

S-Matrix®

Fusion QbD®

QUALITY BY DESIGN SOFTWARE SYSTEM

GC METHOD DEVELOPMENT GUIDE – EMPOWER CDS



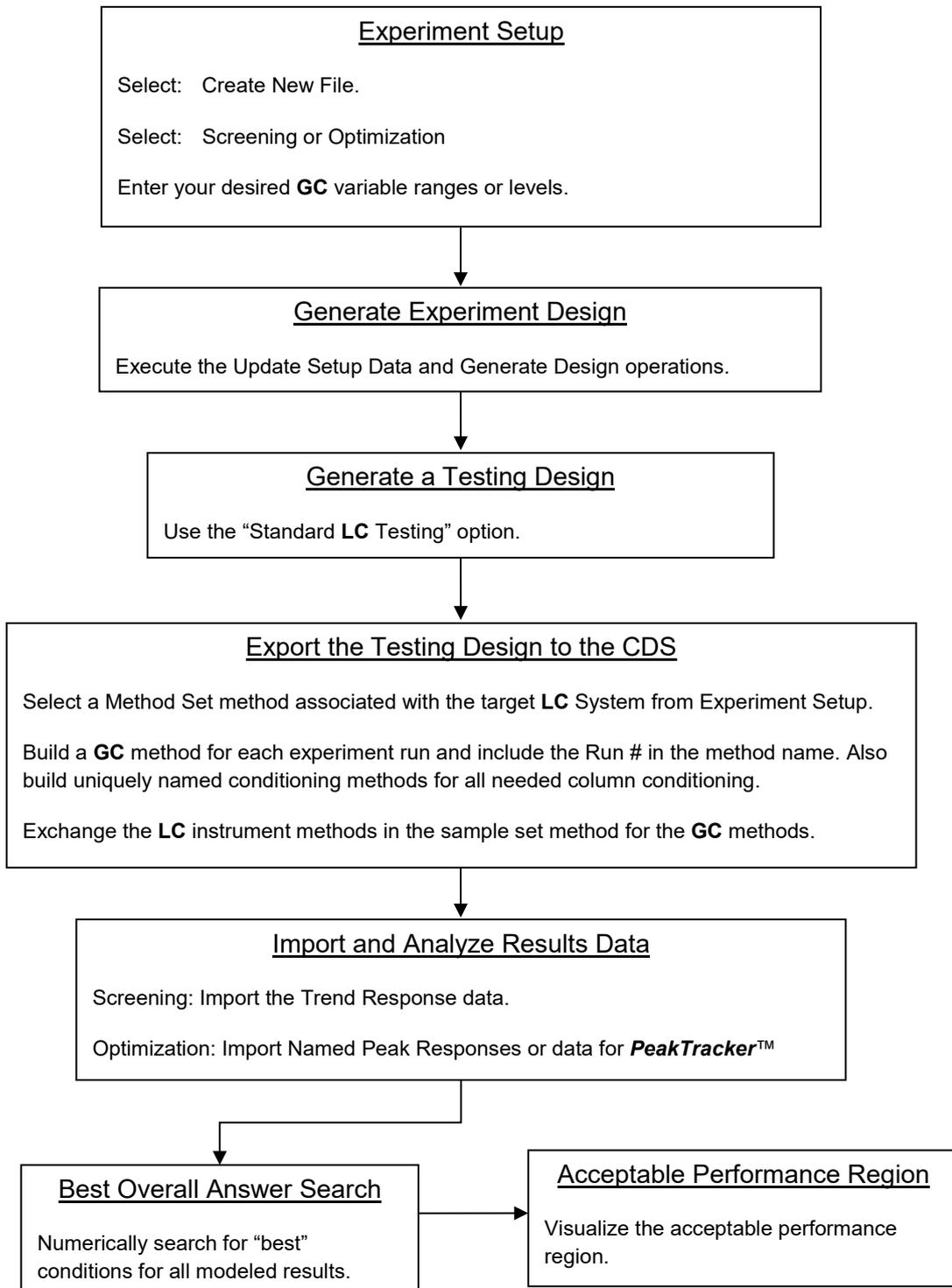
S-Matrix Corporation
www.smatrix.com

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Overview of the Workflow

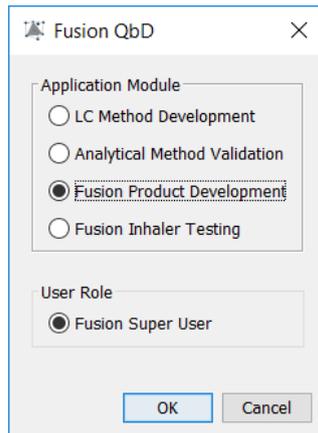
GC Method Development in Fusion QbD is done using the Fusion Product Development Module (FPD). Below is a general workflow.



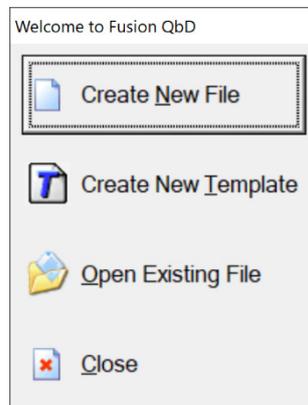
Create the GC Method Development Experiment Design

The Fusion Product Development module is used for creating GC Method Development experiments. In this example, we will describe the process for creating a simple GC experiment using the initial hold time and the temperature programming rate.

1. Launch Fusion QbD. Select the 'Fusion Product Development' module.



2. Select the 'Create New File' option.



3. Set the 'No. of Mixture Variables' to zero (0).

Set the 'No. of Process Variables' to your desired number (2 in this example). Enter your variable settings

- Initial Hold Time Continuous LB = 0.0 UB = 5.0
- Temperature Ramp Rate Continuous LB = 10.0 UB = 30.0

Name	Units	Type	Lower Bound	Upper Bound
Initial Hold Time	Minutes	Continuous	0.0	5.0
State <input checked="" type="radio"/> Variable <input type="radio"/> Constant				
Name	Units	Type	Lower Bound	Upper Bound
Temperature Ramp Rate	Deg/Min	Continuous	10.0	30.0
State <input checked="" type="radio"/> Variable <input type="radio"/> Constant				

Note – you can add parameters and set them as 'State=Constant' if you want to document the constant settings used in the experiment.

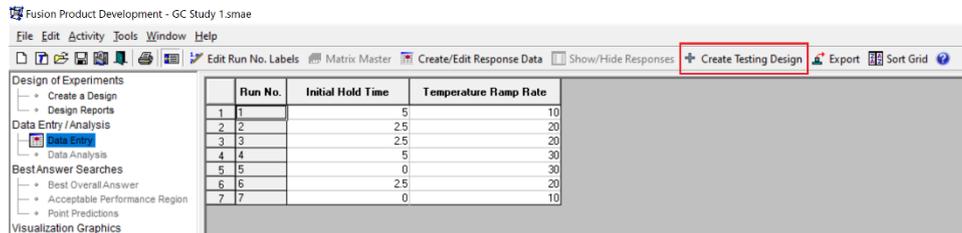
4. Generate the Design.

The screenshot shows the 'S-Matrix' interface for 'Experiment Design'. It includes a sidebar with navigation options like 'Design Reports', 'Data Entry / Analysis', and 'Reporting Toolkit'. The main area displays the 'Experiment Design Matrix' with the following data:

Run No.	Initial Hold Time (Minutes)	Temperature Ramp Rate (Deg/Min)
1	5.0	10.0
2	2.5	20.0
3	2.5	20.0
4	5.0	30.0
5	0.0	30.0
6	2.5	20.0
7	0.0	10.0

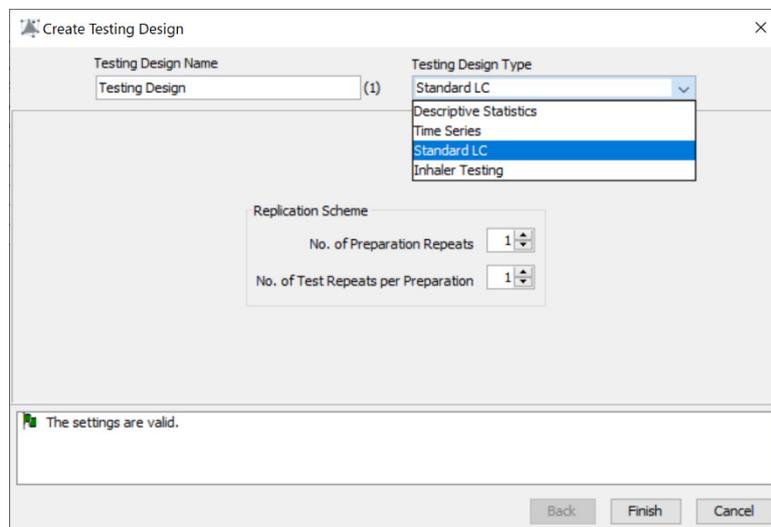
Create the Companion Testing Design

1. In the Data Entry View, click the '+ Create Testing Design' button on the Menu Bar.

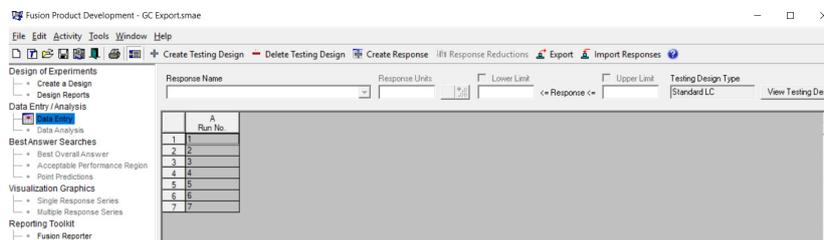


2. Select Standard LC from the 'Testing Design Type' list box.

Use the settings shown in the image below.



3. Save the file with a unique and recognizable file name.

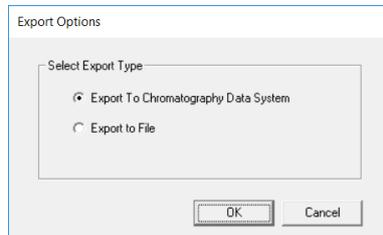
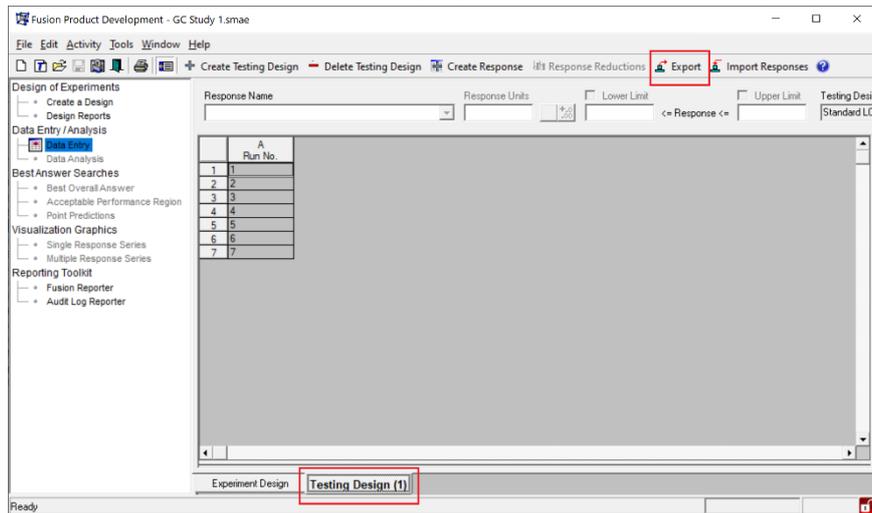


Export the Testing Design to the CDS

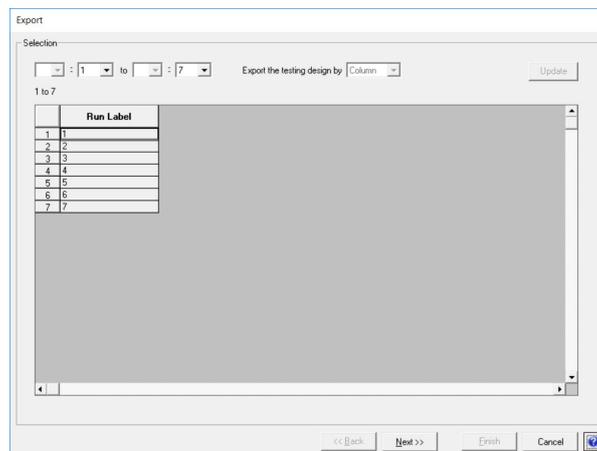
1. Access the Data Entry View and select the 'Testing Design (1)' tab.

Click the 'Export' button on the main menu bar.

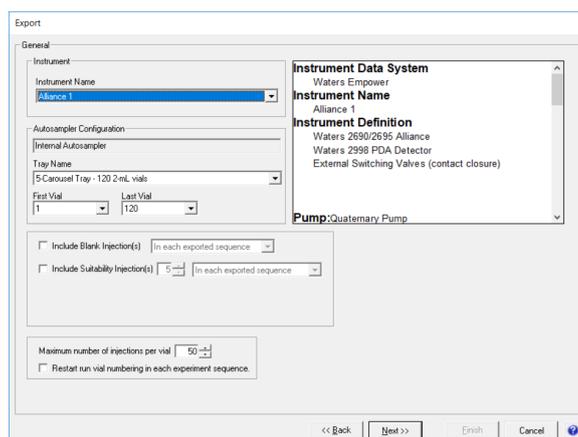
Select on the 'Export to CDS' option on the 'Export Options' dialog.



2. Click 'Next' on the 1st Export wizard dialog pictured below.

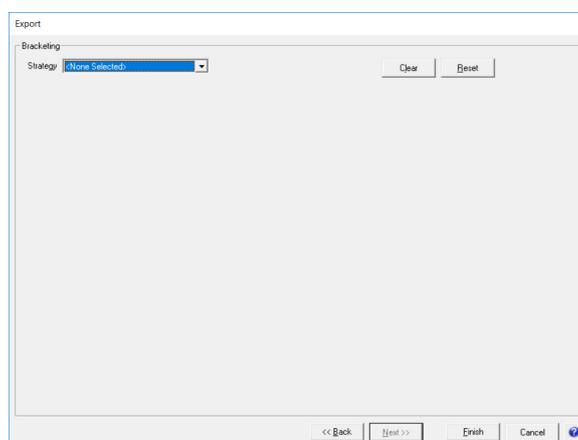


3. Select a valid LC instrument system in the 2nd Export wizard dialog pictured below, and click Next.

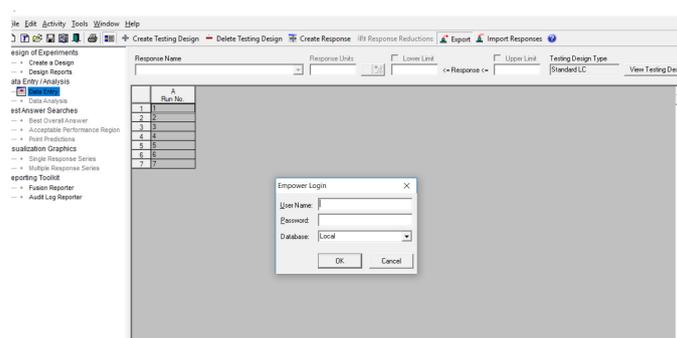


Note – Fusion QbD export automation only works directly with LC instrument systems and methods. Therefore, you must select a licensed LC instrument system. You will match this with the Method Set method you select in Step 6 below, which must be associated with the same LC instrument method and system.

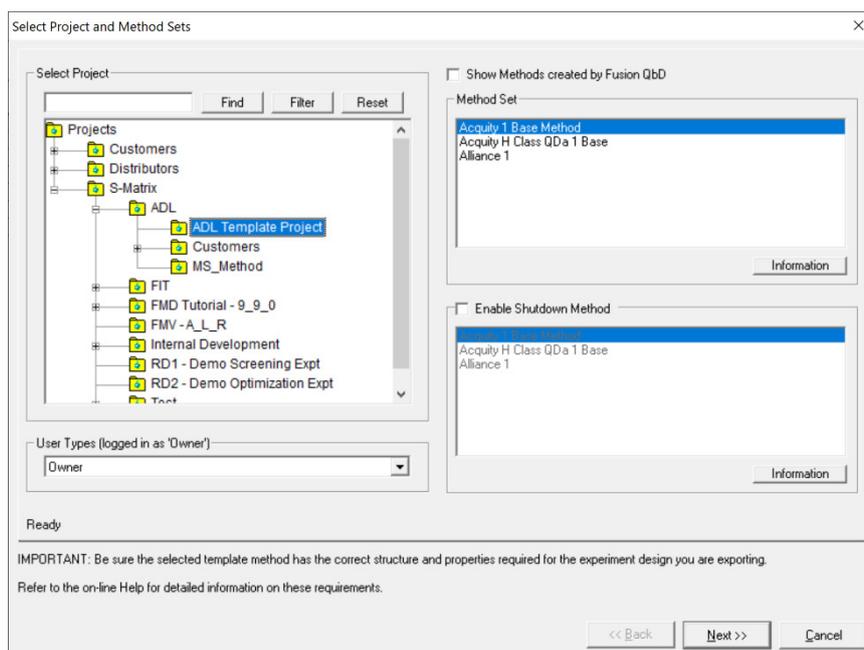
4. Select the ‘None Selected’ option in the Standards Strategy list box within the 3rd Export wizard dialog pictured below, and click ‘Finish’.



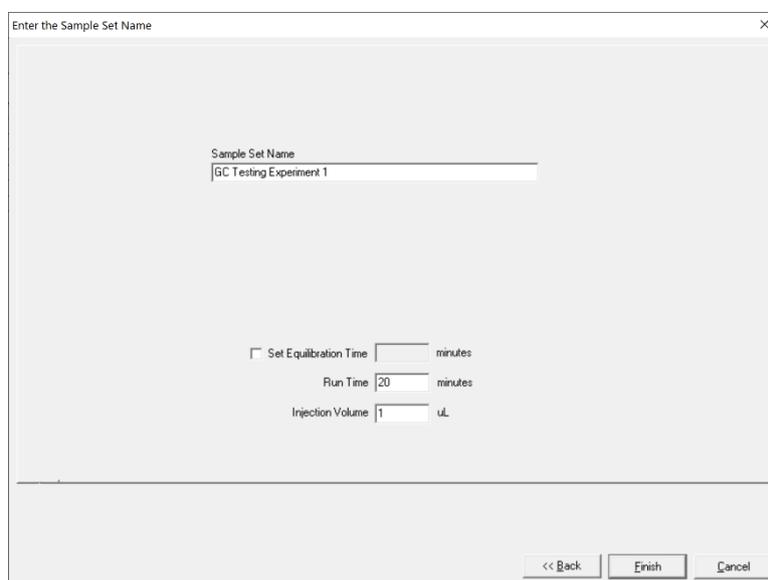
5. Log on to Empower using your Empower logon credentials.



6. In Empower, select the Project and Method Set method which will be used to build the Sample Set method, and click 'Next'.



7. Enter a recognizable name which will be used to name the Sample Set method, Instrument methods, and Method Set methods built as part of the export operation, then click 'Finish'.



IMPORTANT

Run Time and **Injection Volume** – the level settings you enter here will be automatically written to the Sample Set method. You should review and edit these settings as needed in Empower for your experiment run conditions.

Construct the Required GC Methods within the CDS

1. Log on to Empower using your Empower logon credentials.
2. Use the 'Browse Projects' option to navigate to the Empower project in which you exported your experiment design.
3. Open an existing GC instrument method which correctly operates the GC on which you will run your experiment design.
4. Edit the method to contain the correct level settings for all GC parameters you **did NOT include** in your design in terms of your current sample and this experiment.
5. Execute the 'File | Save As...' operation to save the file with a recognizable name. In this example we will use the name "Fusion_GC_Base_Method".
6. With Empower open, launch Fusion QbD, open your GC experiment design file, navigate to the 'Design Reports' View, and select the 'Experiment Design' report from the 'Design Reports list box, as pictured below.

Fusion Product Development - GC Study 1.smae

File Edit Activity Tools Window Help

Design Reports

Experiment Design

Name: Administrator
Company: S-Matrix
Project: Project 1 (User Defined)
Date: 17 FEB 2020 09:07:40 PST [UTC-08:00]

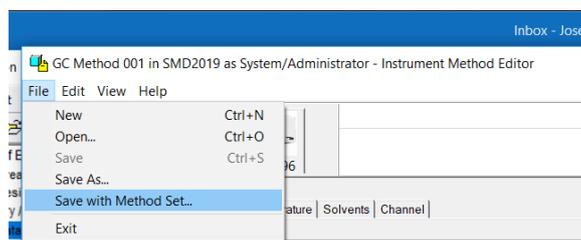
Experiment Design

Experiment Design Matrix

Run No.	Initial Hold Time (Minutes)	Temperature Ramp Rate (Deg/Min)
1	5.0	10.0
2	2.5	20.0
3	2.5	20.0
4	5.0	30.0
5	0.0	30.0
6	2.5	20.0
7	0.0	10.0

7. Open the GC instrument method from Step 5 above. Referring to the Fusion QbD experiment design, edit the GC method to reflect the level settings of the variables in Run No. 1.

- Execute the ‘File | Save with Method Set...’ operation to save the GC Instrument method, and its associated Method Set method, with a recognizable name and a Run 1 extension. In this example we will use the name “Fusion_GC_Study_001”.



- Repeat Steps 7 and 8 above to generate the Instrument Methods and associated Method Set methods required for all the experiment design runs. It is best to do this in the sequential order of the experiment design – for example:

Fusion_GC_Study_001
Fusion_GC_Study_002
...
Fusion_GC_Study_007

Note – doing this in sequential order minimizes mistakes, and supports ease of association of the methods into the associated Sample Set method constructed at the time of export from Fusion QbD.

Edit the Sample Set Method within the CDS

1. Select the Sample Set method which Fusion QbD constructed within your target Empower project, and open it for editing.

Method Name	Method Type	Method Date	Method Id	Old Id
GC Testing Experiment 1_1	Sample Set	2/16/2020 7:54:19 PM PST	1040	
Acquity H Class QDa 1 Base	Method Set	8/15/2019 3:31:00 PM EDT	1019	
Alliance 1	Method Set	8/15/2019 3:36:46 PM EDT	1031	
Acquity 1 Base Method	Method Set	8/15/2019 3:31:00 PM EDT	1022	
Acquity H Class QDa 1 Base	Instrument	8/15/2019 3:31:00 PM EDT	1000	
Alliance 1	Instrument	8/15/2019 3:36:31 PM EDT	1030	
Acquity 1 Base Method	Instrument	8/15/2019 3:31:00 PM EDT	1004	

2. For each experiment run (row) in the Sample Set method, use the Instrument method list boxes within the 'Method Set / Report or Export Method' column to exchange the LC instrument method for the GC method you constructed in the previous section.

Run	Inj Vol (µL)	Label	Sample Name	Level	Function	Method Set / Report or Export Method	Label Reference	Processing	Run Time (Minutes)	Data Start (Minutes)	Next Inj Delay (Minutes)	MS Tune Method	MS Calibration Method	Column Position	Auto Addition
1	10.0	Unk-001-001	1		Inject Samples	GC Method 001		Normal	20.00	0.00	0.00				
2	10.0	Unk-001-002	2		Inject Samples	Alliance 1 Base Method		Normal	20.00	0.00	0.00				
3	10.0	Unk-001-003	3		Inject Samples	Alliance 1 Base Method		Normal	20.00	0.00	0.00				
4	10.0	Unk-001-004	4		Inject Samples	Alliance 1 Base Method		Normal	20.00	0.00	0.00				
5	10.0	Unk-001-005	5		Inject Samples	Alliance 1 Base Method		Normal	20.00	0.00	0.00				
6	10.0	Unk-002-001	6		Inject Samples	Alliance 1 Base Method		Normal	20.00	0.00	0.00				
7	10.0	Unk-002-002	7		Inject Samples	Alliance 1 Base Method		Normal	20.00	0.00	0.00				

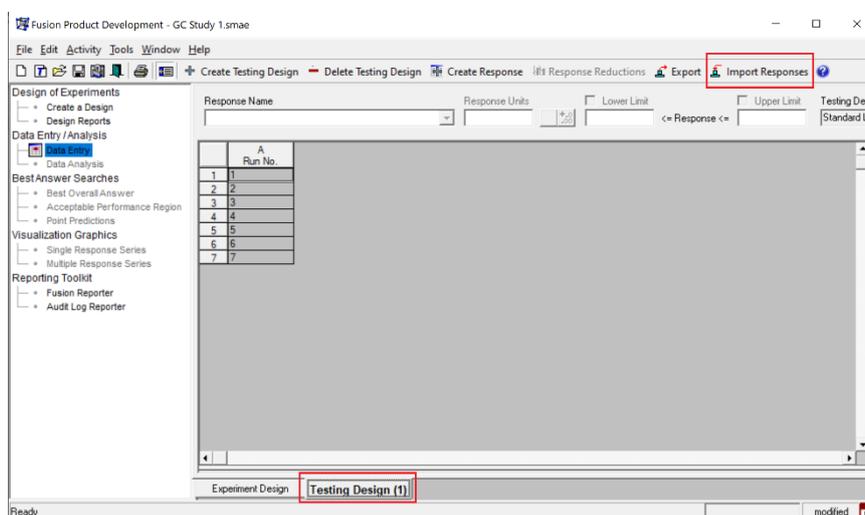
3. Confirm that the run times and injection volumes match the experiment method requirements, and your method times, and save the edited Sample Set method when the exchanges and edits are complete.

IMPORTANT

You should carry out a column conditioning run to bake your column prior to starting your experiment run. You will also need to manually insert rows column conditioning with appropriately constructed conditioning methods as required to support changes between experiment runs.

Run your Experiment within the CDS and Import Your Results

1. Prepare your GC system. Load and execute the Sample Set in Empower.
2. After running the experiment on the GC, process the completed Sample Set into a Results Set using an appropriate processing method. Review the processed results to correct any integration issues.
3. Launch Fusion QbD and access the Fusion Product Development module.
4. Open your experiment file, and access the Data Entry View.
5. Select the 'Testing Design (1)' tab, and import your experiment chromatogram results for analysis and visualization.



Note – refer to the Empower Data Exchange module under the Help menu in Fusion QbD for tips with integration and the Fusion QbD import operation.