find a
method

download
1-click workflow

run, process,
report

AppsLab Library: Chromeleon eWorkflows

AppsLab Library of Analytical Applications
Chromeleon 7.2

Software Version 2.2 • November 2016

thermoscientific

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Document History

Revision: 1.1. This manual is the original manual.

Table of Contents

1 Introduction

1.1   About this Document

This manual provides instructions for using Chromeleon eWorkflows downloaded from Thermo Scientific™ AppsLab Library of Analytical Applications.

The following topics are covered:

- What is an eWorkflow?
- Importing a Chromeleon eWorkflow
- Launching an eWorkflow
- Running the Sequence
- AppsLab Library eWorkflows: Default Settings
- Customizing an eWorkflow

1.2   Document Conventions

The following formatting is used throughout the document to indicate text with special importance.

Note: Indicates information of special interest.

Tip: Indicates information that will help you to use the software more efficiently.

1.3   Requirements

Chromeleon eWorkflows can only be used with Chromeleon 7 or higher.

It is possible to export the results of an eWorkflow in the Adobe® Acrobat® PDF format. Acrobat Reader version 5.0 or higher is needed to read these reports.

1.4   Other Documentation

Other documents provided with Thermo Scientific™ Dionex™ Chromeleon™ Chromatography Data System software provide more information about Chromeleon eWorkflows and Chromeleon. Their scope is described in the *Document Overview*, which is included with the Chromeleon installation media in printed form. The documents are also available in electronic form on the installation disk in the **Documents** folder.

Tip: The *Glossary* describes Chromeleon-specific terms and common abbreviations used throughout the documentation. The *Quick Start Guide* provides information about the daily use of Chromeleon 7.

2 What is an eWorkflow?

An eWorkflow is an electronic procedure that guides users through their entire application, from samples to final results. It assists you in creating an appropriate sequence with predefined associated files and a well-defined structure:

- name and storage location of the sequence

- list of the appropriate instruments

- injection list with a default set of structured injections

- default injection volume, calibration standards, weight, dilution factor, custom variables, etc.

- selected instrument methods, processing methods, view settings and report templates

- additional documents, for example this user manual (**AppsLab Library - eWorkflow - English.pdf**)

- The processing method and report templates ensure the data is processed correctly and final calculations are readily available.

The AppsLab Library allows you to download eWorkflows for use with Chromeleon 7. eWorkflows downloaded from AppsLab Library allow you to quickly and easily run the application in your own laboratory. The eWorkflows downloaded from AppsLab Library typically contain the following files:

- instrument method

- processing method

- report template

- view setting

- custom variable

- **AppsLab Library - eWorkflow - English.pdf** (this user manual)

3 Getting Started

3.1 Importing an eWorkflow

If the AppsLab Library web browser is on the same computer as Chromeleon, an eWorkflow downloaded from AppsLab Library can easily be imported. After download, click the eWorkflow and follow step 4 below.

In the **Import** dialog, **ChromeleonLocal** is selected as the destination data vault. You can select another data vault to import the eWorkflow to from the **Other** drop-down menu and click **Start** (Figure 1).

Note: eWorkflow Tags can be used to restrict the use of eWorkflows to a specific user group. No eWorkflow Tag should be preselected with an eWorkflow from AppsLab Library (Figure 1).

If the AppsLab Library web browser is on a different computer and you need to transfer the eWorkflow to your Chromeleon computer, follow these steps to import the eWorkflow into Chromeleon:

1. In the Chromeleon Console select the **eWorkflows** category.
2. In the menu click **File**, **Import Chromeleon Data**.
3. Select the eWorkflow file and click **Open**.
4. Select the data vault into which you want to import the eWorkflow and click **Start** (Figure 1).
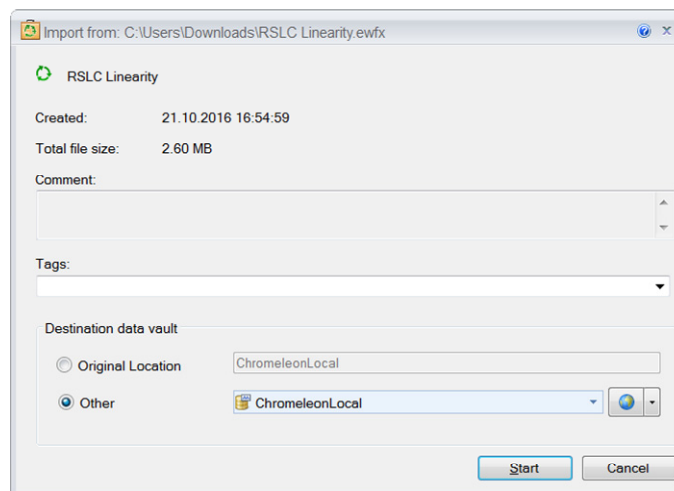
Figure 1: eWorkflow import – Select Data Vault

The eWorkflow is now imported and visible in the list of eWorkflows. The User Manual **AppsLab Library - eWorkflow - English.pdf** is directly accessible.
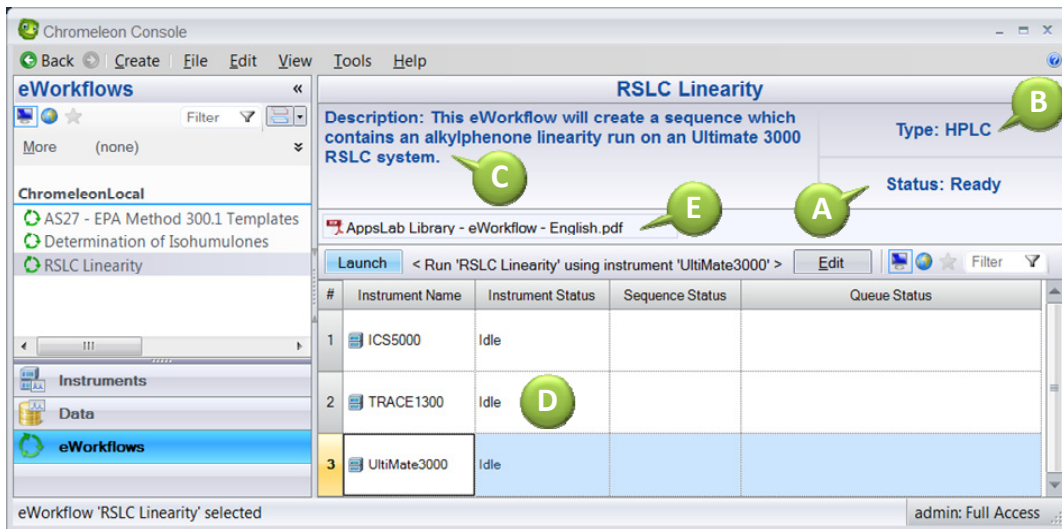
Figure 2: Imported eWorkflow

Table 1: Default eWorkflow General settings

Figure 2	Property	Comment / Setting
A	eWorkflow State	Ready
B	eWorkflow Type	The instrument type the eWorkflow can be used with (HPLC, GC or IC).
C	eWorkflow Description	Description of the purpose of the eWorkflow including the instrument. The description may also provide information about the instrument model to be used.
D	Instruments	No instruments are associated with the eWorkflow. The eWorkflow can therefore be used for all instruments.
E	Attachments	PDF document **AppsLab Library - eWorkflow - English.pdf** (this document). There may be additional attachments, such as the application note PDF or other reference documents in a PDF format.

3.2 Launching an eWorkflow

To create a sequence using a Chromeleon eWorkflow follow these steps:

1. In the Chromeleon Console go to the **eWorkflows** category.
2. Select the eWorkflow (Figure 3A) and the instrument (Figure 3B) to use.
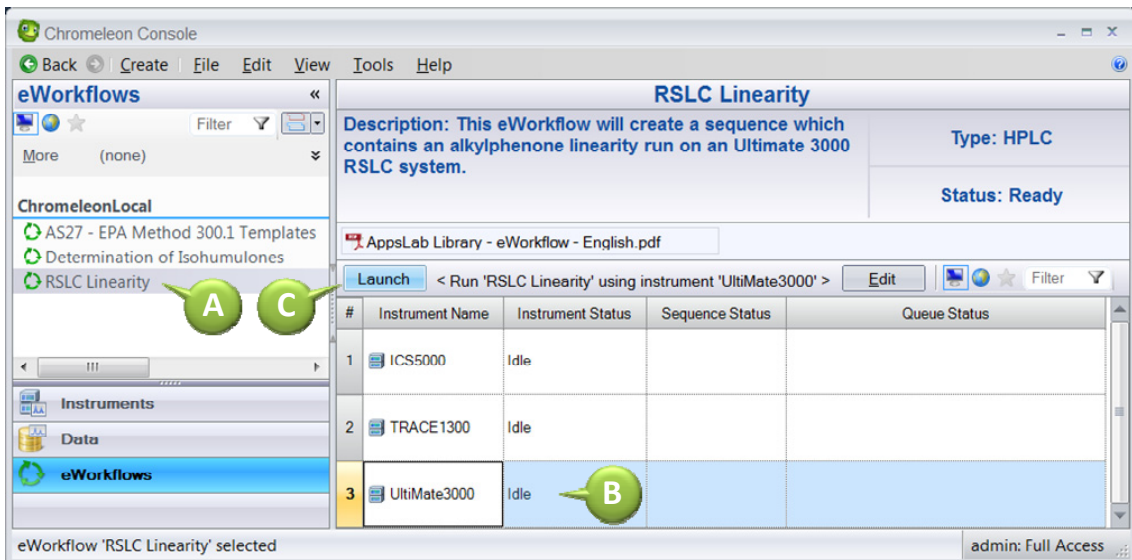
Figure 3: Launching the eWorkflow

3. Click **Launch** (Figure 3C). The eWorkflow Wizard is launched (Figure 4).
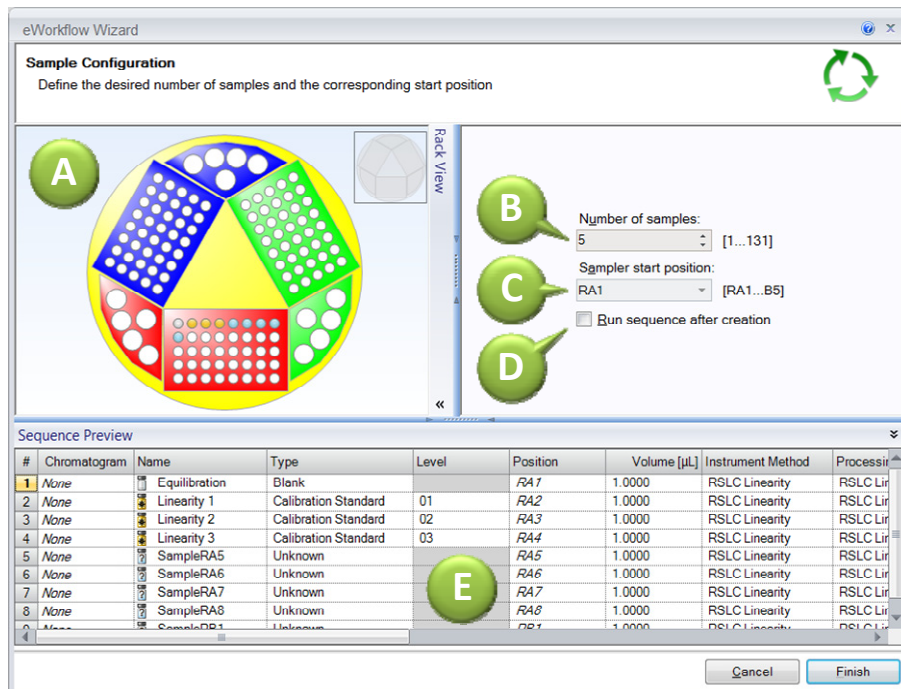
Figure 4: eWorkflow Wizard

Table 2: Settings in the eWorkflow Wizard

Figure 4	Property	Comment / Setting
A	Rack View	Layout of the Autosampler with sample positions
B	Number of Samples	Adapt this setting according to your needs.
C	Sampler Start Position	Adapt this setting according to your needs.
D	Run Sequence after creation	Selecting this setting runs the sequence immediately after creation.
E	Sequence Preview	The sequence structure is already pre-defined as part of the eWorkflow. The Sequence Preview shows the sequence with the number of samples and sampler start position you selected. The preview includes any bracketing according to the bracketing rules set in the eWorkflow.

4. Enter the number of samples and the starting position of the vials in the Autosampler (Figure 4).

5. Click **Finish**. The sequence is now created (Figure 5).
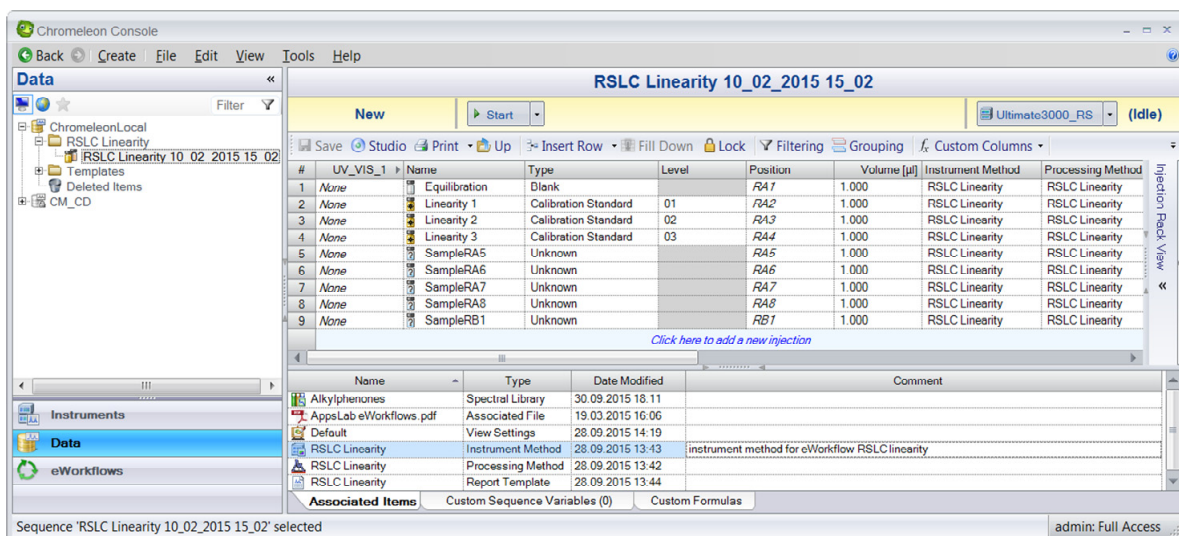
Figure 5: Created sequence

3.3 Running the Sequence

Now that the sequence has been created, it can be started. Follow these steps:

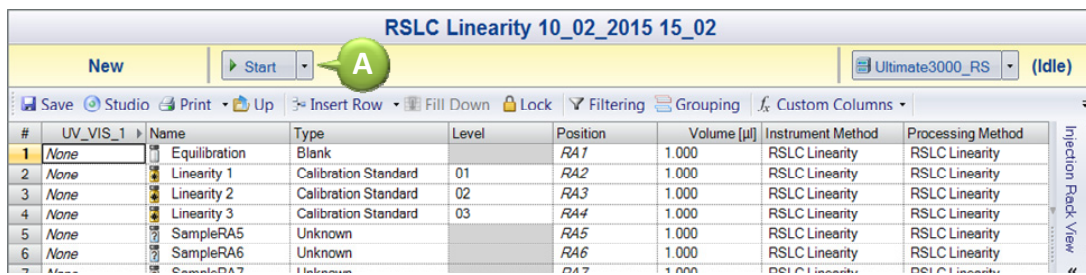1. Select the sequence in the navigation pane.

2. Click **Start** (Figure 6A).

Figure 6: Starting the sequence
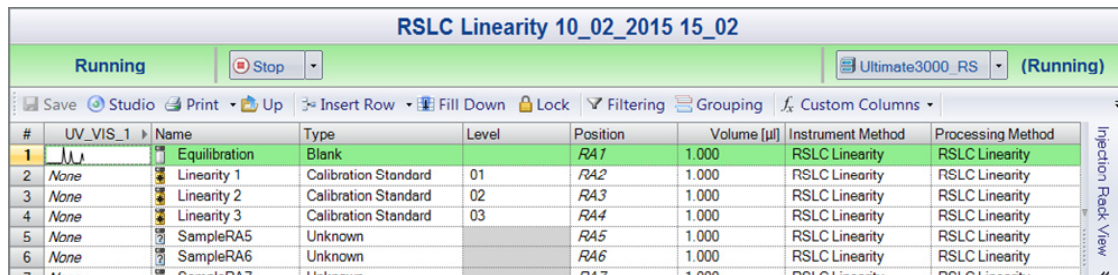
The sequence is now running (Figure 7).

Figure 7: Running sequence

Note: All information in the **Sequence** table can be updated after the sequence has run.

The eWorkflow creates a new folder named after the eWorkflow (e.g., "RSLC Linearity") and a new sequence. The name of the sequence is composed of the eWorkflow name and a date-time stamp (Figure 8).
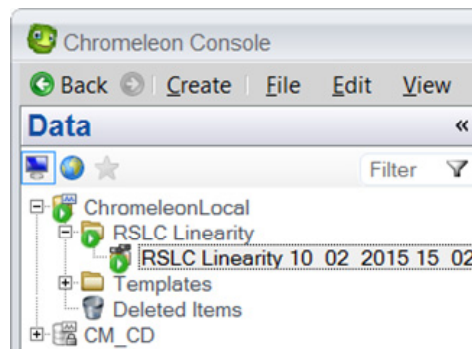

Figure 8: Sequence path and sequence name

4 AppsLab Library eWorkflows: Default Settings

4.1 eWorkflow General

The **eWorkflow General** page is used to specify some general settings for the eWorkflow and to associate instruments, methods, and documents. The eWorkflow General settings for a typical eWorkflow downloaded from AppsLab Library are displayed in Figure 9.
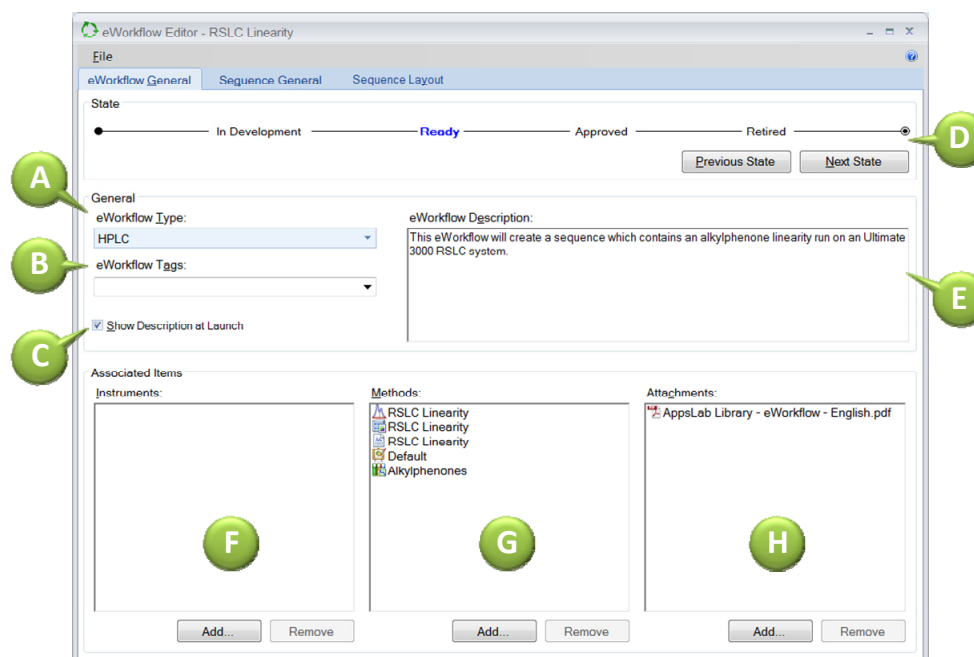
Figure 9: Default **eWorkflow General** page settings

Table 3: Default **eWorkflow General** settings

Figure 9	Property	Comment / Setting
A	eWorkflow Type	The instrument type the eWorkflow can be used with (HPLC, GC or IC).
B	eWorkflow Tags	No eWorkflow tag is associated with the eWorkflow. eWorkflow Tags can be used to restrict the use of eWorkflows to a specific user group.
C	Show Description at Launch	Enabled. Shows an additional page with the eWorkflow description when launching the eWorkflow. This setting can be disabled.
D	eWorkflow State	Ready
E	eWorkflow Description	Description of the purpose of the eWorkflow including the instrument. The description may also provide information about the instrument model to be used.
F	Instruments	No instruments are associated with the eWorkflow. The eWorkflow can therefore be used for all instruments.
G	Methods	Instrument method, processing method, report template, and view settings.

Figure 9	Property	Comment / Setting
H	Attachments	PDF document **AppsLab Library - eWorkflow - English.pdf** (this document). There may be additional attachments, such as the application note PDF or other reference documents in a PDF format.

Note: Chapter 5 describes how these settings can be customized.

4.2 Sequence General

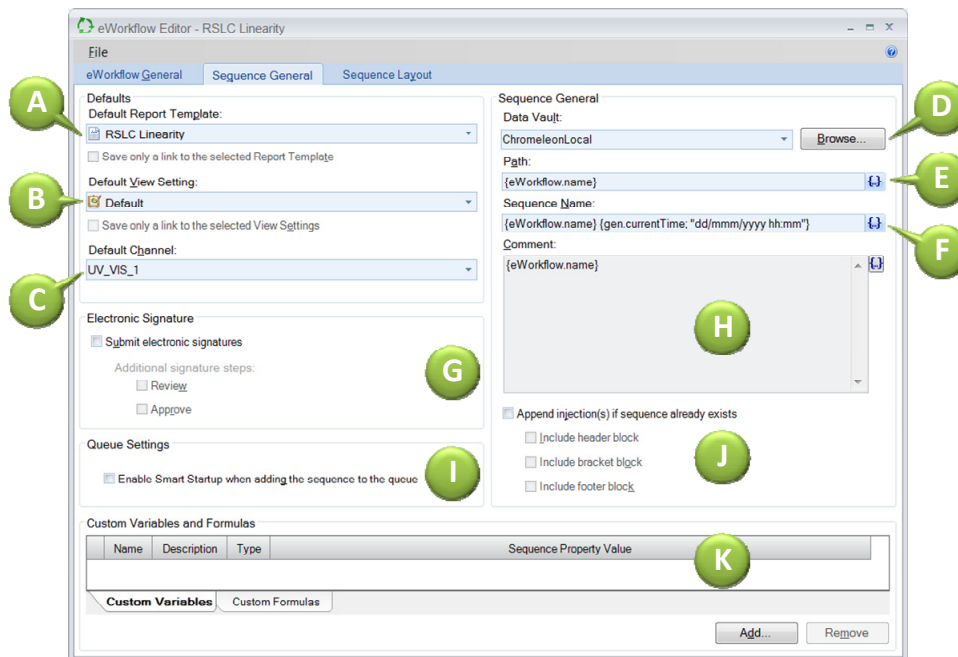The **Sequence General** page is used to specify general settings for the sequence and select a default report and view settings.

Figure 10: **Sequence General** page of an eWorkflow downloaded from AppsLab Library

Table 4: Default **Sequence General** settings

Figure 10	Property	Comment / Setting
A	Default Report Template	Report template to be used as the default template for presenting the data in a report. Typically the report template that is part of the eWorkflow.
B	Default View Setting	View settings to be used as the default settings for presenting the data in the Chromatography Studio. Typically the view setting that is part of the eWorkflow.
C	Default Channel	Defines the channel to be displayed as the default channel when opening an injection. As this depends on the instrument and corresponding instrument method, this is empty.
D	Sequence Name	eWorkflow name followed by current date/time (Example: RSLC Linearity 10_02_2015 15_02)

Figure 10	Property	Comment / Setting
E	Data Vault	ChromeleonLocal
F	Path	Typically the folder the sequence is stored in is named for the eWorkflow (e.g., RSLC Linearity). If this folder does not exist, it will be automatically created when the first sequence is created.
G	Electronic Signature	For regulated (Pharma) applications, all signature steps to submit electronic signatures are checked, to enable a qualified user to electronically sign the sequence and submit, review or approve it. For non-regulated applications, all signature steps to submit electronic signatures are unchecked.
H	Comment	A comment for the sequence. Typically the name of the eWorkflow.
I	Queue Settings	This sequence is created using the <eWorkflow name> (e.g., RSLC Linearity).
J	Append injection if sequence exists	Not used.
K	Custom Variables and Formulas	Not used. This section lists custom variables and formulas used e.g., in the report template.

Note: Chapter 5 describes how these settings can be customized.

4.3   Sequence Layout

The sequence layout defines rules for the sequence layout, for example, the maximum number of unknown samples allowed between calibration standards. The sequence layout helps to create a sequence with a well-defined structure.

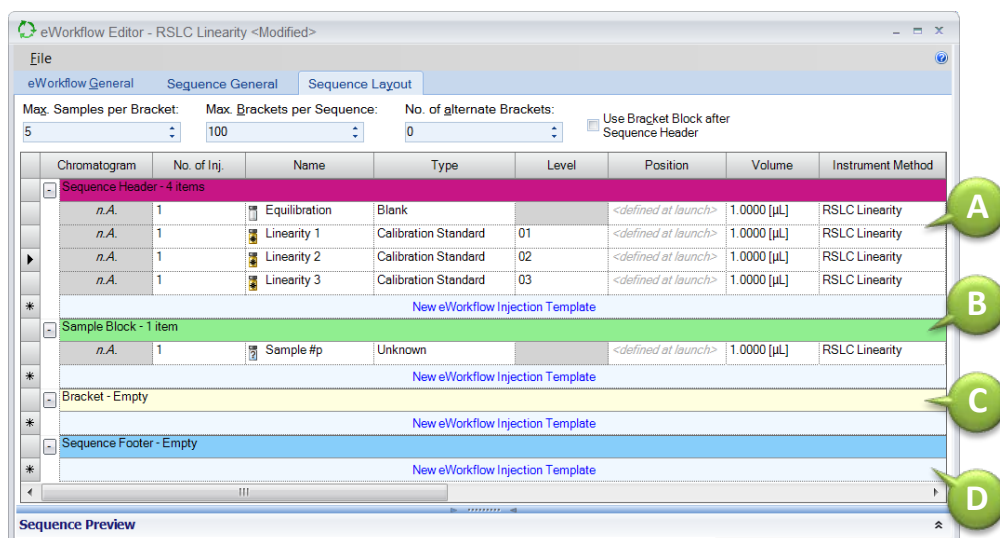A sequence layout comprises four block types, each marked by a different color.

Figure 11: **Sequence Layout** page of an eWorkflow

Table 5: Default **Sequence Layout** settings

Figure 11	Property	Comment / Setting
A	Sequence Header	Injections that always appear at the beginning of a sequence, such as blank injections.
B	Sample Block	The Sample Block includes a line for each sample that needs to be analyzed. The sample block is repeated between brackets. Typically, the Sample Block is pre-populated with one sample named sample #p, where #p indicates the injection position.
C	Bracket	Injections that will be performed between sample blocks (for example, calibration standards). A bracket separates two sample blocks from each other.
D	Sequence Footer	Injections that always appear at the end of a sequence.

4.4 Resulting Sequence

When launching an eWorkflow without making any changes, the resulting sequence will look similar to Figure 12. In particular, an eWorkflow downloaded from AppsLab Library will typically have one sample.

Figure 12: Resulting sequence when launching an eWorkflow

5 Customizing an eWorkflow

The eWorkflow can be customized to fit your needs. To customize an eWorkflow, do the following:

1. In the Chromeleon Console go to the **eWorkflows** category.
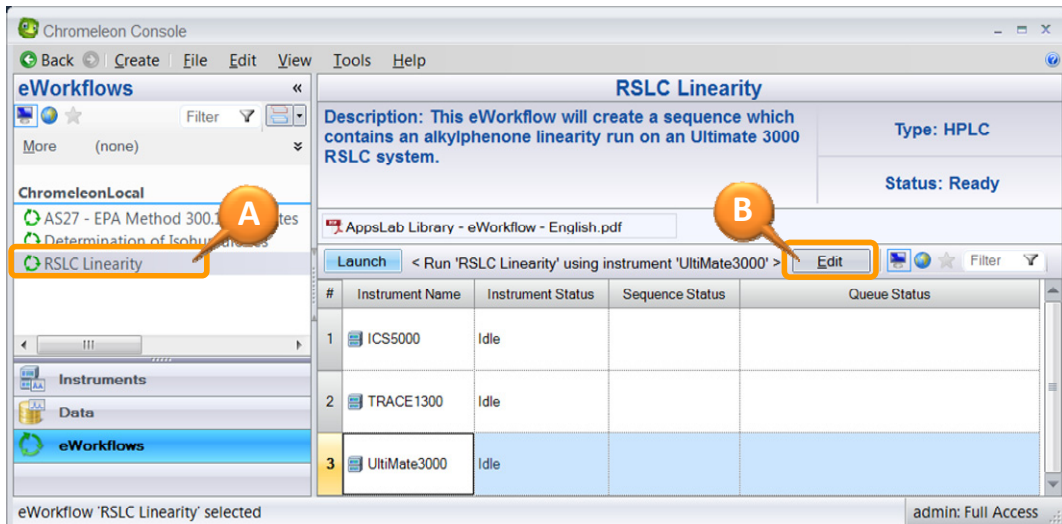2. In the navigation pane select the eWorkflow (Figure 13A).

Figure 13: Start editing the eWorkflow

3. In the work area click Edit (Figure 13B). The eWorkflow Editor opens.
4. To save the eWorkflow with a new name click **File, Save As**.
5. In the **Save eWorkflow** dialog select the data vault (Figure 14A) to store the eWorkflow and enter a name (Figure 14B) for the new eWorkflow.
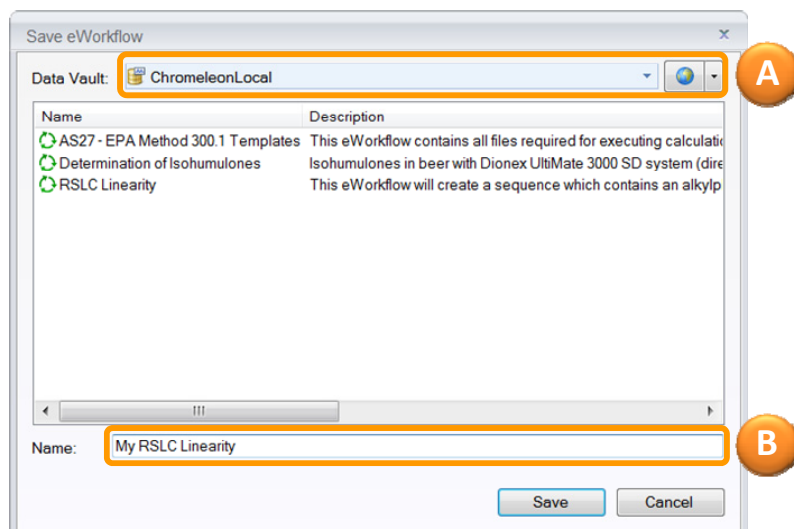
Figure 14: Saving eWorkflow with new name

The eWorkflow can now be customized. The settings to modify are described in sections 5.1, 5.2, and 5.3.

Tip: For an extensive explanation of modifying eWorkflows and defining the sequence layout, refer to the *Chromeleon 7 Help*.

5.1   eWorkflow General

Table 6: Customization for the **eWorkflow General** page

Figure 9	Property	Comment / Setting
A	eWorkflow Type	The instrument type the eWorkflow can be used with (HPLC, GC or IC).
B	eWorkflow Tags	No eWorkflow tag is associated with the eWorkflow. eWorkflow Tags can be used to restrict the use of eWorkflows to a specific user group.
C	Show Description at Launch	Enabled. Shows an additional page with the eWorkflow description when launching the eWorkflow. This setting can be disabled.
D	eWorkflow State	Ready
E	eWorkflow Description	Description of the purpose of the eWorkflow including the instrument. The description may also provide information about the instrument model to be used.
F	Instruments	No instruments are associated with the eWorkflow. The eWorkflow can therefore be used for all instruments.
G	Methods	Instrument method, processing method, report template, and view settings.
H	Attachments	PDF document **AppsLab Library - eWorkflow - English.pdf** (this document). There may be additional attachments, such as the application note PDF or other reference documents in a PDF format.

5.2   Sequence General

Table 7: Customization for the **Sequence General** page

Figure 10	Property	Comment / Setting
C	Default Channel	Defines the channel to be displayed as the default channel when opening an injection. As this depends on the instrument and corresponding Instrument Method, this is empty.
D	Sequence Name	eWorkflow name followed by current date/time (Example: RSLC Linearity 10_02_2015 15_02)
E	Data Vault	ChromeleonLocal
F	Path	Typically the folder the sequence is stored in is named for the eWorkflow (e.g., RSLC Linearity). If this folder does not exist, it will be automatically created when the first sequence is created.
G	Electronic Signature	For regulated (Pharma) applications, all signature steps to submit electronic signatures are checked, to enable a qualified user to electronically sign the sequence and submit, review or approve it. For non-regulated applications, all signature steps to submit electronic signatures are unchecked.
H	Comment	A comment or descriptive text for the sequence. Typically the name of the eWorkflow.
I	Queue Settings	This sequence is created using the <eWorkflow name> (e.g., RSLC Linearity).

5.3   Sequence Layout

Table 8: Customization for the **Sequence Layout** page

Figure 11	Property	Comment / Setting
A	Sequence Header	Injections that always appear at the beginning of a sequence, such as blank injections.
B	Sample Block	The Sample Block includes a line for each sample that needs to be analyzed. The sample block is repeated between brackets. Typically, the Sample Block is pre-populated with one sample named sample #p, where #p indicates the injection position.
C	Bracket	Injections that will be performed between sample blocks (for example, calibration standards). A bracket separates two sample blocks from each other.
D	Sequence Footer	Injections that always appear at the end of a sequence.

Table 9: Customization options for the sequence columns

Sequence Column	Setting
No. of Inj.	Enter the number of injections that should be repeatedly injected from the same vial.
Replicate ID	Enter the replicate ID to indicate the repeated injections for calibration.
Position	This is a non-editable field, which will be filled when creating the sequence.
Volume	Enter the required injection volume.
Instrument Method	Select the correct instrument method. If the eWorkflow can be used on multiple instruments with different instrument methods, leave this field empty.
Processing Method	When the processing method is updated and has a new name, select the correct processing method.
Comment	Enter an appropriate comment for the injection.