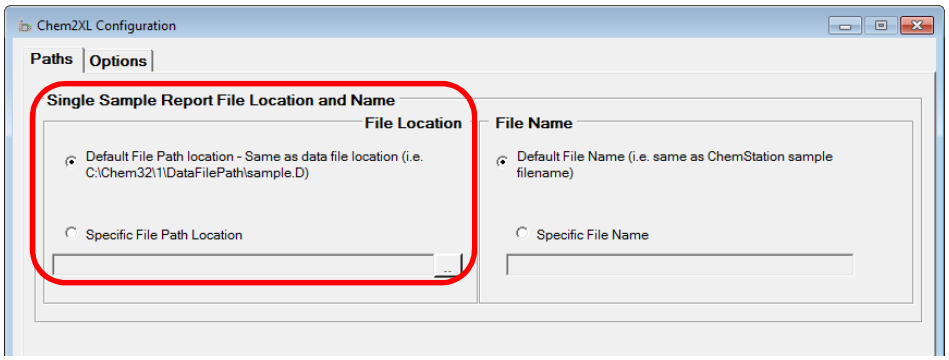


Figure 5.2 Chem2XL Default Single-Sample File location

By default, Multi-Sample reports will be stored in the "Parent" directory of the data files. For example, using the same locations as above, the Multi-Sample report will be stored in c:\chem32\1\data\Demo. (see Figure 5.3)

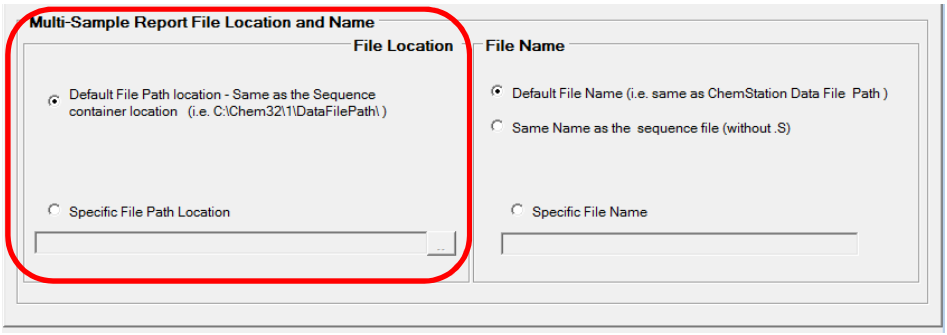


Figure 5.3 Chem2XL Default Multi-Sample File location

Chem2XL Default Report Name

By default, Single-Sample names will be the same as data file name.

For example, a directory named Demo has multiple data directories beneath it: c:\chem32\1\data\Demo\005-0101.D and c:\chem32\1\data\Demo\005-0102.D. The Chem2XL Single-Sample reports will have the same name as the directory, 005-0101.xls and 005.0102.xls respectively. (see Note 1 & 2)

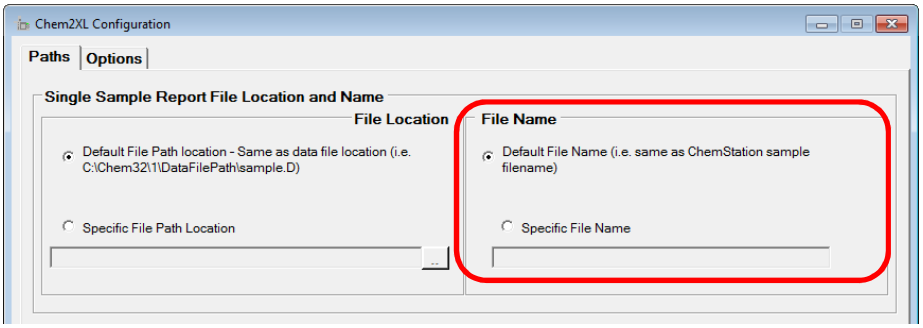


Figure 5.4 Chem2XL Default Single-Sample File Name

Multi-Sample file names by default be the same name as the "Parent" directory. Using the example above, the Multi-Sample report will be named Demo.xls.

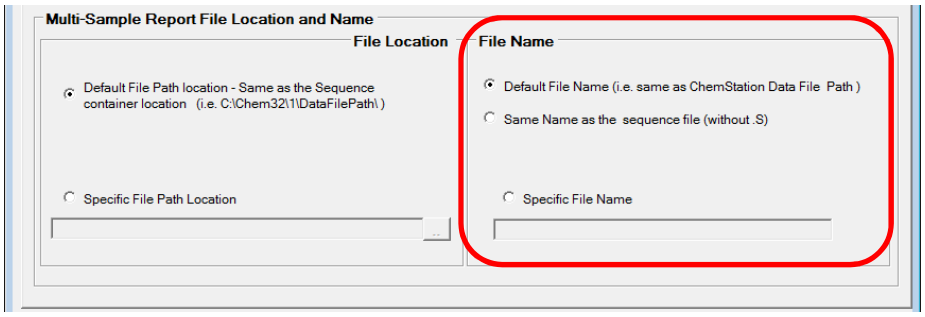


Figure 5.5 Chem2XL Default Multi-Sample File location

If *Same Name as the sequence file (without .S)* is selected, (see Figure 5.5) the name of the sequence will be used for the filename. (see Note 3 & 4)

1. *If Microsoft Excel 2007 or higher is being used, the file extensions will be .xlsx, instead of .xls*
2. *To reduce the chance of overwriting Single-Sample reports saved to a specific location, the Parent folder name will be appended to the path. Each report file will be named the same as the corresponding data file name.*
3. *If a specific location & a specific filename for Multi-Sample reports is selected, all Multi-Sample runs will go to that location/file. This can be useful if it is necessary to save multiple runs or sequences to a single (combined) report file.*
4. *Caution: Multi-Sample report files can get rather large and the possibility exists to exceed the capability of the Excel file when using Excel versions 2003.*

Chem2XL Configuration Options Tab:

From the Options tab, choose which program will be used to view the Chem2XL reports. (see Figure 5.6) It is strongly recommended to select *Microsoft Excel Read Only*. Select *Microsoft Excel Read/Write* only if you close Excel before creating new Chem2XL files. If Excel has the file open for Read/Write and Chem2XL attempts to write to that file, an error will occur.

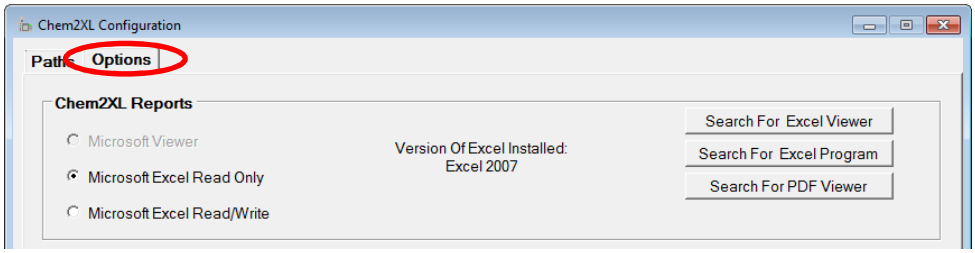


Figure 5.6 View Reports

Microsoft Excel Viewer for Excel 2007 or higher is not supplied with the Chem2XL installation files. In this case, reports by default will be viewed with Excel in the Read Only mode.

Chromatogram Signals: If more than one signal is loaded, Chem2XL will not output the x,y data. If you encounter an error message indicating you should have only one signal loaded, click the ChemStation File menu item, then click "Load Signal…". When the Load Signal dialog box appears, choose one of the signals and click OK.

Chromatogram Export

So you can create/customize your own Chromatogram charts, Chem2XL has the ability to export X, Y data pairs that represent the chromatographic signal. The *Export Every nth Data Point* entry is used to determine the number of data points skipped while outputting data to Excel. Each data pair will be placed on a row on the spreadsheet. Too many data points, however, will slow the Chem2XL output process and possibly exceed Excel's capabilities. If long runs with a high number of data points are expected, you should enter a number larger than 1 to reduce the number of data points. (see Figure 5.7)

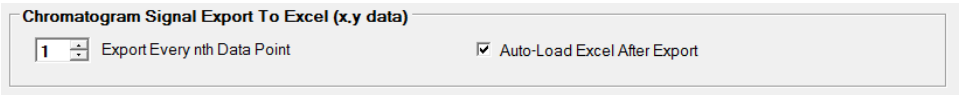


Figure 5.7 Chromatogram x, y output

After saving the configuration, click on the Chem2XL menu item and select *Export Chromatogram Signal to Excel*. (see Figures 5.8 & 5.9)

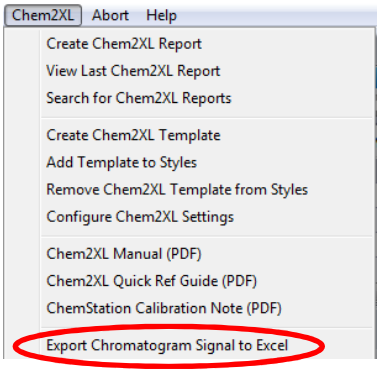


Figure 5.8 Exporting the Chromatogram

	A	B	C
1			
2	Data File:	C:\CHEM32\1\DATA\DEMO\DEM	
3	Sample Name:	isocratic standard	
4	Sample Info:	DAD : slit 2n - all in peak spec	
5	Instrument:	Instrument 1	
6	Operator:		
7	Inject Date/Time:	27-Feb-06, 13:41:39	
8	Report Date:	3/12/2014	
9	Report Time:	10:46:12 PM	
10	Signal:	DAD1 A,	
11	Detector:	DAD1	
12	Title:	DAD1 A, Sig=254,4 Ref=off (DEM	
13			
14	X-Data	Y-Data	
15	-0.015833333	1.083374023	
16	-0.0125	1.091480255	
17	-0.009166667	1.100540161	
18	-0.005833333	1.111030579	
19	-0.0025	1.123428345	
20	0.000833333	1.135826111	
21	0.004166667	1.147270203	
22	0.0075	1.155853272	

Figure 5.9 Chromatogram sample output

Chem2XL Configuration Options Tab:

If the "Output Date as text" is selected, dates may not be sortable. However, other issues can make this preferable in some cases. When a date is put on a spreadsheet and formatted as date, it is actually put on the spreadsheet as a number. Because of the way Excel treats numbers, if the length of the date is wider than the cell into which it is placed, the resulting display will be: ######. This can be fixed of course by making the cell wider, however this may not always be desirable. If it is displayed as text, it can extend beyond the cell width.

DEFAULT DATE-TIME FORMAT

When Chem2XL receives a date from the ChemStation, that date can be converted to one of many different formats. If the Chem2XL Template has been formatted with a particular date format, Chem2XL will attempt to format the date using that format.

Chem2XL will use the following priority to format dates:

1. If the Chem2XL Template has a date format, that format will be used.
2. If the Template has a "General" format, Chem2XL will use the format that is set up in the "Configure Chem2XL Settings" menu item.

For example:
If the ChemStation date is formatted as "dd-MMM-yy, hh:mm" (13-Apr-12, 10:52:01) and the date location on the Template is formatted as "yyyy-mm-dd hh:mm:ss", then Chem2XL will attempt to output the date using the format found on the Template.
If the Template has "General" format for the date location, then the date format selected in the "Configure Chem2XL Settings" will be used. For the pre-configured date formats in Chem2XL see figure 5.10.

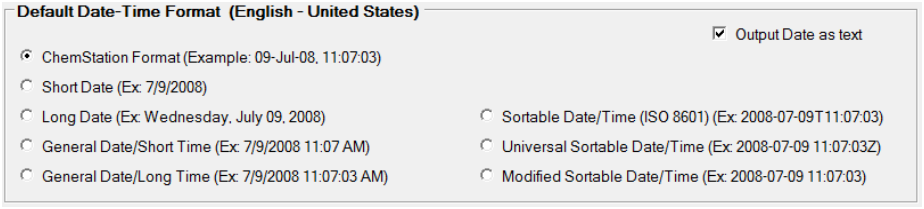


Figure 5.10 Pre-configured date formats

MISC OPTIONS:

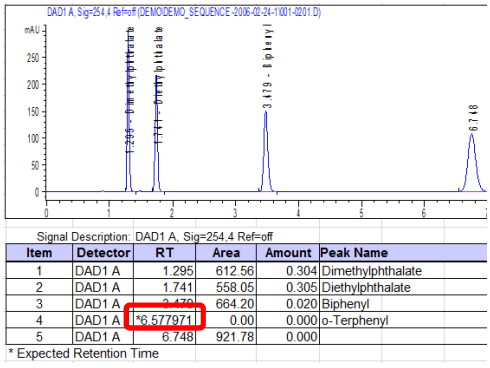
WHEN RETENTION TIME IS NOT FOUND

If a Calibration Table has been set up and one of the named compounds is not detected, Chem2XL will output the expected Retention Time if you have selected *When Retention Time Is Not Found…*
An asterisk will be placed in the same cell to help you identify the undetected compound. (see figures 5.11 & 5.12)

Chem2XL Configuration Options Tab:

1. *If your reports don't have the need for Peak Performance Statistics, unclick this to allow faster processing.*

2. *If the same compound is detected from two different detectors, and Multi-Sample reports are being used, the first compound detected could be overwritten on the spreadsheet.*



Item	Detector	RT	Area	Amount	Peak Name
1	DAD1 A	1.295	612.56	0.304	Dimethylphthalate
2	DAD1 A	1.741	558.05	0.305	Diethylphthalate
3	DAD1 A	3.479	664.20	0.020	Biphenyl
4	DAD1 A	*6.577971	0.00	0.000	o-Terphenyl
5	DAD1 A	6.748	921.78	0.000	

* Expected Retention Time

Figure 5.12 Undetected compound output

MISC OPTIONS:

WHEN RETENTION TIME IS NOT FOUND

If a Calibration Table has been set up and one of the named compounds is not detected, Chem2XL will output the expected Retention Time if you have selected *When Retention Time Is Not Found…*
An asterisk will be placed in the same cell to help you identify the undetected compound. (see figures 5.11 & 5.12)

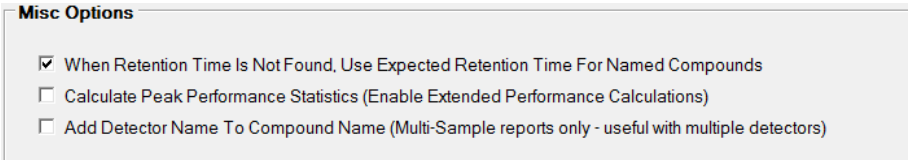
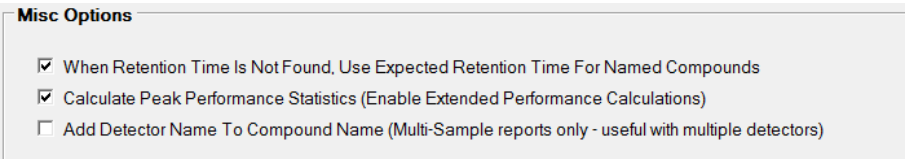


Figure 5.11 Miscellaneous Options

CALCULATE PEAK PERFORMANCE

Check the *Calculate Peak Performance Statistics* box if the Chem2XL report will have any system suitability or peak performance statistics. ChemStation does not produce these calculations by default and therefore it is necessary to select this option to produce the data. (see Note 1)



ADD DETECTOR NAME TO COMPOUND NAME

Add Detector Name To Compound Name is important when multiple detectors are used. Clicking this button assures that all compounds are reported properly on the report if the same compound is detected on two or more detectors. This is important only when outputting Multi-Sample reports. (see Note 2)

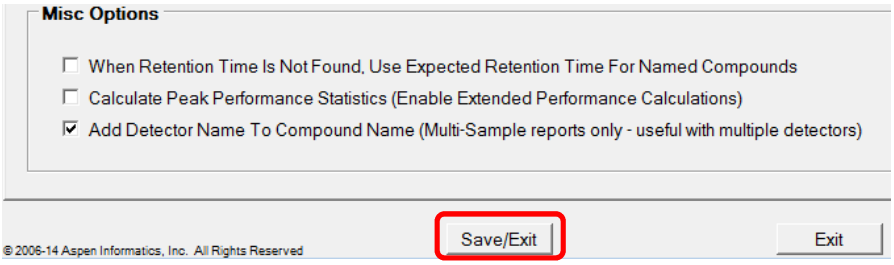


Figure 5.13 Miscellaneous Options

Make sure to click *Save/Exit* after each change. Your selections won't be saved if this button isn't used. (see Figure 5.13)

Search

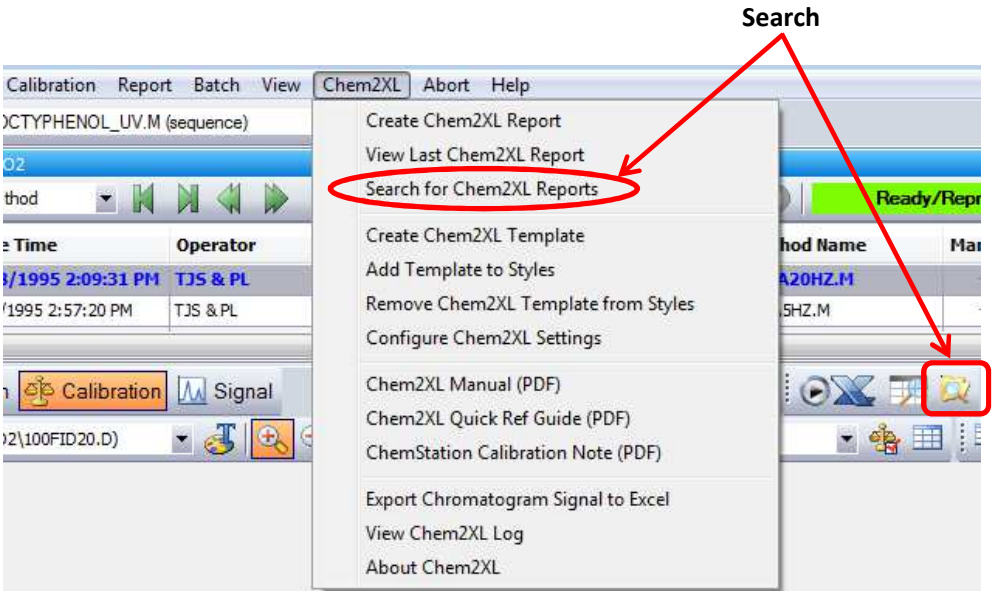


Figure 6.1 Chem2XL Search Utility

The Chem2XL search can be accessed from the ChemStation main menu or from the Chem2XL file icon. The Search Utility will locate Chem2XL reports. The search utility has a number of useful criteria. The search criteria that can be used to query are:

- ◊ Directory path
- ◊ File names (wildcards can be used such as *)
- ◊ Date ranges
- ◊ Keywords within Excel reports (note wildcard searching the default)

Once the list of files is displayed, they can be viewed/edited by double clicking the file. To aid in finding a file within the list, sort the list alphabetically or by date created by clicking on the File or Date heading.

Search

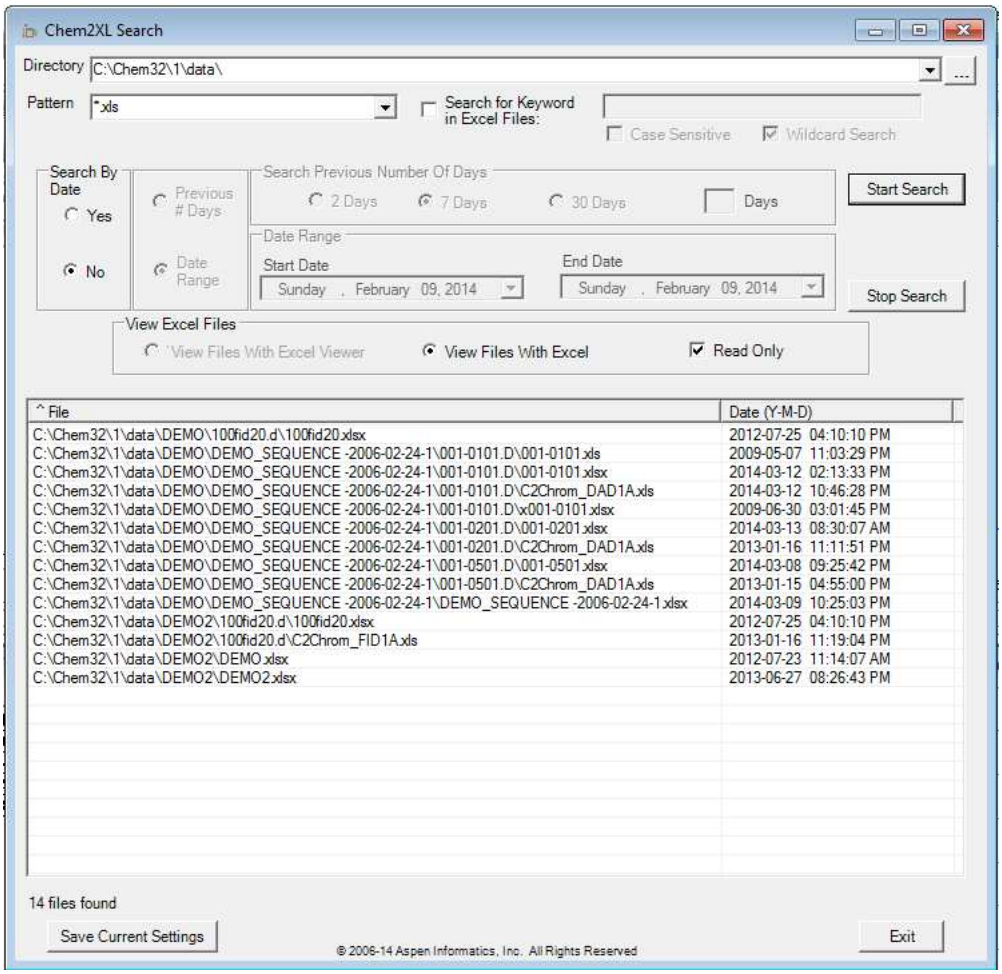


Figure 6.2 Chem2XL Search Utility

*To find all files that contain a particular compound name, enter the name into the "Search for Keyword" text box. Two check boxes below the text box allow further refining of search. If Case Sensitive is checked, upper and lower case characters must match exactly. The Wildcard Search box will allow substitute characters to be found by using the * character. Example *ethylphthalate will find Diethylphthalate and Dimethylphthalate.*

1. To begin SEARCH, enter location of search in the Directory field. The Directory drop-down box is pre-configured with several default locations. Another option to define the search locations is to click on the box with three dots (to the right of the Directory field). From here, navigation to your hard drive is possible to begin the search.

   Search Utility will find all files in the selected directory (folder) as well as those below the selected directory location (directories/folders below the selected location if more directories/folders exist). The default Patterns are *.xls (Excel report files) and *.xlt (Excel template files).

2. To search for a particular KEYWORD within the Excel files, click the *Search for Keyword in Excel Files* box. A text box will now be enabled to allow you to enter any desired text to search for. See Note on left.

3. Date searches may also be incorporated by clicking the desired choice and or entering a Start and End Date.

4. To save the settings in the search utility press the Save Current Settings button located in the bottom left of the screen (optional).

Support Services

Aspen informatics provides software support contracts for an additional fee to extend telephone support and software update services for Chem2XL. Software support helps to improve productivity for system managers and operators of Chem2XL. Support contracts also provide software updates throughout the term of the contract.

Questions

Support questions can be made by emailing support@chem2xl.com. Software support response time is within 2 business days. General software support includes Chem2XL installation and problem analysis and resolution. Aspen Informatics will work to isolate your problem to the covered software product and inform you if the problem is with another application, networking or hardware issues of possible. Support provides the latest product information on the latest product features and known problems and solutions, plus operational advice and assistance.

Bugs - reporting of software problems should be done by sending an email to support@chem2xl.com describing the issue in detail. Typical information needed in the support email include but are not limited to error message, screen captures of the error, usage scenarios, problem reproducibility, and problem description. Please include version of: Windows, ChemStation, Excel and Chem2XL.

Updates

Updates for Chem2XL can be downloaded from Chem2XL website. Software updates are available during the warranty period (90 days following purchase) or for the term of the software support agreement.

Customization

Chem2XL is a very flexible and powerful report generator for the Agilent ChemStation. Chem2XL report templates offer the power of MS Excel and can be created and modified to produce sophisticated reports. Depending on the use and needs, customization can be purchased on a project basis. Customization service can include but are not limited to customizing Chem2XL, template creation, and modifications to the Agilent ChemStation. Support of customized software is based on the project complexity and soft-ware support contracts are quoted as an additional item to Chem2XL support.

Requirements

- ◊ ChemStation B.01.01 through B.04.xx (B.02.01 through B.04.xx is recommended)
- ◊ Microsoft Excel 2007 or higher
- ◊ Microsoft Windows 7 or higher (32bit or 64bit)
- ◊ Microsoft dot net runtime 2.0 or higher
- ◊ For Hardware requirements, see the Agilent ChemStation Specifications

Excel Limitations

Feature	Maximum Limit	
	Excel 2003	Excel 2007-2010
Open Workbooks	Limited by available memory & system resources	Limited by available memory and system resources
Worksheet size	65,536 rows x 256 cols	1,048,576 rows x 16,384 cols
Column width	255 Characters	255 Characters
Row height	409 points	409 points
Page breaks	1000 horizontal & vertical	1026 horizontal & vertical
Length of cell contents (text)	32,767 characters. Only 1,024 display in a cell; all 32,767 display in formula bar.	32,767 characters.
Sheets in a workbook	Limited by available memory (default is 3 sheets)	Limited by available memory (default is 3 sheets)
Colors in a workbook	56	16 million colors (32 bit with full access to 24 bit color spectrum)
Cell styles in a workbook	4,000	64,000
Named views in a workbook	Limited by available memory	Limited by available memory
Custom number formats	200 to 250, depending on language version of Excel installed.	200 to 250, depending on language version of Excel installed.
Names in a workbook	Limited by available memory	Limited by available memory
Windows in a workbook	Limited by system resources	Limited by available memory
Panes in a window	4	4
Linked sheets	Limited by available memory	Limited by available memory
Scenarios	Limited by available memory	Limited by available memory
Changing cells in a scenario	32	32
Adjustable cells in Solver	200	200
Custom functions	Limited by available memory	Limited by available memory
Zoom range	10 percent to 400 percent	10 percent to 400 percent
Reports	Limited by available memory	Limited by available memory
Sort references	3 in a single sort; unlimited when using sequential sorts	64 in a single sort; unlimited when using sequential sorts
Undo levels	16	100
Fields in a data form	32	32

Excel Calculation Limits

Feature	Maximum Limit	
	Excel 2003	Excel 2007-2010
Number precision	15 digits	15 digits
Largest number allowed to be typed into a cell	9.99999999999999E+307	9.99999999999999E+307
Largest allowed positive number	1.79769313486231E+308	9.99999999999999E+307
Smallest allowed negative number	-2.2251E-308	-2.2251E-308
Smallest allowed positive number	2.229E-308	2.2251E-308
Largest allowed negative number	-1E-307	-9.99999999999999E+307
Length of formula contents	1,024 characters	8,192 characters
Iterations	32,767	32,767
Worksheet arrays	Limited by available memory.	Limited by available memory.
Selected ranges	2,048	2,048
Arguments in a function	30	255
Nested levels of functions	7	64
Number of available worksheet functions	329	341
Earliest date allowed for calculation	January 1, 1900 (January 1, 1904, if 1904 date system is used)	January 1, 1900 (January 1, 1904, if 1904 date system is used)
Latest date allowed for calculation	December 31, 9999	December 31, 9999
Largest amount of time that can be entered	9999:59:59	9999:59:59

Sample Information Fields

The items listed are available in Chem2XL reporting. Chem2XL has two main categories of information, Sample Information fields and Peak Information fields.

Sample information fields describe the individual samples that are analyzed and reported.

Acquisition Instrument Name is the name of the instrument that the sample run was originally run on. This value is setup in the ChemStation configuration editor.

Data File: The name of the ChemStation raw data file .
(ex. C:\Chem32\1\Data\April6-2006\Sample1.D)

Dilution: Can be used to compensate for changes in sample volume that occur during sample preparation. Dilution is a numeric value used generally to calculate final concentration of a sample. The value will be used in the ChemStation to calculate final concentration/amount if a calibration calculation type is setup in the ChemStation. The value is entered in the ChemStation sequence table.

Injection Date-Time: Date and Time the sample was injected into the instrument. The timestamp is from the original acquisition instrument internal clock when the sample was run.

Inj: Inj is the injection number from the sequence table.

Injection Volume: Amount of sample that was injected. The units will depend on the sampling device used during analysis. By default LC is dis-
played in milliliters and GC runs are micro liters.

Internal Standard Amount: In the ChemStation this value can be used to compensate for injection variability when the corresponding ISTD calculation type is selected.

Method: Name of the method used to acquire/analyze the sample(s) for a given sequence line.

Multiplier: A scaling factor applied to calculation results before they are reported. Multiplier is a numeric value used generally to calculate final concentration of a sample. The value will be used in the ChemStation to calculate final concentration/amount if a calibration calculation type is setup in the ChemStation. The value is entered in the ChemStation sequence table.

Operator: Name of the operator or user creating the sequence or run.

Sample Amount: Total amount of sample used in the analysis. Sample amount is a numeric value used generally to calculate final concentration of a sample. The value will be used in the ChemStation to calculate final concentration/amount if a calibration calculation type is setup in the ChemStation. The value is entered in the ChemStation sequence table.

Sample Information: an extra field that allows longer description of the sample.

Sample Name: A user-entered name identifying the sample run. Alternates names: sample ID.

Sequence Path includes the name of the sequence used including the path.

Signal Description: The detector used to run the original samples

Vial Location: An identifier for the location from which the current sample will be drawn. For instruments configured with an automatic sampler, this identifier represents the vial's/well's physical location in the sample tray.

Peak Detail Fields

The items listed are available in Chem2XL reporting. Chem2XL has two main categories of information, Sample Information fields and Peak Information fields.

Peak Information fields contain information such as retention time, area, amount and peak performance calculations such as resolution and tailing factor.

Amount: The calculated amount of sample being analyzed. For amount to be calculated you must first build a calibration table and the run calibration standards.

Area: Area is calculated area under the chromatographic peak. Depending on the detector the units vary.

Area Percent: Area percent is calculated from the total area summation (Area Sum) in the chromatogram.

Area Sum: The Area Sum is the total area of all peaks in the chromatogram.

Compound Group: Compound group is a number representing the group to which a calibrated peak belongs. For Chem2XL to output a compound group value you must setup a ChemStation calibration table that has at least one component that is grouped.

Correlation Coefficient: The correlation coefficient gives a measure of the fit of the calibration curve between the data points.

Detector: The detector is the description of the detector used to analyze the sample.

Height: is the response height of the chromatographic peak.

Height Percent: Height percent is calculated from the height of the individual peak in the chromatogram divided by the total height summation (Height Sum).

Height Sum: Height Sum is the total area of all peaks in the chromatogram .

Intercept: The intercept is point at which a linear equation passes through the y axis. In the slope intercept form of a linear equation (y=mx+b) the intercept is represented by b. For Chem2XL to output linear equation information you must build a calibrated method in the Agilent ChemStation and select linear curve fit.

Peak Name: Peak name is the name which is assigned to a peak in the ChemStation calibration table.

R (Correlation Coefficient): The closeness of fit of the data point to the line of regression. A number from 0.0 to 1.0. A 0 value equals no correlation , and 1.0 equals perfect fit.

Retention Time (RT): The time that elapses between injection and elution of a solute is called the retention time (LC and GC) or migration time (CE) tR

Relative Retention Time (RRT): Retention/ migration times are characteristic for the compounds they represent, but they are not unique. Comparisons are normally made in terms of relative retention using a time reference substance.

Signal to Noise Ratio: The Signal-Noise Ratio/Temp. Stability test is used to verify signal to noise performance of the detector and the column temperature stability. For Chem2XL to output signal to noise you must setup a noise range under -> Reports – System Suitability -> Edit Noise Ranges

Slope: The slope is used in quantification of a standard curve (linear regression). The slope represents the rate at which a line increases or decreases. In the slope intercept form of a linear equation (y=mx+b) the slope is represented by m. For Chem2XL to output linear equation information you must build a calibrated method in the Agilent ChemStation and select linear curve fit.

Symmetry (Tailing Factor): For a description of the system suitability (performance) calculations please see the Agilent manual “Understanding Your ChemStation”.

Width: The peak width is the width of the band within the column, which increases the longer the solute stays in the column.

System Suitability

System Suitability (peak performance) Items available in Chem2XL			
Plates	Plates Tangent	Plates 5 Sigma	Plates Statistical
Width	Half Width	Width Half Height	Width 5 Sigma
Width Tangent	Width Tailing	USP Tailing	Selectivity
Resolution Half Width	Resolution Tangent	Resolution 5 Sigma	Resolution Statistical
Statistical Moment 0	Statistical Moment 1	Statistical Moment 2	Statistical Moment 3&4
kPrime: For Chem2XL to output k', you must fill in the ChemStation column information (void volume)			

NOTE 1: For a complete description of the system suitability (performance) calculations, please see the Agilent manual "Understanding Your ChemStation".

NOTE 2: Microsoft Excel must be purchased separately and is not included with Chem2XL.

NOTE 3: ChemStation, ChemStore and OpenLAB ECM are registered trademarks of Agilent Technologies. Chem2XL is used in cooperation with Agilent Technologies.

Excel is a registered trademark of Microsoft Corporation.

What is Chem2XL?

Chem2XL is a custom report generating tool for the Agilent ChemStation that utilizes Microsoft Excel.

What does Chem2XL do?

Chem2XL allows users to create templates to export data to Microsoft Excel spreadsheets. Reports are then saved as MS Excel files, saved as a .pdf (with .pdf generating software), or printed. MS Excel files can then be used for future manipulation.

Why should my lab use Chem2XL?

If your lab spends time manually entering data into a spreadsheet, or uses a calculator to report data, Chem2XL will automate the process, eliminate entry errors and save valuable time and resources.

How does Chem2XL work?

Chem2XL builds user defined sophisticated templates that can be used to automate reporting of single samples or summarize results from sequences in the ChemStation.

Can Chem2XL create templates with custom calculations?

Yes. Chem2XL can be used to build single and multi sample templates that automatically generate ChemStation reports. Templates can be built with custom calculations adding the calculating power of Microsoft Excel to your reporting.

What types of calculations are compatible with Chem2XL reports?

Most Excel functions can be utilized in Chem2XL reports. Examples include Sum, Stdev, Average, Lookup functions, and many others.

Can Chem2XL generate Microsoft Excel files directly from the ChemStation?

Yes. Chem2XL can automatically or manually generate single or multi-sample reports directly into Excel file formats.

What is the difference between a single-sample and a multi-sample report?

Chem2XL creates two categories of report formats, single and multi-sample. A single-sample report contains information pertaining to one sample run/ injection. A multi-sample report contains data from any number of sample runs/injections. For example a multi-sample report can create a summary report containing a row of data for each sample in a sequence. You can use multi-sample reports to help you trend or perform statistics on data.
data.

Where does Chem2XL save the Excel Report files?

By default Chem2XL saves Single-Sample Excel report files to the ChemStation data file directory:
(Ex. C:\Chem32\1\Data\Demo\005-0101.D\005-0101.xls)

By default Multi-Sample reports are saved in the parent directory of the ChemStation data directories:
(Ex. C:\Chem32\1\Data\Demo\Demo.xls)

What instruments will Chem2XL work with?

Chem2XL is designed to work with the LC/GC/AD/LCMS/CE ChemStations.

Is Chem2XL compatible with the Agilent ChemStore database?

Yes. Chem2XL report generation will function with ChemStore. Single-sample Chem2XL report files are stored inside the raw data file directory and therefore will be included when ChemStore stores data files in the database.

Is Chem2XL compatible with the Agilent OpenLAB Enterprise Content Manager (ECM)?

Yes. Chem2XL report generation will function with OpenLAB ECM®. Single-sample Chem2XL report files are stored inside the raw data file directory and therefore will be included when ECM® stores data files in OpenLAB®. As an additional benefit, if you also have Excel Remediation services for OpenLAB, Chem2XL will have an internal audit trail thereby helping with validation.

Will Chem2XL function without Microsoft Excel installed?

No.

Can I use the Microsoft Excel viewer instead of installing Excel?

No. However, Chem2XL can use the Excel viewer to display Chem2XL reports. Chem2XL needs Excel loaded on the PC to generate reports as well as create and edit templates.

Can Chem2XL be run in the ChemStation data analysis only version?

Yes.

What is the best naming convention for Chem2XL templates?

Templates can be named based on ChemStation methods, instruments, calculation types, projects, analysis names, or chemical compounds. It is recommended that Chem2XL templates names reflect the function of the template so that it will be easy for users to relate the name to it's function.

Can Chem2XL reports have color Chromatograms?

Yes, however you need to install a color printer driver and have it selected as the default printer for ChemStation to output the chromatogram in color.

Is there a Chem2XL website?

Yes: http://www.chem2xl.com.

Is Chem2XL supported?

Yes. Inquiries will be answered at support@chem2xl.com.