

Strategy for Designing Electronic Lab Notebook Workflows Both Flexible Enough for R&D and Comprehensive Enough for Regulated Work

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Purpose

Electronic laboratory notebook (ELN) workflows are typically designed for either research or regulated use. Documentation requirements for regulated sample analysis are unnecessarily comprehensive and rigid for free-form research. Creating and validating separate templates targeted for different uses is inefficient. Presented here is a widely applicable, strategy for designing practical ELN workflows (templates), whereby the same template can be used across the full range of regulatory requirements, from non-regulated R&D to fully regulated sample analysis.

Key Features of Strategy:

- Validating a single, multifunctional template is more efficient than validating multiple templates targeting different experiment types.
- Valuable ELN functionality is made available and practical for R&D experiments to whatever extent desired by the end user for any given experiment.
- Experiments performed during R&D, where 21CFR Part 11 compliant documentation and error checking are not required, are prevented from use in support of regulated sample analysis.

Simple Concept Yields Significant Flexibility

Logic embedded into each workflow is written to turn on and turn off specific functionality based upon the type of experiment selected.

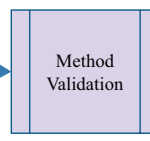
Four experiment types are provided as options in Bioanalytical methods within an ELN:

Run Identification Table	
	Entry
Study	0022-1058
Run	002
Run Type	
System Suitability Study	0022-1058 S5
System Suitability Run	2
_BAM	BAM.0002
BAM Version	BAM.0002.02
_BAM Title	Analysis of Methadone and EDDP in Human Plasma by LC-MS-MS
_Validation Level	Regulated



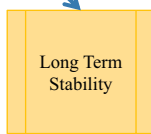
No mandatory user entries nor error checking, yet still provides useful ELN functionality as desired:

- Accurate, reproducible calculations
- Comprehensive record of equipment, supplies, and reagents used
- Screen captures, notes, and data files easily retrievable and shared



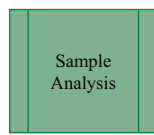
- All mandatory user entries and error checking required, except QC need not be within stability (not yet established)

- Fresh Calibrators are required
- System Suitability is not required (not yet established)



- All mandatory user entries and error checking required, except for ensuring long term QCs are within stability (not yet established)

- Fresh Calibrators are required
- System Suitability is required



- All mandatory user entries and error checking required
- Calibrators and QCs must be within established stability
- System Suitability is required

Both yield standard Experiment ID (circled in red)

Note the Experiment ID has a leading "MD" (method development) **automatically** applied for use in segregating this data from regulated use. Numerous other error checks are not applied.

Status	
Instrumental_Analysis	MD-IA-BAM.0002.02-0022-1056-001
Is BAM Template Appropriate For This Sponsor?	Yes
Is BAM Template Appropriate For This Study?	NA
Correct BAM Version and Regulatory Status?	NA
All Mandatory Fields Complete?	NA
Passed All Field Checks?	NA
System Suitability Acceptable?	NA
Template Formulas Intact?	NA

Status	
Instrumental_Analysis	IA-BAM.0002.02-0022-1056-001
Is BAM Template Appropriate For This Sponsor?	Yes
Is BAM Template Appropriate For This Study?	Yes
Correct BAM Version and Regulatory Status?	Yes
All Mandatory Fields Complete?	Yes
Passed All Field Checks?	Yes
System Suitability Acceptable?	Yes
Template Formulas Intact?	Yes

Results

Validated ELN workflows provide diverse utility throughout method development, method validation, and sample analysis. With the embedded logic strategy described above, any workflow functionality of interest during method development is available without requiring undue, or impractical, regulatory compliance. For example, numerous (even expired) reagents could be tested during method development to determine the resulting level of carryover, without halting the experiment if the reagents or results were unacceptable. However, these same workflows are also sufficiently flexible and comprehensive for use during method validation and sample analysis to confirm a litany of mandated acceptance criteria. Despite using the same validated workflows, however, data obtained during method development is segregated from use in support of regulated studies via automatically applied experiment naming conventions.

Conclusion

This strategy allows research chemists to benefit from the same useful ELN workflow functionality required for regulated work without incurring unwarranted regulatory burden.