

Using Agilent Fraction Collectors in Thermo Scientific Chromeleon with ICF Integration

Technical Note

Information and Recommendations

Agilent Fraction Collectors in Chromeleon environment behave differently compared to what is described in the Driver Online Help. Note the following specifics:

- Built-in intelligence can only be applied among Agilent modules via CAN. Therefore, ensure to use an Agilent-only instrument LC system for fraction collection.
- *ICF integration:*
 - Currently, the use of Agilent Fraction Collectors in Chromeleon is *only* supported using the ICF integration.
 - Define a **Stoptime** for any Agilent Fraction Collector (FC)/Fraction Collector Cluster (FCC) as for internal calculations, for example time-based fractionation, the FC/FCC **Stoptime** is needed. Ensure that the defined run time is in sync with the chosen sample run time.
- *Agilent Drivers for Chromeleon*
 - Using Fraction Collectors with Agilent Drivers for Chromeleon is *not yet* supported. Some rudimentary features are available, but these are not supported.
 - Agilent Drivers for Chromeleon is the recommended instrument control in Chromeleon as the ICF integration is phasing out. However, ICF integration is currently the only supported control for fraction collection. Future Agilent Drivers for Chromeleon will include fraction collection support and offer enhanced user experience for control.

NOTE

The use of Agilent Fraction Collectors in Chromeleon with the ICF integration is only recommended for routine applications where users know upfront how many fractions they will collect during a run. When there is overfill, the system does not abort and fill the next valid location. The use in research environment is not recommended (status 02/2022).

Single Fraction Collection Setup

Configuration

Online Help:

- 1 The LC Drivers offer various configuration changes. To apply these changes, use the instrument tile in the dashboard.

The changes are applied on the fly and written back to the instrument.

- 2 For hardware-related changes, modify the instrument.

ICF Integration

- 1 For the G1364A/B/C/D and G5664A Fraction Collectors:

- a Go to the **Reconfigure Modules** tab in the Home ePanel to access the configuration settings.

- b Change the parameters and click **Apply**.

The changes are applied after an automatic reconnect to the instrument.

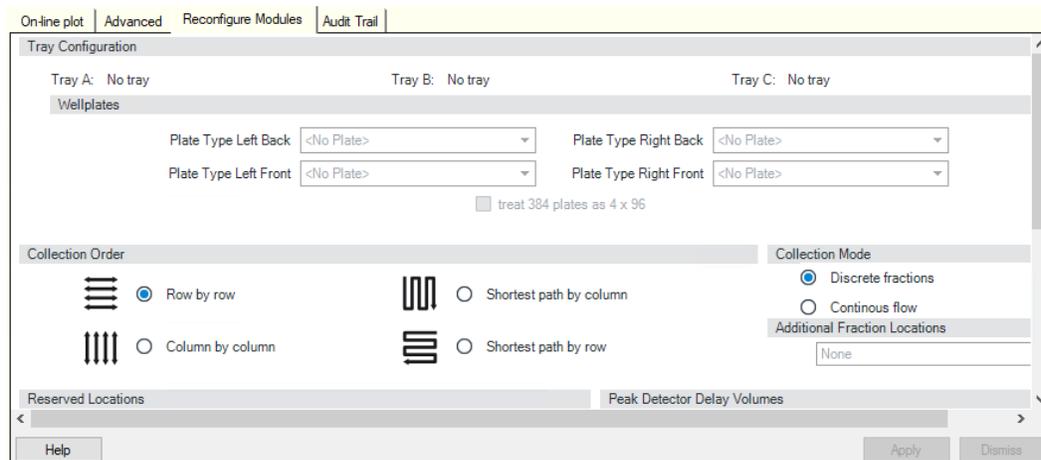


Figure 1 Module reconfiguration window

Single Fraction Collection Setup

- 2 For the G1364E/F, G7166A, G7158B, G7159B, and G5664A Fraction Collectors:
 - a Right-click into the instrument tile of the Fraction Collector in the Home ePanel and select **Modify**.
 - b Select the configuration settings you want to change.
A configuration dialog opens.
 - c Change the parameters and click **OK**.
The changes are applied after an automatic reconnect to the instrument.

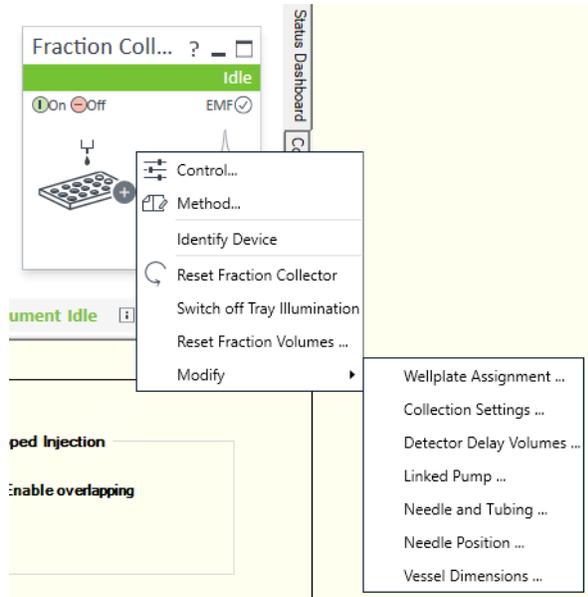


Figure 2 Instrument tile

Method Window

Online Help: The FC method window offers the option to load a reference chromatogram to perform a fraction preview.

ICF integration: Starting with ICF 3.0, this feature is only present in CDS, which offers a selection of a reference chromatogram. Before ICF 3.0, the option is present, but will run into an error.

Start Locations

Each CDS has its own approach where and how to set the fraction start locations. In Chromeleon, the following information applies for **Fraction Start Location**.

- Set the **Fraction Start Location** in the Home ePanel, in the **Advanced** tab, section **Fraction Collection**.
- Use one of the following *formats*, depending on the tray/container used in the fraction collector::
 - Px-Row-Column (for example P1-B-1)
 - Linear addressing (for example vial 1)
- The **Fraction Start Location** can be left empty. In this case, fractioning starts at the first location vial 1/P1-A-1 and continues using the next location based on the selected fraction order until the end of the sequence.
- Enter an *absolute location* and each run of the sequence will start again with this location (see Note on pooling).
- The **Fraction Start Location** does not offer *logic positions*, such as **Next Location**, **Next Row**, etc. as options.
- The **Fraction Start Location** does not offer **Pooling**. **Pooling** start fraction collection at the same position as in the previous run and keep track of the fraction fill state to prevent overfills.

NOTE

Using an absolute start location, each run of a sequence starts at the same location, so this option is a kind of “pooling”. However, this setup does not warn the users or stop the sequence if there are overfills. When reaching the maximum fill volume, the fraction collector advances to the next valid position and may contaminate fractions of the previous run. Therefore, the user must know the expected fractions upfront and needs to intervene if correction is necessary.

- A **Custom Column** can be used to assign different fraction start locations per sequence run.

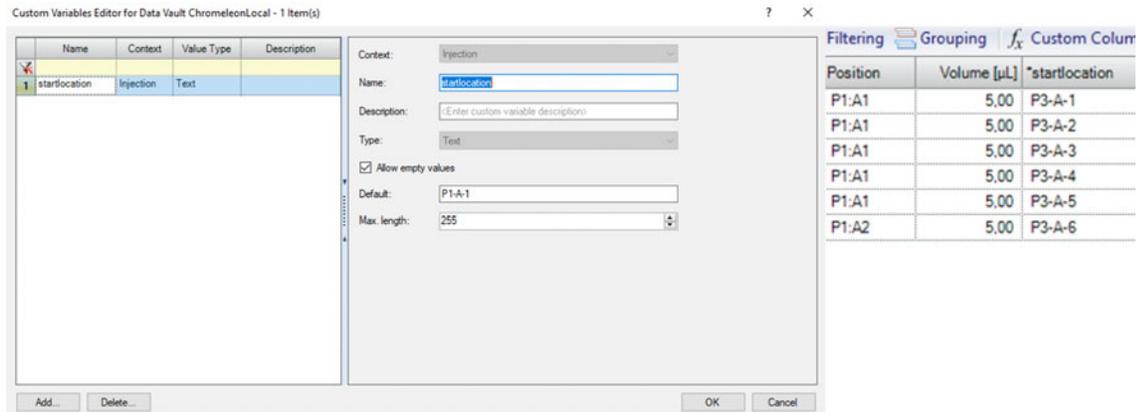


Figure 3 Custom variables editor

NOTE

The start position is used even if the position was used in prior runs or is already completely filled. The user needs to calculate upfront how many fractions will be collected, otherwise it is possible that the run collects in already used/occupied locations.

Reporting

- Manual fractioning is possible, the action is recorded in the audit trail. They are recorded, marked as information not as manual action.

Line	Date	Time	Concentration	System	Event
3	07.02.2022	11:51:34 +01:00	0,338	LCSystem	Analytical result /AFC.0.FractionData: 3 results
4	07.02.2022	11:51:31 +01:00	0,289	LCSystem	G1364E-AN84294568 - End of fraction
5	07.02.2022	11:51:31 +01:00	0,288	LCSystem	G1364E-AN84294568 - Manual stop fraction
6	07.02.2022	11:51:29 +01:00	0,248	LCSystem	G1364E-AN84294568 - Manual start fraction
7	07.02.2022	11:51:29 +01:00	0,248	LCSystem	G1364E-AN84294568 - Begin of fraction
8	07.02.2022	11:51:26 +01:00	0,201	LCSystem	G1364E-AN84294568 - End of fraction
9	07.02.2022	11:51:26 +01:00	0,195	LCSystem	G1364E-AN84294568 - Manual stop fraction
10	07.02.2022	11:51:23 +01:00	0,146	LCSystem	G1364E-AN84294568 - Begin of fraction
11	07.02.2022	11:51:23 +01:00	0,146	LCSystem	G1364E-AN84294568 - Manual start fraction
12	07.02.2022	11:51:20 +01:00	0,101	LCSystem	G1364E-AN84294568 - End of fraction
13	07.02.2022	11:51:20 +01:00	0,099	LCSystem	G1364E-AN84294568 - Manual stop fraction
14	07.02.2022	11:51:18 +01:00	0,073	LCSystem	G1364E-AN84294568 - Begin of fraction
15	07.02.2022	11:51:18 +01:00	0,065	LCSystem	G1364E-AN84294568 - End of fraction

Figure 4 Audit trail

- If enabled, the chromatogram indicates the collected fractions graphically. The example shows time-based fractioning.

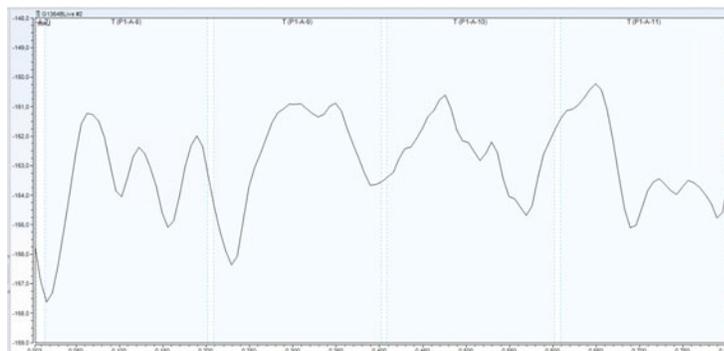


Figure 5 Chromatogram

- The chromatogram displays the first location of each fraction in darker shade. When there is overflow, subsequent locations are marked in lighter shade.
- You can use the built-in Chromeleon **Tube report** for reporting. You can also use custom variables if they are defined and set up.

The screenshot shows the 'Tube Report' dialog box in the Chromeleon software. The dialog is open over a data table. The table contains the following data:

Line	Pos.	Start	End	Volu
1				
2		min	min	ml
4	P1-B-7	0,001	0,105	
5	P1-B-8	0,203	0,266	
6	P1-B-9	0,307	0,349	
7	P1-C-1	0,389	0,434	
8	P1-C-2	0,476	0,524	
9	P1-C-3	0,572	0,616	
10	P1-C-4	0,659	0,707	
11	P1-C-5	0,753	1,000	

The dialog box includes various options for report generation, such as 'Results', 'Integration', 'Peak Summary', 'Calibration History', 'Data Audit Trail', 'Test Cases', 'Frame Table', 'Tentative Identification', 'IPD Components', 'IPD Processes', 'NTMS Processes', 'Processing Method', and 'Instrument Method'.

Figure 6 Tube report

- The fraction trigger reason (Detector signal, manual trigger, or overflow) is not reported.

Fraction Collection Cluster

Supported Clusters

Supported clusters with ICF A.02.05 / LC Driver A.02.19:

- Up to 3 G7159B main FCs with G9322A, 1 G7166A recovery FCs in Cluster
- Up to 3 G1364E main FCs with G9322A, 1 G7166A recovery FCs in Cluster
- Up to 3 G1364E main FCs with G9322A, 1 G1364E recovery FCs in Cluster
- Up to 3 G7166A main FCs

Setup/Configuration

- 1 In the Configuration Manager, define the cluster.
- 2 Manually adjust the **Device name**.

NOTE

Chromeleon has some naming limitations. Do not use spaces. Only the alphanumeric characters a..Z and 0..9 and the underscore (_) are allowed. The field is limited to 24 characters.

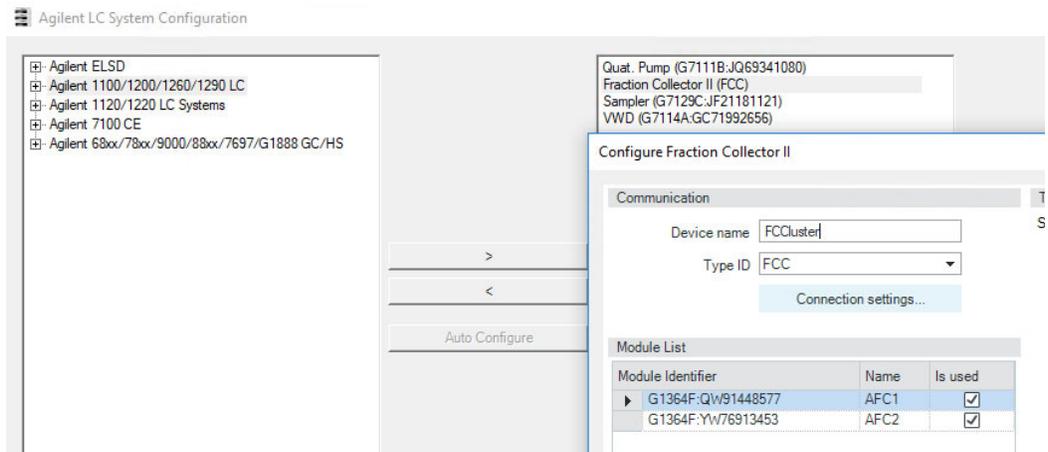


Figure 7 System configuration

- 3 Shorten the 2D signal names to conform with Chromeleon naming conventions.

Gen	FractionCollector_AFC1DelaySensor	FCCluster: AFC1 Delay Sensor [counts]	FCCluster: AFC1 Delay Sensor [counts]	0	0	counts	1,000
Gen	FractionCollector_AFC1Temperature	FCCluster: AFC1 Temperature [°C]	FCCluster: AFC1 Temperature [°C]	0	0	°C	1,000
Gen	FractionCollector_AFC2DelaySensor	FCCluster: AFC2 Delay Sensor [counts]	FCCluster: AFC2 Delay Sensor [counts]	0	0	counts	1,000
Gen	FractionCollector_AFC2Temperature	FCCluster: AFC2 Temperature [°C]	FCCluster: AFC2 Temperature [°C]	0	0	°C	1,000

Figure 8 2D signal names

- 4 Manually enter the min/max values for the signal names.
 - Delay Sensor: -2097152 / 2097152
 - Temperature: -128 / 128

Start Locations

- There is *no fraction start location* on the Home ePanel when a cluster is configured. The system starts at vial 1/P1-A-1. You can also use custom column to set up a start location.
- Some cluster topologies offer the option to recover samples and solvents from the waste line of the fraction collector. To set a recovery start location, right-click the instrument tile of the Fraction Collector Cluster in the Home ePanel and click **Modify ... Recovery Settings**.

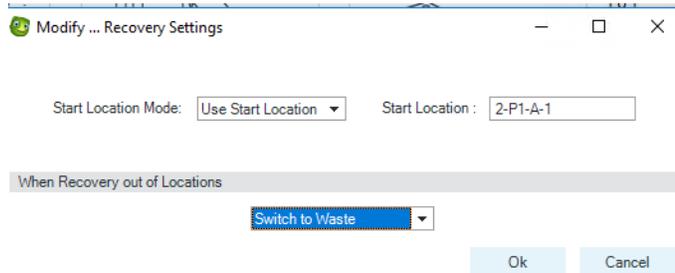


Figure 9 Recovery settings

Features Requiring LC Driver 3.0 or Higher

New modules and new features require LC Driver updates. The current Chromeleon versions (status 02/2022) do not support any LC driver above A.02.19 SR2 (included in ICF 2.6).

That means that any feature released with LC Driver 3.0 or higher for an existing fraction module is not available to the user. See [Table 1](#) on page 8.

Table 1 Driver features

LC Driver	Feature
3.0	Increased capabilities for analytical-scale Fraction Collector II Clusters Up to three collectors can be combined with dedicated rotary valves to collect fractions. For Recovery Collection, up to three more modules can be attached using a G9322A Agilent 1260 Infinity II Clustering Valve. For more information, see Agilent LC&CE Driver 3.0 Release Note (https://www.agilent.com/cs/library/technicaloverviews/public/LC-and-CE-Driver-Release-Note-3-0.pdf).
3.1	New module support: G7158B Open-Bed Sampler <i>and</i> Fraction Collector Support of autoscale cluster combination of modules to allow for seamless switching between analytical scouting runs and preparative-scale purification within the same sequence. For more information, see Agilent LC&CE Drivers 3.1 Release Note (https://www.agilent.com/cs/library/technicaloverviews/public/LC-and-CE-Driver-Release-Note-3-1.pdf).
3.2	Enhanced support of G7158B 1290 Infinity II Preparative Open-Bed Autosampler and Fraction Collector in Fraction Collector Cluster The LC and CE Drivers now support clustering of the G7158B with up to two more Fraction Collector modules and up to three more Recover Collector modules.
3.3	G4734B Preparative 6-column selector valve, 600 bar (5067- 6722) (Works as generic valve till LC Driver 3.3)
3.4	Flow gradients during fractioning