

Chromatography: Revvity's Signals™ Notebook Driving Digital Transformation using Scitara's Digital Lab Exchange, DLX™

Summary

Integration between Informatics systems and HPLC CDS platforms are very common requests within the lab. The ability to set up a chromatography run in an Electronic Lab Notebook (ELN) or LIMS (for example), send the sample list to a CDS, and then seamlessly retrieve the processed results is highly desirable but is often still a manual or semi-manual process.

This use case illustrates how Scitara's DLX can be integrated with Revvity's Informatics' Signals research management platform to provide a seamless interactive experience with CDS systems.

Challenge

The desired workflow is bi-directional and requires a dialog between the systems. Within the Signals Notebook, the user will have a complete or partial sample list that they want to send to a CDS. That list may need to be augmented with additional information before the samples are acquired and processed. When data processing is complete, the processed results need to be transferred back from the CDS to the Signals Research platform. The challenge is making this data exchange as seamless and easy as possible while maintaining data integrity and a chain of custody for the data.

For the purposes of illustration, this example will use Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) software, but the same process is readily achievable with other leading CDS platforms.

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signals

Simplify and enhance
experimental procedures
and data handling with a
single button click

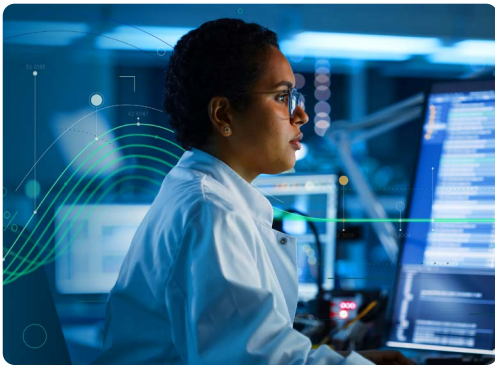
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Solution

Using Scitara DLX, an external action may be configured in the relevant Signals Notebook table where the user is building the sample list. When the user has accumulated all of the relevant data within Signals and is ready to send the list to Chromeleon and create a sequence, the external action link is selected. This launches a dialog inside of a Signals Notebook iFrame and prompts the user for needed information. Since the prompts are based on a dynamic Chromeleon lookup based on the Chromeleon SDK, the number of required prompts can be minimized by having more information at hand in advance and pre-loading this information.

The following information may be configured as part of the sequence creation process:

- ☐ The Chromeleon instance to be used
- ☐ User credentials (important in regulated environments and for data integrity in general)
- ☐ The Chromeleon folder where the sequence will be stored
- ☐ The instrument to be used (optional)
- ☐ A sequence preview where methods may be dynamically selected, and missing parameters entered, such as injection volume or carousel position

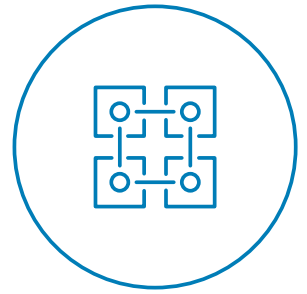


Any additional information added to the sequence as part of the sequence creation process can be written back to Signals Notebook as well as sent to Chromeleon to keep Signals and Chromeleon in sync.

When the samples have been processed, the user may retrieve the processed results from another external action selection within Signals Notebook. The user experience may be as simple as a single button click that retrieves

all processed results associated with the sequence name. The user may also browse their accessible Chromeleon locations and select their desired results.

The user experience is under customer control based on the Scitara DLX Orchestration and may be modified by the customer administrator at any time if the workflow requirements change. It is also possible to route data to multiple locations in parallel (for example, send CDS results to the Signals Platform and to a data lake in parallel).



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PARTNER USE CASE

SignalsNotebook

Quick Find

Christopher Jahn

DLX Demo Notebook

DLX Demo

Contents

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Experiment Contents

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Samples Table

2 of 1000 items

ID	Description	Batch	Sample Type	Amount	Actual Weight	Weight taken on	Analyst Name	Comments	Equipment Id	Status	Created Date	Attached Docs	Template
Sample 511	Some Description	123-456	Unknown	1.6 g	1.652 g	Oct 17, 2022, 01:00 PM	Christopher Jahn	Sample is Green	Lab Balance	Complete	Oct 11, 2022, 09:29 PM	(3) View and Manage	Samples (CT)
Sample 512	Some Description	123-456	Unknown	1.6 g	1.654 g	Oct 17, 2022, 01:00 PM	Christopher Jahn	Sample is Blue	Lab Balance	Complete	Oct 11, 2022, 09:29 PM	(3) View and Manage	Samples (CT)

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Orchestrations

Orchestration name: Signals

+ Add Filter

Signals Add Sample

Triggers by an event or

Signals Chromeleon

User-triggered

Signals Chromeleon

User-triggered

Signals Create Chro

User-triggered

Signals Create Weig

User-triggered

Signals Chromeleon Create Sequence

Started by Christopher Jahn 2 minutes ago, completed in 1 minute

User Triggered

User-triggered

Connection Action

GetTable action completed

User Input

User input completed

User Input

User input completed

User Input

User input completed

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Signals Chromeleon Create Sequence

Started by Christopher Jahn less than a minute ago

Step 2 of 5

Log in to Chromeleon

Username*

cmadmin

Password

•••••

Role (optional)

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Signals Chromeleon Create Sequence

Started by Christopher Jahn 1 minute ago

Step 4 of 5

Sequence data

New sequence name*

MySampleList1.71.6Oct2022

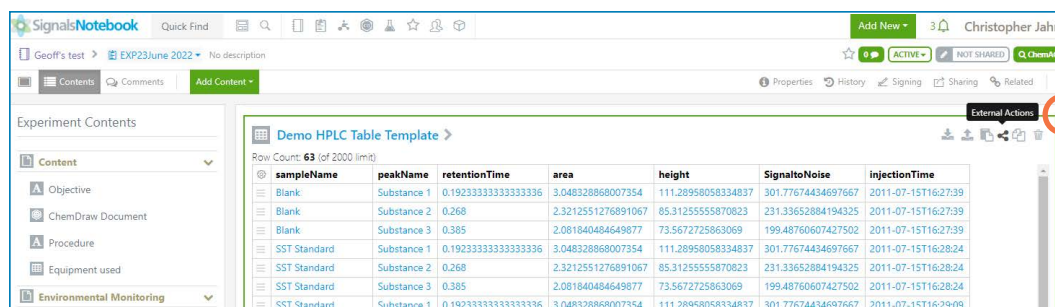
Sequence Template

Sample ID	Vial Position	Injection Volume	Instrument Method
Test123	A1	10	Generic Screening (Vanquish)
Test945	A2	15	Generic Screening (Vanquish)

..... Add samples weight data automatically to a CDS run ...

..... Initiate CDS sequence creation by selecting an external action menu choice in Signals Notebook, prompting user log-in and subsequent configured steps.

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Signals Notebook

Quick Find

Add New + 3 Christopher Jahn

Geoff's test > EXP23/June 2022 No description

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Experiment Contents

Content

- Objective
- ChemDraw Document
- Procedure
- Equipment used
- Environmental Monitoring

Demo HPLC Table Template

Row Count: 63 (of 2000 limit)

sampleName	peakName	retentionTime	area	height	SignaltoNoise	injectionTime
Blank	Substance 1	0.19233333333333336	3.048328868007354	111.28958058334837	301.77674434697667	2011-07-15T16:27:39
Blank	Substance 2	0.268	2.3212551276891067	85.3125555870823	231.33652884194325	2011-07-15T16:27:39
Blank	Substance 3	0.385	2.081840484649877	73.5672725863069	199.48760607427502	2011-07-15T16:27:39
SST Standard	Substance 1	0.19233333333333336	3.048328868007354	111.28958058334837	301.77674434697667	2011-07-15T16:28:24
SST Standard	Substance 2	0.268	2.3212551276891067	85.3125555870823	231.33652884194325	2011-07-15T16:28:24
SST Standard	Substance 3	0.385	2.081840484649877	73.5672725863069	199.48760607427502	2011-07-15T16:28:24
SST Standard	Substance 1	0.19233333333333336	3.048328868007354	111.28958058334837	301.77674434697667	2011-07-15T16:29:09

External Actions

.....After the sequence is complete and the data processed, the results may be uploaded seamlessly into Signals Notebook.

Benefits

With the integration of DLX and Signals Notebook, the manual process of collecting and entering data is mitigated. In addition, the likelihood of an error is greatly reduced by removing the possibility of human error when manually entering data.

- ☐ Seamless bi-directional integration between Signals Notebook and CDS systems
- ☐ Configurable user input based on workflow needs
- ☐ Direct retrieval of CDS processed results back to Signals Notebook
- ☐ Route data to multiple locations in parallel
- ☐ Full digital chain of custody for data integrity and compliance support

