Agilent OpenLAB Chromatography Data System A.02.01 HF03 - Updates

1. OpenLAB CDS ChemStation C.01.06 HF03

Sequence Table updates

In OpenLAB CDS ChemStation version C.01.06 and C.01.07, the sequence table is updated with new features. Introduced with C.01.06, the data file name will change to **OnlineEdited** while editing a sequence.

For users who update the sequence table, while acquiring data on a regular basis, the recommendation is to use the **Name Pattern** option. This option will enable users to edit the sequence and have the data file names updated based on the pattern selected. A user can put fixed characters into the field then add a token to the file naming. When using this feature, there is a limit of 40 characters for the data file name.

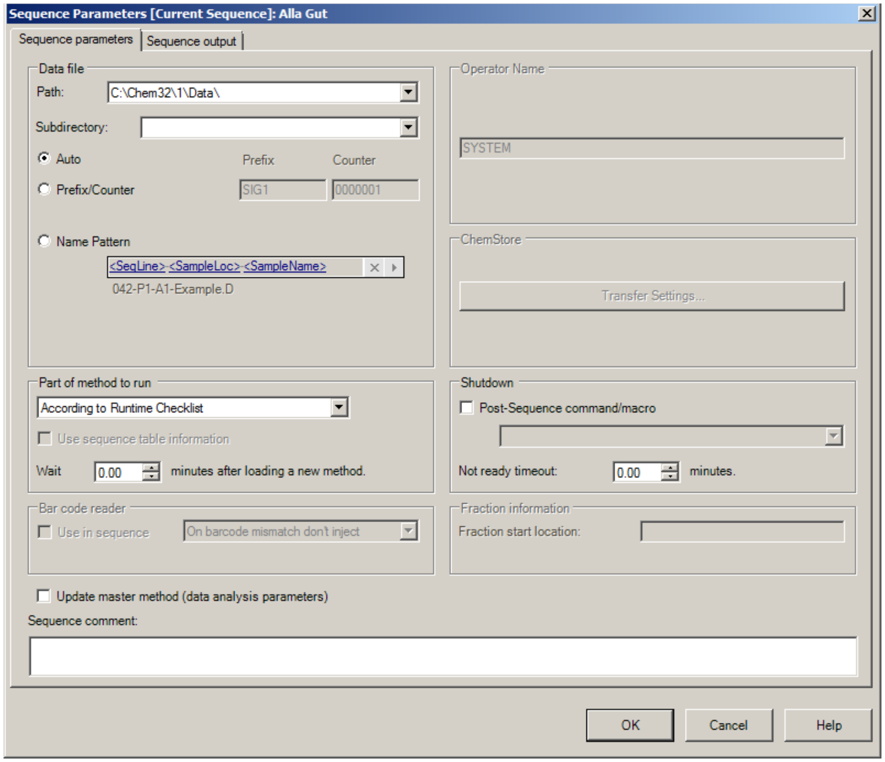
If you use the **Auto**, **Prefix/Counter**, or **Manual** technique, and add lines to a running sequence, the default filename will be **OnlineEdited#.D**, where # is incremented for each additional line.

Setting up the Data File Name (in Sequence Parameters dialog)

The following options are available to specify data file names:

- Auto
- Prefix/Counter
- Name Pattern
- Manual

NOTE The default option for new sequence templates is **Name Pattern**. This is also the recommended technique if you want to add sequence lines while a sequence is already in acquisition.



Sequence Parameters [Current Sequence]: Alla Gut

Data file
Path: C:\Chem32\1\Data\
Subdirectory:
● Auto
○ Prefix/Counter Prefix: SIG1 Counter: 0000001
○ Name Pattern <SeqLine>-<SampleLoc>-<SampleName>
042-P1-A1-Example.D

Operator Name: SYSTEM

Part of method to run: According to Runtime Checklist
☐ Use sequence table information
Wait 0.00 minutes after loading a new method.

Shutdown
☐ Post-Sequence command/macro
Not ready timeout: 0.00 minutes.

Bar code reader
☐ Use in sequence On barcode mismatch don't inject

Fraction information
Fraction start location:

☐ Update master method (data analysis parameters)
Sequence comment:

Figure 1 Sequence Parameters dialog

Name Pattern

Use tokens to create the data file names for each sequence line.

Eg. **<Sequence Line>-<Sample Location>-<Sample Name>**

If your instrument supports different injection locations (GC with back and front injector), you can provide different patterns for each location. For example, use a prefix with an indication for the injection location:

GC with back and front injector

- **F-<Sequence Line>-<Sample Location>-<Sample Name>** for front runs, and
- **B-<Sequence Line>-<Sample Location>- <Sample Name>** for back runs.

NOTE The data file names are resolved at the moment the run starts. The sequence table will therefore not contain any data file names.
The resolved data file names can contain up to 40 characters. Longer names will be truncated. If a resolved name is not unique, a counter value will be appended.

Data file (in Sequence Table)

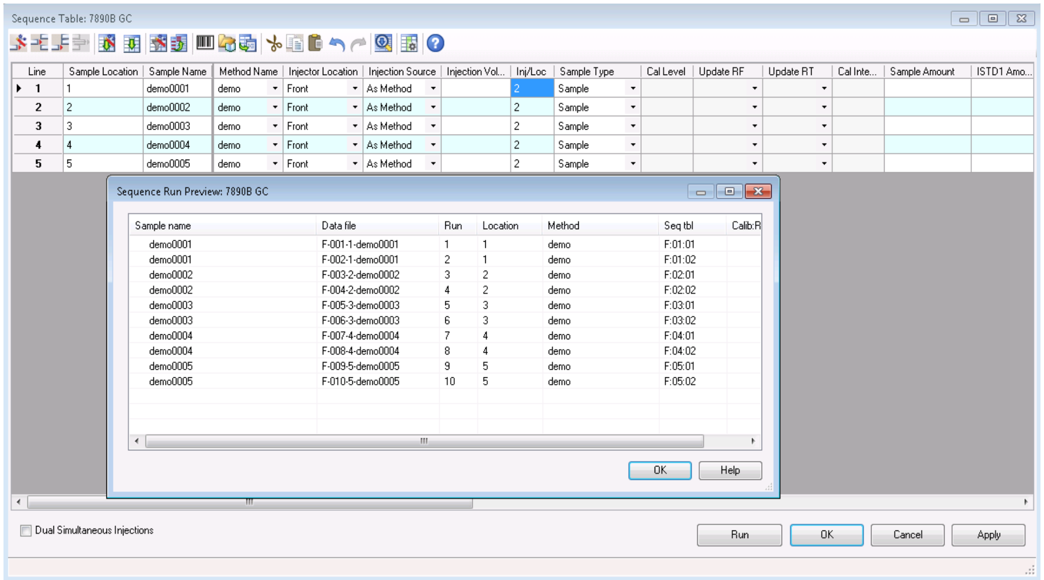
The **Data File** field in the **Sequence Table** is the name of the file where data collected from acquisition or analysis is stored. Use the select tokens for the data file name.

You can select from the following tokens:

Sample Name	The information that has been barcoded or typed into the field
Sample type	Type of samples QC sample, calibration, sample
Sample location	Vial or location of the sample vial or wellplate location
Method	Method name of the sample for the line of the sequences
Sequence line	The current line in the rolled out sequence
Replicate Number	The number per vial injections (note if editing a running sequence this will still be 1)
Date	Date at time of acquisition of the sample
Time	Time stamp at time of acquisition of the sample

Some suggestions for use of the Data File Naming Token feature are the following:

- If you want to add sequence lines while a sequence is already under acquisition, we recommend using the **Name Pattern** naming scheme, and leaving the **Datafile** column in the Sequence Table empty. After editing the sequence, the system will automatically generate a data file name when the sample beginning acquisition.
- If you manually enter a name into the **Data file** column of the Sequence Table, that name will be used as the data file name for that run, overriding the **Auto**, **Prefix/Counter**, or **Name Pattern** naming scheme.
  - With other naming schemes, the default filename will be **OnlineEdited#.D**, where # is incremented for each additional line when editing the sequence.
  - Deleting lines from a running sequence can lead to serious inconsistencies, especially if the sequence is paused and then restarted.
- The tokens **Date** and **Time** are incompatible with the execution of Partial Sequence.
- The feature **Write barcode to sample name** with the **Name Pattern** Token **<SampleName>** will produce the result of *no Sample Name* for the Data File.
  A suggestion would be use the other tokens available for the data file name.

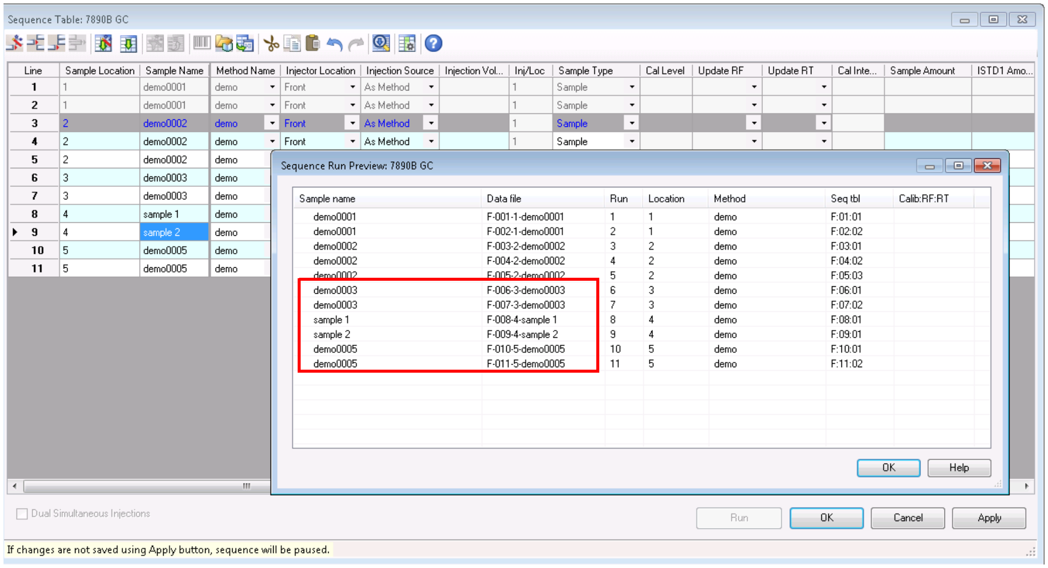


Line	Sample Location	Sample Name	Method Name	Injector Location	Injection Source	Injection Vol...	Inj/Loc	Sample Type	Cal Level	Update RF	Update RT	Cal Inte...	Sample Amount	ISTD1 Amo...
1	1	demo0001	demo	Front	As Method		2	Sample						
2	2	demo0002	demo	Front	As Method		2	Sample						
3	3	demo0003	demo	Front	As Method		2	Sample						
4	4	demo0004	demo	Front	As Method		2	Sample						
5	5	demo0005	demo	Front	As Method		2	Sample						

Sample name	Data file	Run	Location	Method	Seq tbl	Calib:R
demo0001	F-001-1-demo0001	1	1	demo	F:01:01	
demo0001	F-002-1-demo0001	2	1	demo	F:01:02	
demo0002	F-003-2-demo0002	3	2	demo	F:02:01	
demo0002	F-004-2-demo0002	4	2	demo	F:02:02	
demo0003	F-005-3-demo0003	5	3	demo	F:03:01	
demo0003	F-006-3-demo0003	6	3	demo	F:03:02	
demo0004	F-007-4-demo0004	7	4	demo	F:04:01	
demo0004	F-008-4-demo0004	8	4	demo	F:04:02	
demo0005	F-009-5-demo0005	9	5	demo	F:05:01	
demo0005	F-010-5-demo0005	10	5	demo	F:05:02	

☐ Dual Simultaneous Injections

Figure 2 **Sequence prior to running samples**: The data file names will be as displayed unless there is an edit in the sequence, then the data file names will be updated according to the name token selection in Sequence Parameters. In this example **<SeqLine><SampleLoc><Sample Name>** Name Pattern tokens were used.



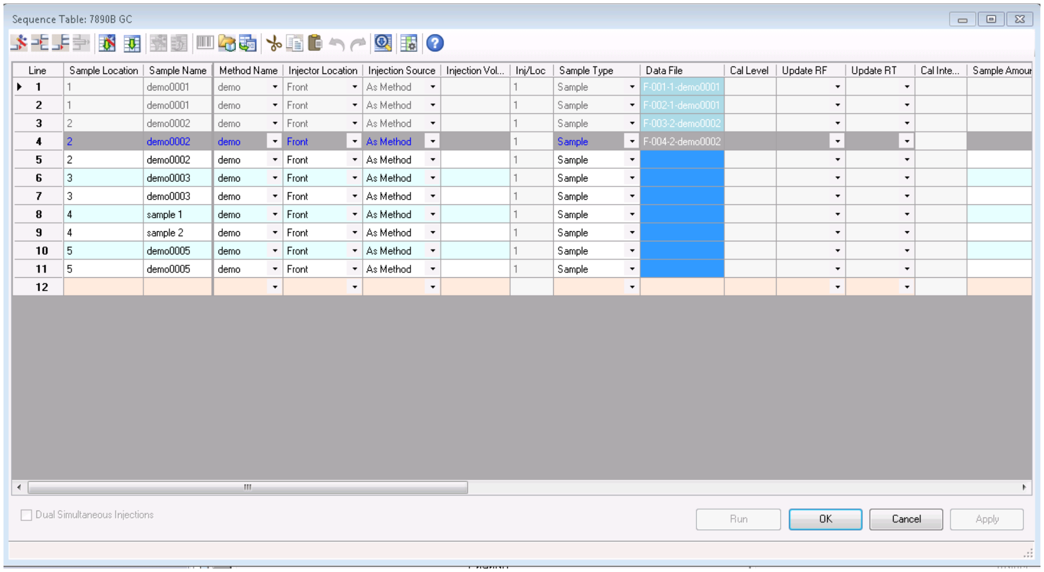
Line	Sample Location	Sample Name	Method Name	Injector Location	Injection Source	Injection Vol...	Inj/Loc	Sample Type	Cal Level	Update RF	Update RT	Cal Inte...	Sample Amount	ISTD1 Amo...
1	1	demo0001	demo	Front	As Method		1	Sample						
2	1	demo0001	demo	Front	As Method		1	Sample						
3	2	demo0002	demo	Front	As Method		1	Sample						
4	2	demo0002	demo	Front	As Method		1	Sample						
5	2	demo0002	demo											
6	3	demo0003	demo											
7	3	demo0003	demo											
8	4	sample 1	demo											
9	4	sample 2	demo											
10	5	demo0005	demo											
11	5	demo0005	demo											

Sample name	Data file	Run	Location	Method	Seq tbl	Calib:RF:RT
demo0001	F-001-1-demo0001	1	1	demo	F:01:01	
demo0001	F-002-1-demo0001	2	1	demo	F:02:02	
demo0002	F-003-2-demo0002	3	2	demo	F:03:01	
demo0002	F-004-2-demo0002	4	2	demo	F:04:02	
demo0002	F-005-2-demo0002	5	2	demo	F:05:03	
demo0003	F-006-3-demo0003	6	3	demo	F:06:01	
demo0003	F-007-3-demo0003	7	3	demo	F:07:02	
sample 1	F-008-4-sample 1	8	4	demo	F:08:01	
sample 2	F-009-4-sample 2	9	4	demo	F:09:01	
demo0005	F-010-5-demo0005	10	5	demo	F:10:01	
demo0005	F-011-5-demo0005	11	5	demo	F:11:02	

☐ Dual Simultaneous Injections

If changes are not saved using Apply button, sequence will be paused.

Figure 3 **Preview Running Sequence**: In this example you can see the data file names have been updated according the name token selection in **Sequence Parameters**.



Line	Sample Location	Sample Name	Method Name	Injector Location	Injection Source	Injection Vol...	Inj/Loc	Sample Type	Data File	Cal Level	Update RF	Update RT	Cal Inte...	Sample Amour
1	1	demo0001	demo	Front	As Method		1	Sample	F-001-1-demo0001					
2	1	demo0001	demo	Front	As Method		1	Sample	F-002-1-demo0001					
3	2	demo0002	demo	Front	As Method		1	Sample	F-003-2-demo0002					
4	2	demo0002	demo	Front	As Method		1	Sample	F-004-2-demo0002					
5	2	demo0002	demo	Front	As Method		1	Sample						
6	3	demo0003	demo	Front	As Method		1	Sample						
7	3	demo0003	demo	Front	As Method		1	Sample						
8	4	sample 1	demo	Front	As Method		1	Sample						
9	4	sample 2	demo	Front	As Method		1	Sample						
10	5	demo0005	demo	Front	As Method		1	Sample						
11	5	demo0005	demo	Front	As Method		1	Sample						
12														

Figure 4 The data files names are automatically filled in just prior to acquisition of the sample. In this example **<SeqLine><SampleLoc><Sample Name>** Name Pattern tokens were used.

2. Intelligent Reporting

For data acquired by ChemStation C.01.06 or higher the Report Template Editor has been updated for the fields

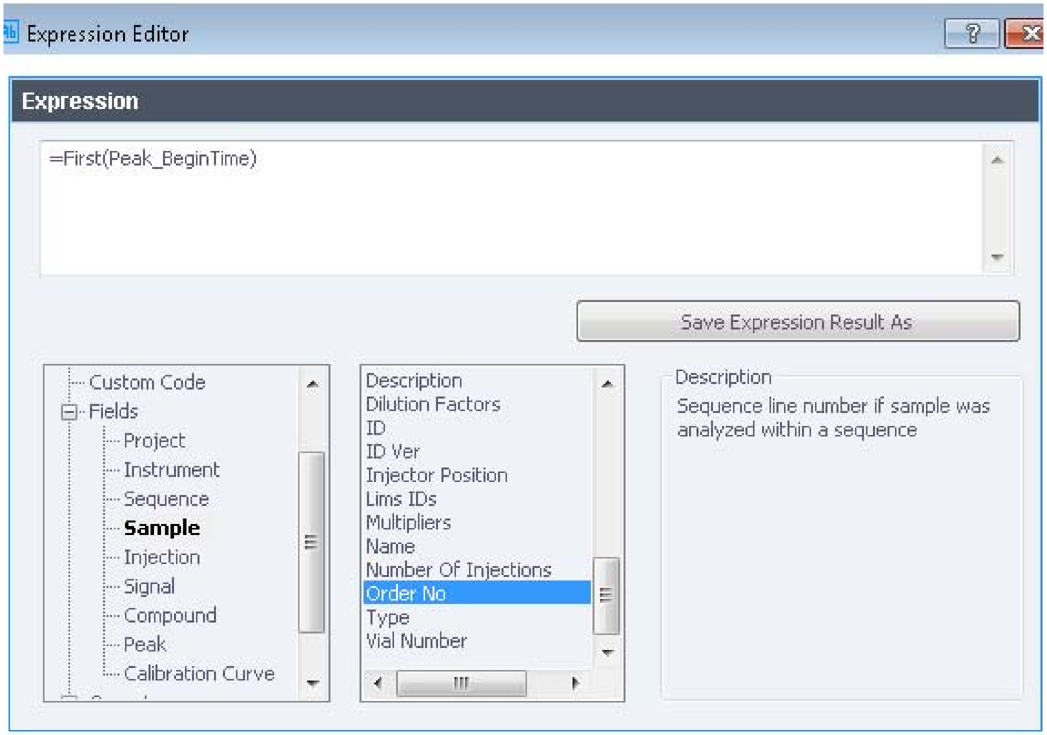
SAMPLE_ORDERNO, and
SAMPLE_ACQUISITIONORDERNO.

To show the line number of an injection in the sequence table on the report, always use the field **Sample Acquisition Order No.** This option directly matches to the sequence table order.

Only if the sequence template specifies multiple injections for a line, to group and sort injections that originate from the same template line, use the field **Sample Order No**. The field **Sample Order No** contains the sequence table line number of the first injection for a template line.

Sequence line number:

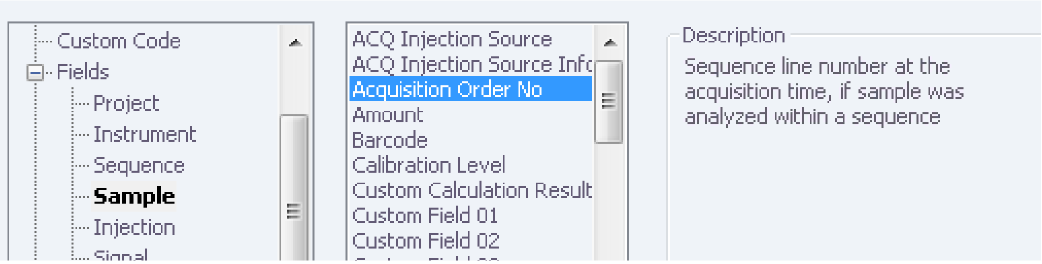
If a sequence template specifies multiple injections for the line, this field contains the line number of the first of these injections in the rolled out sequence table.



`=First(Peak_BeginTime)`

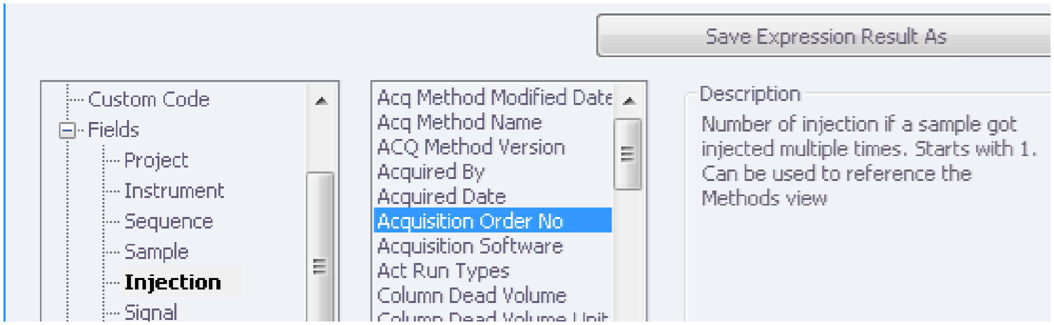
Sequence line number if sample was analyzed within a sequence

Figure 5 **Sample, Order No:**
Sequence line number of the first injection for a sequence template line.



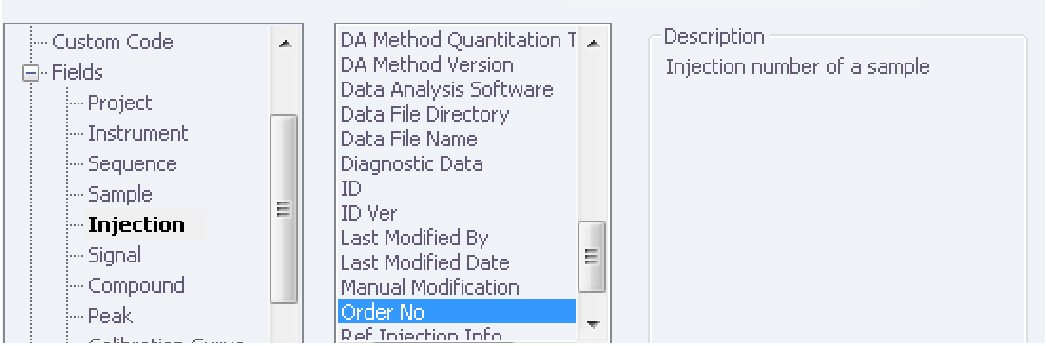
Sequence line number at the acquisition time, if sample was analyzed within a sequence

Figure 6 **Sample, Acquisition Order No:**
The sequence line number when the sample is acquired.



Number of injection if a sample got injected multiple times. Starts with 1. Can be used to reference the Methods view

Figure 7 **Injection, Acquisition Order No**:
Number of injection per vial.
Note, if the sequence was edited during acquisition, this number maybe only be one.



Injection number of a sample

Figure 8 **Injection, Order No**:
Injection number of a sample.

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