

Streamlining Workflows in Chromatography Laboratories

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INTRODUCTION

At a basic level, all chromatography workflows are similar—samples are injected, chromatographic separations are performed, data is captured, and results are generated. Where workflows differ is in the details, such as instrument conditions, injection sequence requirements, data evaluation process, and techniques by which results are calculated. Setting up these different details is a time consuming and error-prone process.

For example, a chromatographic analysis in regulated laboratories typically requires that a user configures a sequence with a set number of system suitability injections, calibration standards, and check standards. In addition, it is often required to perform duplicate or triplicate injections of each sample for analysis, and to repeat bracketing standards at regular intervals. After acquisition of data, a user typically has to process the data according to rules described in the standard operating procedure, and then calculate the results. An error in any one of these steps can invalidate the data and require that all samples are run again.

This poster describes a new software solution that streamlines all chromatography workflows, significantly reducing the time taken between receiving a sample for analysis and producing the final result.

AN INTRODUCTION TO eWORKFLOWS

eWorkflows are a set of rules within the Dionex Chromeleon® Chromatography Data System software that capture all of the characteristic aspects of a chromatography workflow. Users only need to provide a minimum amount of information when starting their chromatographic experiment. When using an eWorkflow, the user will only need to select an instrument, enter the number of samples for analysis and starting vial position, and then hit go.

When an eWorkflow is executed, it automatically builds all elements of a chromatography sequence:

- Provides a list of all available and suitable instruments
- Provides the correct sequence name and storage location
- Creates an injection list following the rules of the workflow
- Defines all important injection settings (Injection Volume, Injection Type, Calibration Levels, Dilution Factors, etc.)

- Provides all custom variables necessary for this workflow
- Provides all associated objects for the sequence (Instrument and Processing methods, Reports)
- Includes attachments for reference (such as PDF documents)
- Shows only those data fields that are necessary for the workflow

This automated process significantly reduces the number of steps required to create a sequence of injections. In addition, the instrument method selected contains the correct settings for running the analysis, the processing method contains the appropriate peak detection and calibration settings, and the report correctly calculates all necessary results. This further minimizes the number of steps and amount of time it takes to get to the final result.

RUNNING AN eWORKFLOW

All eWorkflows are organized in the eWorkflows Category (Figure 1). The navigation pane provides an overview of all eWorkflows available for the user (Figure 1A). For the selected eWorkflow the Work Area (Figure 1B) provides a list of all instruments in the network which are suitable to run the selected eWorkflow, including their current status. In addition any attached documents (such as method SOP) are immediately accessible.

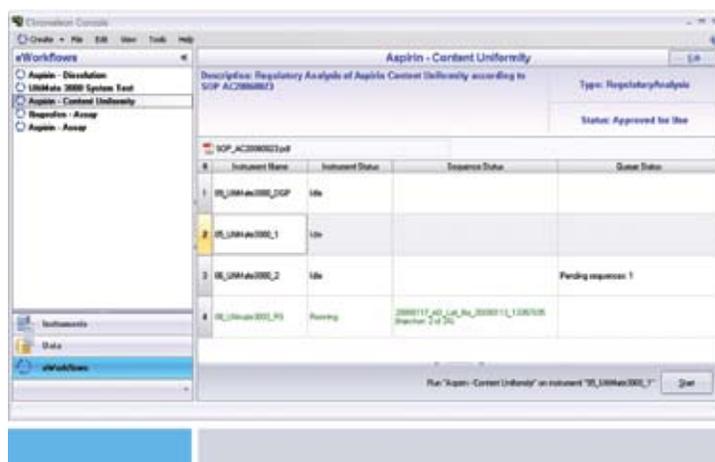


Figure 1. eWorkflows category showing all available eWorkflows.

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When a suitable instrument is selected, the user is only a few mouse clicks away from starting a run.



Figure 2. Select an Instrument to run the eWorkflow.

The eWorkflow wizard is initiated with the start button (Figure 2). Simply enter the number of samples to analyze and their start position in the autosampler (Figure 3).

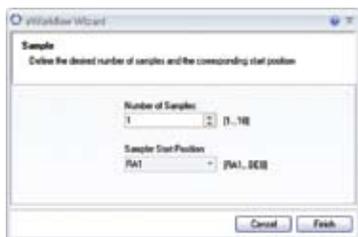


Figure 3. Enter number of samples to analyze.

The sequence is automatically created according to the sequence layout defined in the eWorkflow and ready to start (Figure 4).

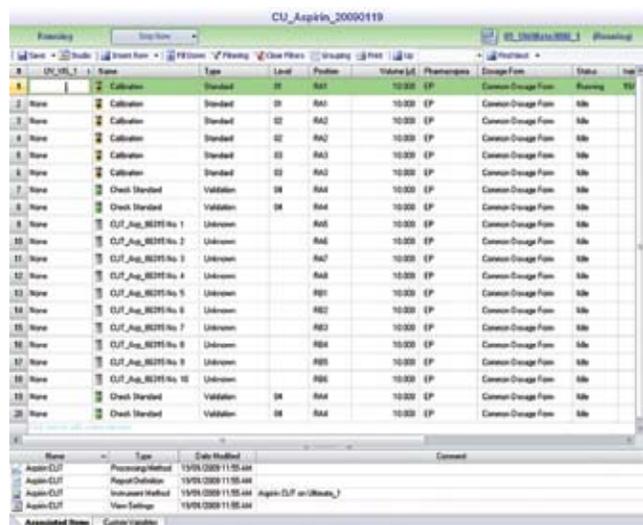


Figure 4. Run the sequence.

The sequence includes the correct processing method, with all detection parameters and peak table, and the correct report template. The results are calculated immediately (Figure 5).

Uniformity of Dosage Units Report

General			
Product Batch Number	85315	Target Content %	102.0
Peak Name	Aspirin	Correction Factor	1.050
CU# Number	156781	Min. Acceptance Value LT	15.0
Class	UV_VIS_1	Lower Amount Limit	Not needed if n=10!
Dosage Form	Common Dosage Forms	Upper Amount Limit	Not needed if n=10!
Pharmaceutical	EP		
Results			
		n = 10	
Mean		110.5	
Standard Deviation s		2.5	
Reference Value M		102.0	
Acceptance Value AV		14.4	
Test Result		Test passed	

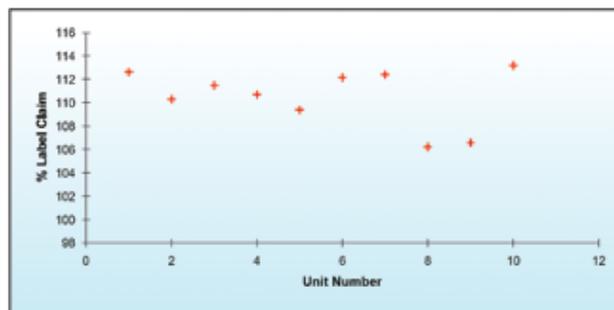


Figure 5. Report the final results.

These few steps are all a user needs to know to run and report any analysis that has been implemented as an eWorkflow.

eWORKFLOW EDITOR

eWorkflows are easily created and customized using the eWorkflow Editor. This editor consists of three parts:

- eWorkflow General
- Sequence General
- Sequence Layout

eWorkflow General

In the General Settings page (Figure 6), it is possible to specify all settings related to the eWorkflow.

The most important part is setting the associated items. Here it is possible to define on which instruments the eWorkflow is allowed to run, to define which methods may be used, and to attach external documents (for example, an electronic document of the procedure). Methods and attached documents can be either added to the eWorkflow, or included as a link. The latter has the advantage that multiple eWorkflows can link to the same file and the file can be updated independently from the eWorkflows using it.

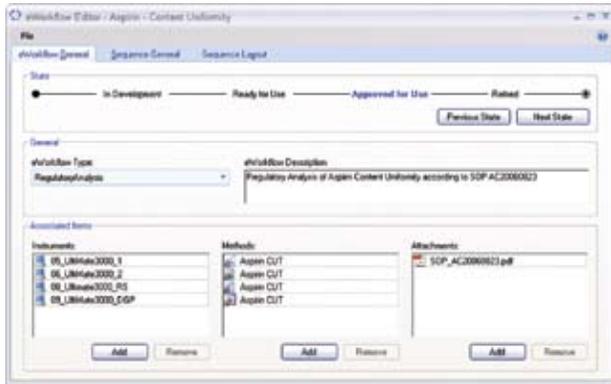


Figure 6. General eWorkflow settings.

Sequence General

The Sequence General page provides general sequence options (Figure 7), such as sequence name and location. The option to use report formulas in the sequence name and sequence location ensures data storage in the correct location, as well as using a unique name. For example, when using report formulas it is possible to structure sequence locations according to the instrument name, user name, etc.

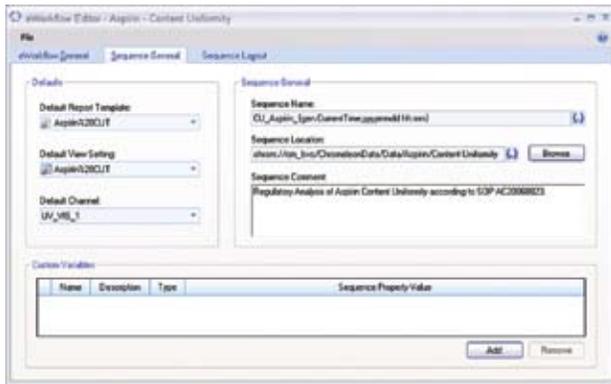
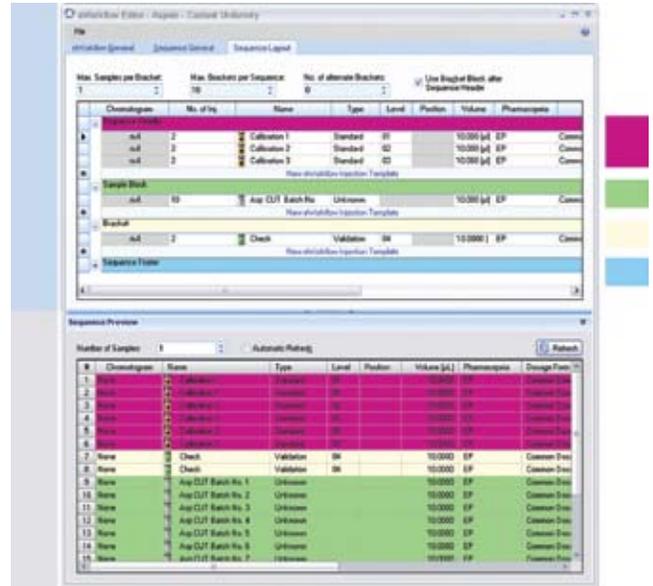


Figure 7. General Sequence settings.

Sequence Layout

The most important part of the eWorkflow Editor is the Sequence Layout page. Here, the sequence layout rules are defined. The upper area (Figure 8A) gives the possibility to restrict the number of samples and brackets in the sequence. It also allows the use of alternating brackets.



Figures 8. Sequence Layout settings.

The Sequence Header (A1) defines injections that will always appear at the beginning of the sequence. The Sample Block (A2) contains the injections that need to be performed for each physical sample that needs analyzing. The Bracket (A3) defines injections that need to be performed for each bracket. The Sequence Footer (A4) defines injections that need to be performed at the end of the sequence, for example a shutdown method. Finally the Sequence Preview (Figure 8B) shows a sequence that would be created according to the set rules.

The eWorkflow editor allows for any combination of these areas to be used allowing for maximum flexibility. For example, if the method does not require bracketing standards then this area can be left blank.

The flexibility of the Sequence Layout settings allows creating eWorkflows for every chromatography laboratory, whether it is quality control or research and development and independent of the industry. It is also possible to define every type of analysis, regulated, quality control, method development or open access, using eWorkflows.

SUMMARY

The eWorkflow solution streamlines workflows in chromatography laboratories. With the eWorkflow editor one can easily setup workflow rules that users can readily follow—rules defining basic structure and requirements for the workflow. Once the eWorkflow has been defined, a user can set up and start an analysis in significantly less time than traditionally required. Using eWorkflows also ensures that all steps are followed correctly, reducing the need for additional verification, and saving additional laboratory time.

eWorkflows significantly improve efficiency in chromatography laboratories.

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LPN 2257-01 06/09
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