The ChemStation Treasure Chest
Part 3: Microsoft Excel reporting for ChemStation with add-on software Chem2XL

Technical Note

Introduction

Most ChemStation users are very familiar with performing routine tasks with their software. Are you also aware of the hidden treasures buried within ChemStation? This series of Technical Notes will give you tips and tricks on how to improve your labs outcome by using ChemStation's hidden features.

ChemStation connects very well to external programs. For example, the partner software Chem2XL® from Aspen Informatics™ creates custom reporting solutions by utilizing the power of MS Excel®. Many labs use Excel or a calculator for calculations after GC /LC runs to meet data reporting needs. This Technical Note describes how Chem2XL eliminates manual transcription time and errors, ultimately increasing accuracy and productivity.

How Chem2XL works

Chem2XL automates the reporting process of the Agilent Chem-Station by sending data results directly from the ChemStation into Excel spreadsheets.

Chem2XL is integrated into the ChemStation menu allowing the user to set up and use report templates with a single mouse-click. Templates automate the reporting process and can be set up to handle sophisticated reporting calculations. Two types of templates can be created with Chem2XL, a single sample template (one sample per report) or a summary template (multiple samples per report). The generated reports are then saved for future use, or can be printed or saved as a PDF file (with PDF generation software). Built into Chem2XL are some basic templates that can be selected and used right after loading the software. One of the powerful features of Chem2XL is in the tem-plates that are created for both single sample report and multi-sample reports. In the following we will create a single sample report template.

Step 1: Create a Template:
• From the ChemStation menu press the Chem2XL drop-down menu, select *Create Chem2XL Template* (figure 1).
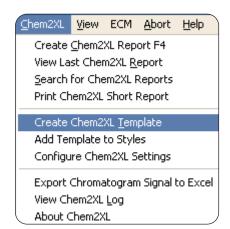

Figure 1
Chem2XL menu - *Create Chem2XL template.*

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- The *Chem2XL Setup Wizard* is now in view (figure 2). Select the items to be included on the report.
- Figure 2 is an example of how to set up a single sample report template.

Step 2: After clicking *Create Template* (or editing an existing template with *Open Template*), the Excel sheet opens, showing the items which were selected in the Wizard. You will see only placeholders on the Excel sheet, because in the template stage no data has been entered into the report. In Excel, you may add a column, and/or custom calculations (such as a column which shows whether your sample passed or failed). In figure 3, an equation is used to test whether the resolution is in the specified range. Conditional formatting is also applied to give passing cells a green color and failing cells a red color. You can enter simple or sophisticated formulas in the cells of the template, depending on your needs.

Step 3: After you have finished editing the template, name and save the template.

Step 4: Back in ChemStation, add the template to the ChemStation report styles by selecting *Add Template to Styles* under the Chem2XL menu (figure 4).
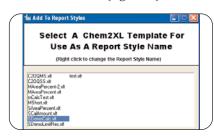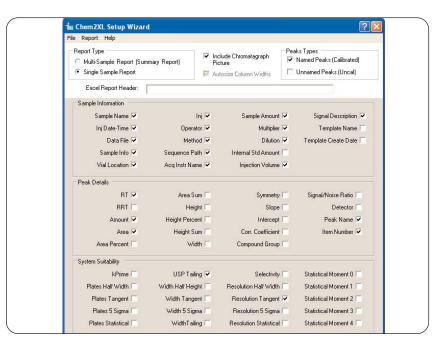
Figure 2
Chem2XL report template wizard.

Figure 3
Creating a Chem2XL template with formula and conditional formatting.

Figure 4
Add Chem2XL report template to ChemStation styles.

Note: Each method can have a separate template that is used for reporting.

Step 5: In the *ChemStation Report* dropdown menu, select *Specify Report*, then select your template under *Report Style* (figure 5).
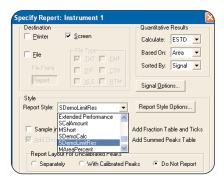

Figure 5
Select the Chem2XL template from ChemStation Report styles

Step 6: You have now added your customized report template to the ChemStation reports and are ready to produce a Chem2XL report by pressing the *Create Chem2XL Report* button. Chem2XL reports can be run inter-actively or automated along with sequence acquisition or process-ing. See example reports in figures 6, 7 and 8. Note that you will need to save the method when you change report styles.

Figure 6
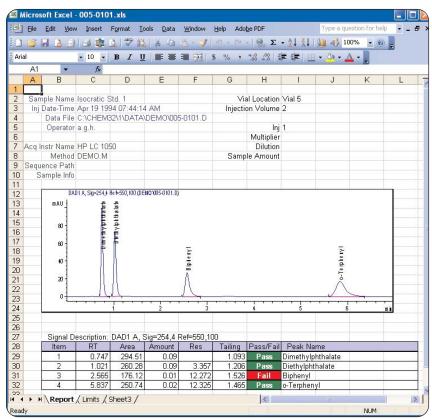**Chem2XL toolbar buttons (ChemStation revision B.02.01 or higher).**

Figure 7
Chem2XL example: Single sample report with Pass/Fail for tailing factor.

Figure 8
Chem2XL Example: Multi-sample sequence report.

Summary

- Chem2XL enables you to quickly create comprehensive report templates in a very short time.

- These templates can be reused again. Chem2XL eliminates manual transcription time and errors, ultimately increasing accuracy and productivity.

- Chem2XL reports can also be saved (along with ChemStation data) inside Agilent's Enterprise Content Manager (ECM). With ECM, Excel Remediation is used to add audit trail and compliance to spreadsheets, further enhancing data integrity.

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