The ChemStation Treasure Chest

Part 1: Create a calibration table in virtually no time

Technical Note

Introduction

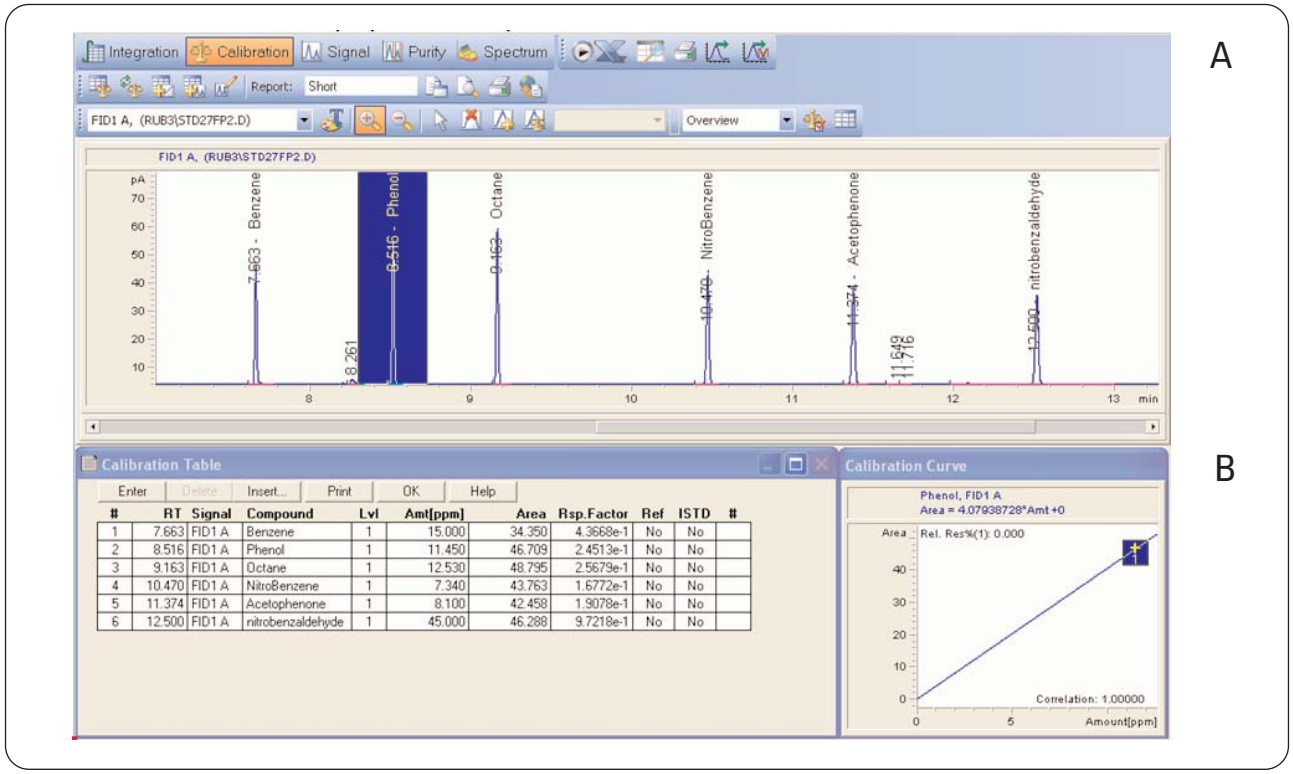
Most ChemStation users are very familiar with performing routine tasks with their software. Are you also aware of the hidden treasures buried within ChemStation?
This series of Technical Notes will give you tips and tricks on how to improve your labs outcome by using ChemStation's hidden features.

Creating an idenfication/calibration table

One area that many ChemStation users find helpful is having the ChemStation identify their peaks. The ChemStation can identify peaks based on retention time as well as their spectral composition. The section below focuses on creating a simple identification/calibration table.

1. From the *Data Analysis* view, load the data file of a sample or standard you have run with ChemStation B.02.01 or higher that contains the peaks of interest. Select the signal you wish to use for quantization. Select *Use current method* in the toolbar of the navigation table
2. Load the method that you used to acquire the data.
3. Make sure you have properly integrated the peak(s) of interest. Tip: To minimize edits to the calibration table, remove unwanted peaks.
4. Make sure that your method is set to display peak names on chromatograms. To do so, click *Signal Options* from the *Graphics* menu. In the dialog box, mark the check box for *Compound Names*.
5. From the Calibration menu, click *New Calibration Table*.
6. In the *Calibrate...* dialog box, click OK to keep the defaults.
7. In the calibration table, locate the cells for *Compound* and *Amt [ng/µL]* (amount). For *Compound*, type the name of each peak. For *Amt [ng/µL]*, type the known quantity for the compound. If the amount is unknown or not important, then type the number 1.
   Tip: To delete a line in the calibration table, click in the grey area to the left of the row to select the row (the selected peak is shown in blue on the chromatogram), then click the *Delete* button.
8. Save the calibration table as part of the method. From the *File* menu, click *Save > Method* or *Save as > Method*.
9. If you want the report to print the amount for each compound, you need to change the report calculation type. From the *Report* menu, click *Specify Report*. Under *Quantitative Results*, change *Calculate* to *ESTD* (external standard) or *ISTD* (internal standard). If you do not wish to calibrate and simply want peak names for identification purposes, then choose *Percent*.

Now you have a simple calibration table that will identify peaks and prints the compound names on reports (Figure 1).



#	RT	Signal	Compound	Lvl	Amt[ppm]	Area	Rsp.Factor	Ref	ISTD	#
1	7.663	FID1 A	Benzene	1	15.000	34.350	4.3668e-1	No	No	
2	8.516	FID1 A	Phenol	1	11.450	46.709	2.4513e-1	No	No	
3	9.163	FID1 A	Octane	1	12.530	48.795	2.5679e-1	No	No	
4	10.470	FID1 A	NitroBenzene	1	7.340	43.763	1.6772e-1	No	No	
5	11.374	FID1 A	Acetophenone	1	8.100	42.458	1.9078e-1	No	No	
6	12.500	FID1 A	nitrobenzaldehyde	1	45.000	46.288	9.7218e-1	No	No	

Figure 1.
The software automatically labels the identified peaks in the chromatogram (A), after you have created the calibration table (B).

Create sophisticated reports with the add-on software Chem2XL from Agilent's partner Aspen Informatics

For advanced reporting, we recommend the Chem2XL® add-on software. It allows you to create single sample or summary (multi-sample) reports using Microsoft® Excel. The software adds buttons for Excel-export to the Chem-Station user interface (Figure 1). You can create custom Excel templates and then process your samples through them, producing reports with custom calculations and the formatting capabilities of MS Excel. Further information about Chem2XL is available at Aspen's website www.chem2xl.com.

Another quantitation tip

To remove the area labels that the software displays on the chromatogram after manual integration, type a simple command on the ChemStation command line: *delann chromreg,,5*. To repeat the command as needed, simply press the F3 key.

Online answers available 24/7

The ChemStation software includes many time-saving features. To learn more, view our LC ChemStation frequently asked questions (FAQs) website, where you will find expert answers to questions from ChemStation users: www.agilent.com/chem/chemstation-faqs

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