

Sequence Summary with Intelligent Reporting for OpenLAB ChemStation

INTRODUCTION AND BACKGROUND

Sequence Summary Reporting (SSR) is the recommended technique for generating reports for data that spans multiple datafiles (i.e., multiple injections) collected as part of a sequence in Agilent ChemStation software.

ChemStation Revisions C.01.01 and higher (officially referred to as OpenLAB CDS ChemStation) generate result data acquired via a single run or via sequences (multiple injections of samples or calibration standards) in a specific file format called ACAML (Agilent Common , which is used by Intelligent Reporting. To use Intelligent Reporting for data acquired with ChemStation revision older than OpenLAB ChemStation, the data must first be reprocessed using ChemStation C.01.01 or higher.

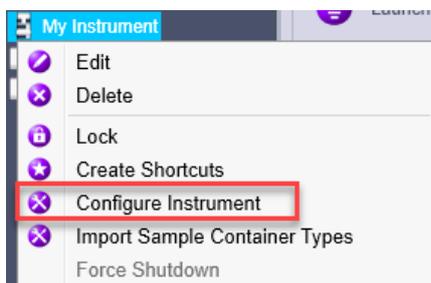
Intelligent Reporting templates are individual files, similar to sequence templates or sequence files, but with a .RDL extension. The default location for the report templates in the local file system is C:\Chem32\REPSTYLE. Upon installation of ChemStation, the software provides several predefined report templates that can serve as a starting point to create customized templates. When data files are acquired, the report templates referenced in the acquisition method are copied into the result set on the same level as the data files for which they will be used.

The sequence file (.S) dictates, among other settings, not only the order in which injections or data acquisition will proceed, the method(s) to be used for acquiring data, and the subdirectory in which the data will be stored, but also whether a SSR will be generated upon completion of the sequence or upon reprocessing of the data result set. The report is output whenever the option to output a sequence summary report is selected in the sequence parameters and the sequence is either processed for the first time or upon any subsequent reprocessing when the setting is enabled in sequence parameters.

INSTRUCTIONS TO CONFIGURE AND OUTPUT A SEQUENCE SUMMARY REPORT

The following will describe how to create a sequence summary report using an Intelligent Report template. This example will also show how to make one modification and output the results.

1. First, ensure that the Intelligent Reporting option in the instrument configuration is on. This option can be found in the OpenLAB Control Panel, in the configuration for the instrument being used for this task. Right-click on the instrument and select "Configure Instrument":

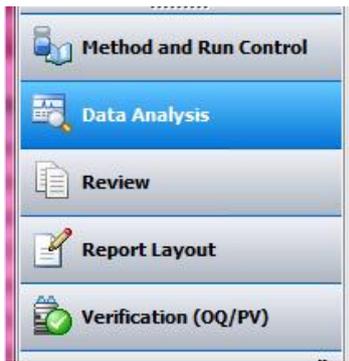


2. The instrument configuration includes an option to "Enable Intelligent Reporting," which will allow editing of Intelligent Report templates in the ChemStation Report Layout view and ensure that there is no confusion with respect to classic report templates, since those will not be visible in the Report Layout view.

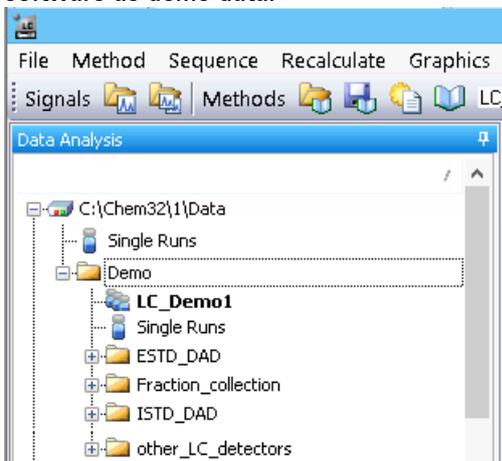




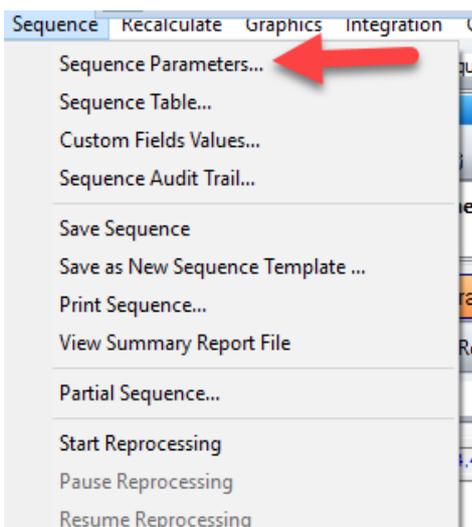
- To output a sequence summary report, navigate to Data Analysis.



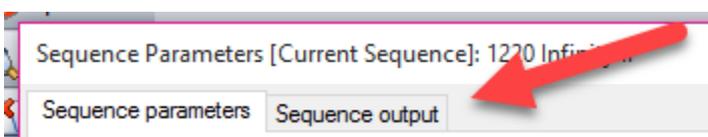
- Load the appropriate Data Result Set (also known as Sequence Container), which is the set of data collected as part of a sequence in ChemStation. In this example, we are loading the Data Result Set included with the software as demo data:



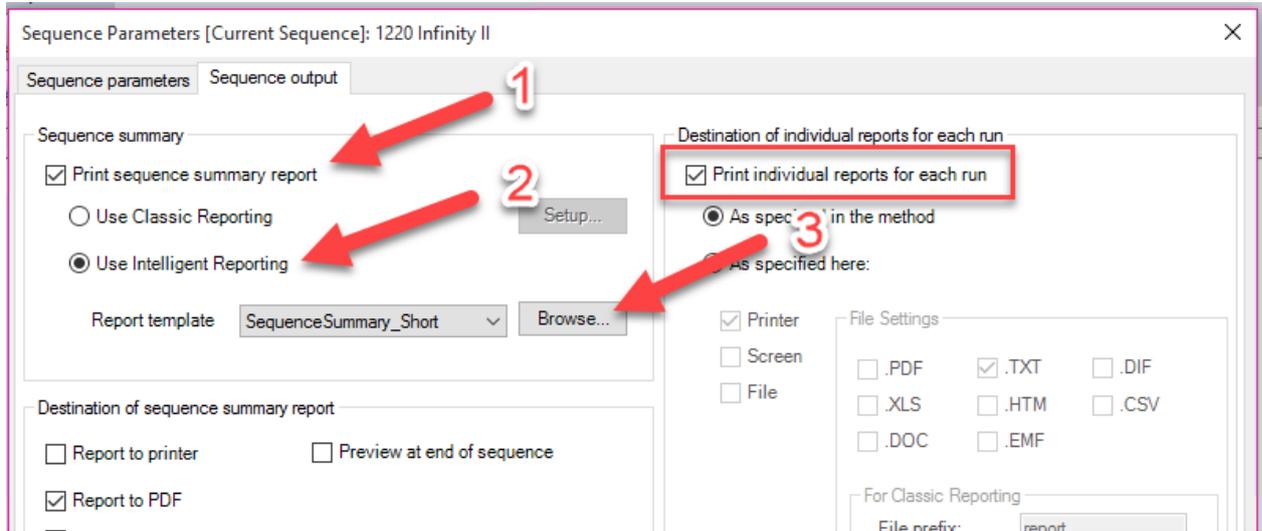
- Navigating to Sequence > Sequence Parameters will allow configuration of the reprocessing options:



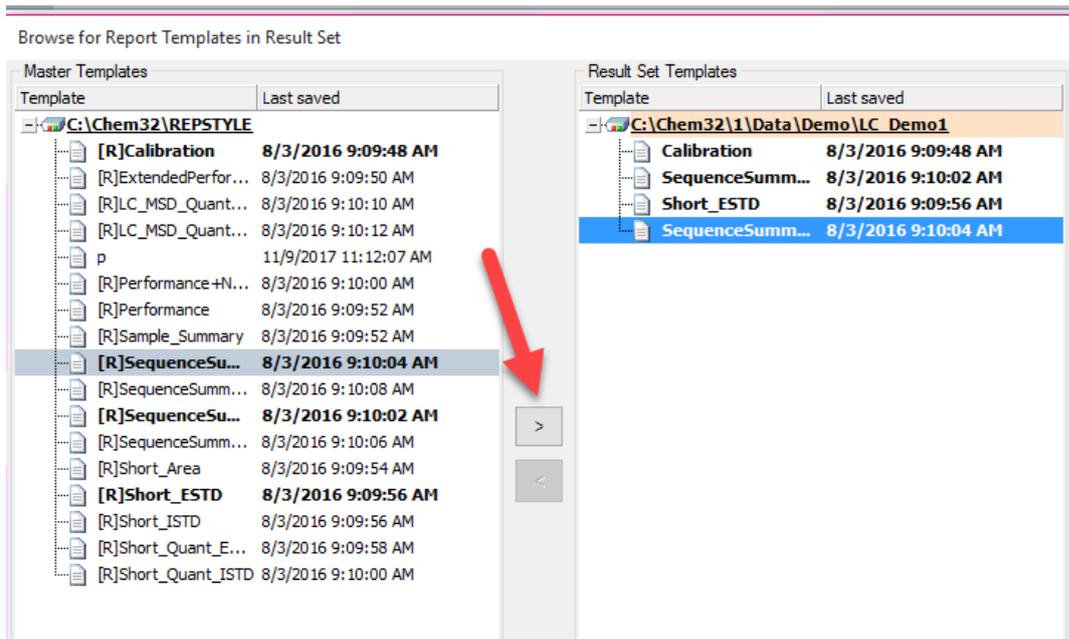
- Select the "Sequence Output" tab:



7. Select "Print sequence summary report" (1) as well as "Use intelligent reporting." (2) Go to "Browse" (3) (Note: there is an additional option to print individual reports for each run, which will be saved in each folder corresponding to a data file in Windows):

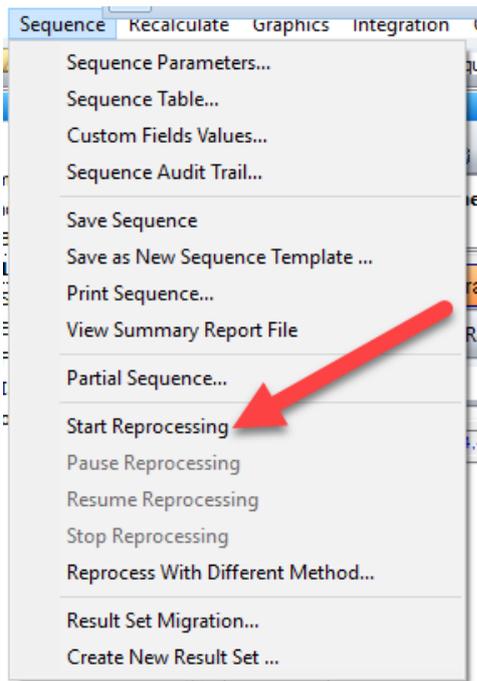


8. Choose the sequence summary report template to be used. Click the arrow to move the template over to the results set. Click "OK":

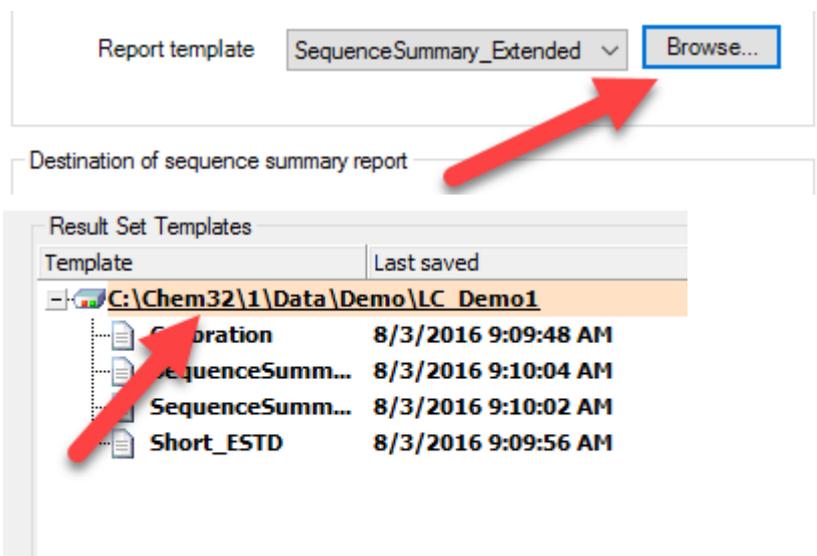




- On the sequence drop down menu, choose "Start Reprocessing" to reprocess the data files in the result set according to the sequence method. At the end of reprocessing, a sequence summary report will be output:



- The report is saved to a specific destination in the format selected, inside the data result set that will have been reprocessed. This path is displayed in the Result Set Templates:

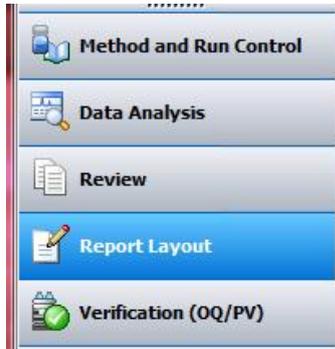


- If the sequence summary report is modified or a different report template is desired, that report must be added to the results set again (see step 8) and the subsequent steps followed again.

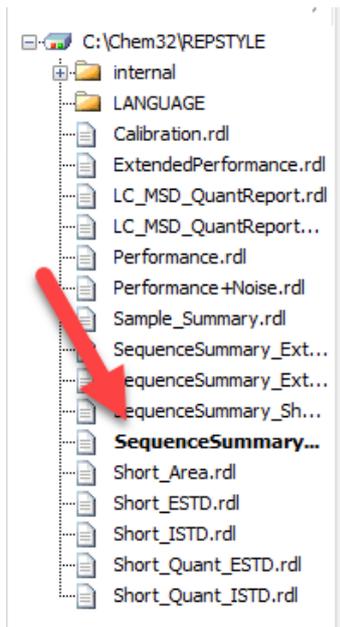
INSTRUCTIONS TO CREATE A CUSTOMIZED SEQUENCE SUMMARY REPORT

The instructions below will cover creating an additional column to calculate more peak area percent results in a sequence summary report using an existing report template (.RDL file) as a starting point. This technique can be used for other calculation columns as needed.

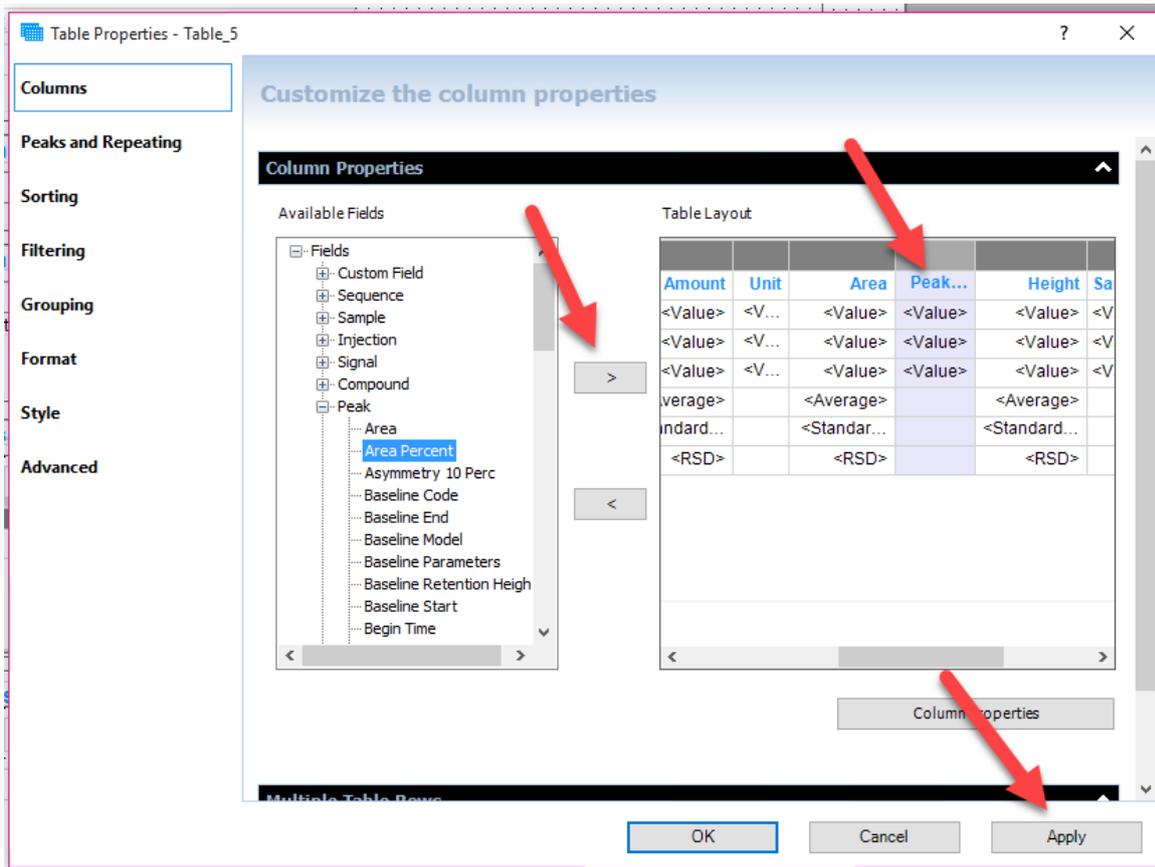
1. First, ensure that the Intelligent Reporting option in the instrument configuration is on (see instructions at the top of this document). Navigate to Report Layout in the bottom left-hand corner of ChemStation:



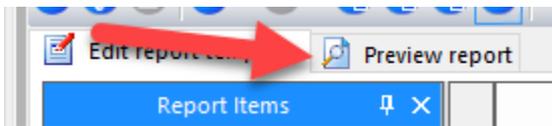
2. Load an existing sequence summary report by selecting it in the navigation pane on the left of the screen or by clicking File > Open Report Template. This example will use SequenceSummary_Standard.rdl:



3. Within the table to be edited, right click and go to "Properties":



6. Select "Preview Report":



7. The report will now show the new column that was added:

Compound: dimethylphthalate Signal: DAD1 A, Sig=254,4 Ref=360,100

Line#	Location	Inj#	Type	RT [min]	Amount	Unit	Peak Area Percent	Height
11	P1-F-03	1	BV	0.451	998.59425	ng/ul	263.27890	21.92
			Mean	0.451	998.59425		263.27890	176.30209
			StdDev	0				0.00000
			RSD	0.000	0.00000		0.00000	0.00000