

Efficient Strategy for Generating Method-Specific Workflows in an Electronic Lab Notebook

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Purpose

One common concern among scientists regarding implementing an electronic laboratory notebook (ELN) is that method-specific workflows (or templates) may either lack sufficient detail to be useful, or require repeated validation exercises for each new method. However, with the widely applicable strategy for designing ELN workflows outlined here, detailed, method-specific templates can be written for any method in a few minutes without requiring additional validation.

Simple Concept Yields Significant Efficiency

The strategy is to keep all **functionality** in PRIMARY templates, which are otherwise devoid of method-specific information. Primary templates are then used to generate SECONDARY templates with the addition of method-specific details via screen captures (Fig. 1) and hidden tables (Fig. 2). Such method details are automatically made visible to the end user, providing all the instructions necessary for completing a given method task. The functionality of a primary template is not impacted by the mere addition of method-specific information. Thus, primary templates need be extensively validated only once. After that, countless method-specific secondary templates may be very efficiently generated without requiring additional template validation.

Fig. 1 Screen Capture in Secondary Template with Method-Specific Information (No functionality requiring validation)

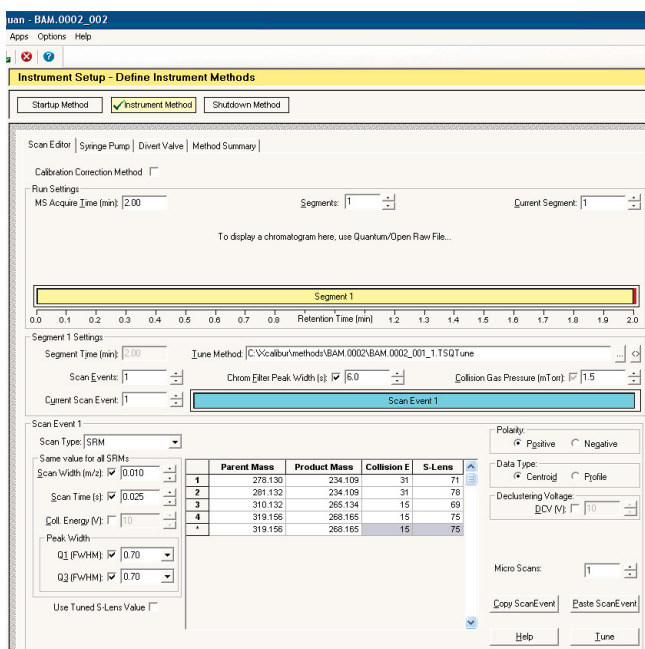


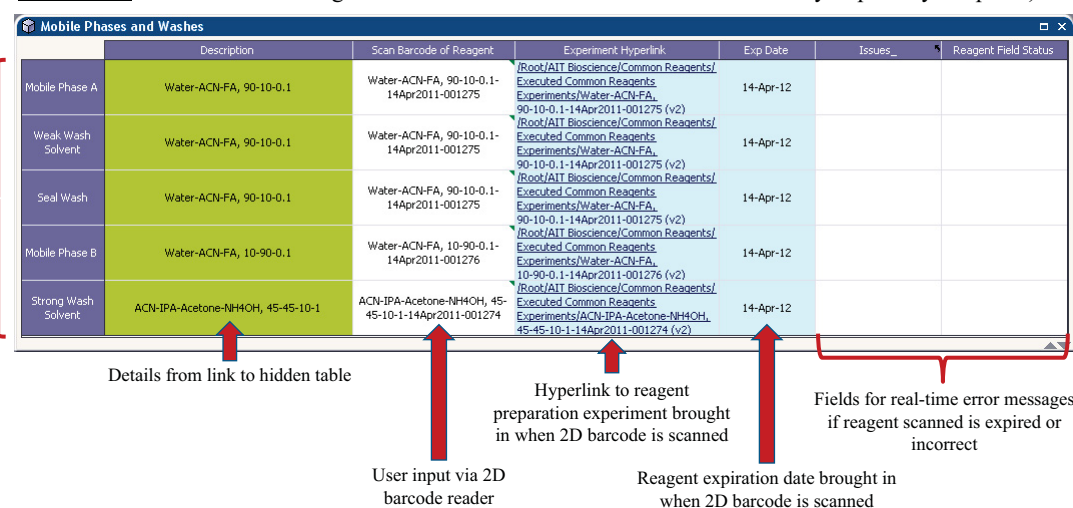
Fig. 2 Hidden Table, Completed in Secondary Template with Method-Specific Information (No functionality requiring validation)

	Analyte 1	Analyte 2
Analyte Name	Methadone	EDDP
Ionization Probe Description	ESI Probe Assembly	ESI Probe Assembly
LC Column	HSS T3 2.1x50	HSS T3 2.1x50
LC Column Temperature (C)	35	35
Injection_Volume (µL)	4	4
Mobile Phase A	Water-ACN-FA, 90-10-0.1	Water-ACN-FA, 90-10-0.1
Weak Wash Solvent	Water-ACN-FA, 90-10-0.1	Water-ACN-FA, 90-10-0.1
Seal Wash	Water-ACN-FA, 90-10-0.1	Water-ACN-FA, 90-10-0.1
Mobile Phase B	Water-ACN-FA, 10-90-0.1	Water-ACN-FA, 10-90-0.1
Strong Wash Solvent	ACN-IPA-Acetone-NH4OH, 45-45-10-1	ACN-IPA-Acetone-NH4OH, 45-45-10-1
Regression Type	Quadratic	Quadratic
Weighting Factor	1/x ²	1/x

Key Features of Strategy:

- ❖ Each type of workflow (ELN template) is developed as a PRIMARY template containing specific functionality that is extensively tested and reviewed. Primary templates contain no method-specific instructions or information.
- ❖ Primary templates contain hidden tables (Fig. 2) where method-specific information is added when SECONDARY templates are generated for each new method. Additional method-specific information can also be easily added via screen captures (Fig. 1). Hidden table content is made available to end-users via links to various user-viewable tables (Fig. 3).
- ❖ Method-specific secondary templates can be quickly generated, as they only differ from each other (and from primary templates) by the specific information (not functionality) included in the hidden tables and screen shots, and thus, do not require additional template validation.

Fig. 3 Example of User-Viewable Table, in Secondary Template (Green cells are from links to information in hidden table in Fig. 2. Other cells result from validated functionality in primary template.)



	Description	Scan Barcode of Reagent	Experiment Hyperlink	Exp Date	Issues_	Reagent Field Status
Mobile Phase A	Water-ACN-FA, 90-10-0.1	Water-ACN-FA, 90-10-0.1-14Apr2011-001275	/Root/AIT Bioscience/Common Reagents/Executed Common Reagents/Experiments/Water-ACN-FA, 90-10-0.1-14Apr2011-001275 (v2)	14-Apr-12		
Weak Wash Solvent	Water-ACN-FA, 90-10-0.1	Water-ACN-FA, 90-10-0.1-14Apr2011-001275	/Root/AIT Bioscience/Common Reagents/Executed Common Reagents/Experiments/Water-ACN-FA, 90-10-0.1-14Apr2011-001275 (v2)	14-Apr-12		
Seal Wash	Water-ACN-FA, 90-10-0.1	Water-ACN-FA, 90-10-0.1-14Apr2011-001275	/Root/AIT Bioscience/Common Reagents/Executed Common Reagents/Experiments/Water-ACN-FA, 90-10-0.1-14Apr2011-001275 (v2)	14-Apr-12		
Mobile Phase B	Water-ACN-FA, 10-90-0.1	Water-ACN-FA, 10-90-0.1-14Apr2011-001276	/Root/AIT Bioscience/Common Reagents/Executed Common Reagents/Experiments/Water-ACN-FA, 10-90-0.1-14Apr2011-001276 (v2)	14-Apr-12		
Strong Wash Solvent	ACN-IPA-Acetone-NH4OH, 45-45-10-1	ACN-IPA-Acetone-NH4OH, 45-45-10-1-14Apr2011-001274	/Root/AIT Bioscience/Common Reagents/Executed Common Reagents/Experiments/ACN-IPA-Acetone-NH4OH, 45-45-10-1-14Apr2011-001274 (v2)	14-Apr-12		

Results

During method development, as various parameters are updated, the hidden table in the validated instrumental analysis template is populated with the method-specific information. Additionally, screen captures of LC and MS/MS parameters such as the mobile phase gradient, tune parameters, and m/z transitions are also brought into the template, providing more instructional detail without impacting previously-validated template functionality. Taking merely minutes to create from a previously validated primary template, such secondary templates provide all necessary method-specific details without requiring additional validation.

Conclusion

This widely applicable design strategy efficiently yields workflows that are sufficiently method-specific to be useful, without requiring additional workflow validation.