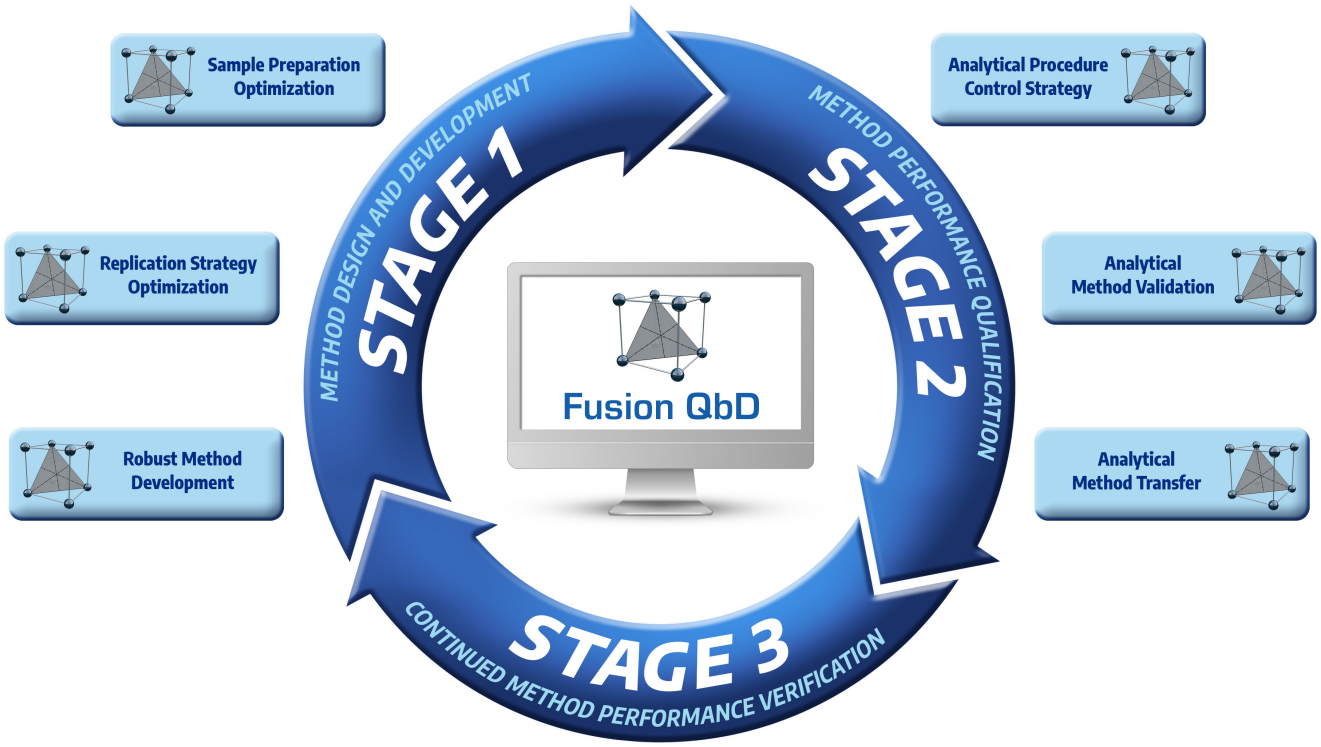
S-Matrix®

Fusion QbD®

QUALITY BY DESIGN SOFTWARE SYSTEM

GC METHOD DEVELOPMENT GUIDE – V 4.0
EMPOWER CDS



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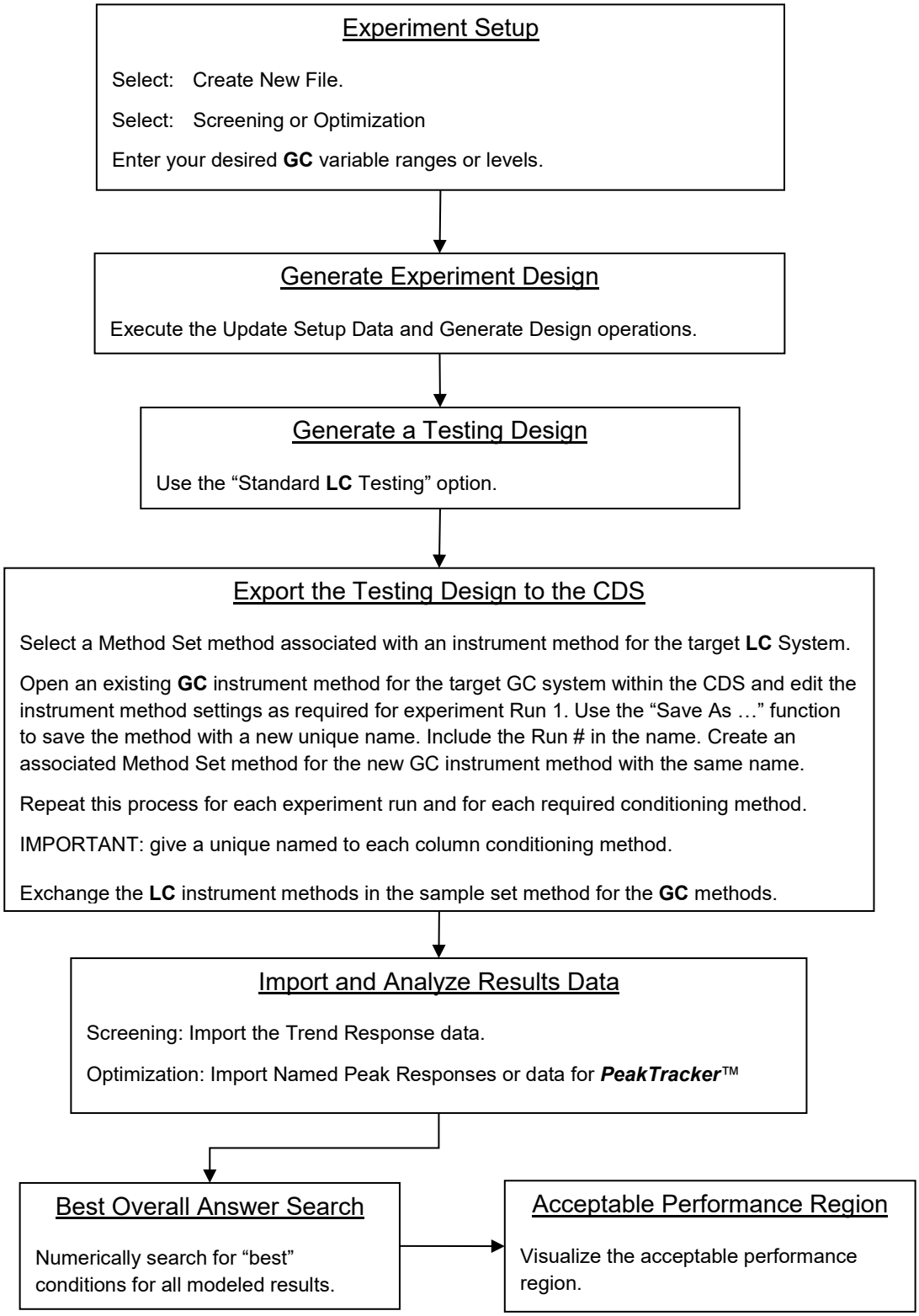
Overview of the Experiment Workflow

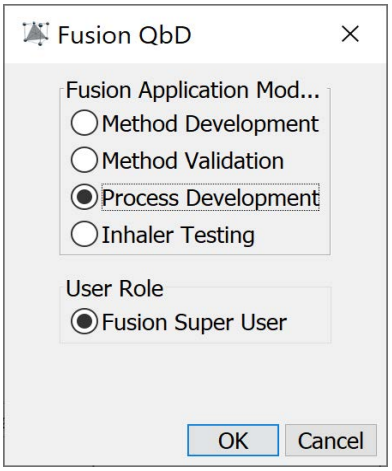
GC Method Development in Fusion QbD is done using the Fusion Process Development Module (FPD). Below is a general experiment workflow.



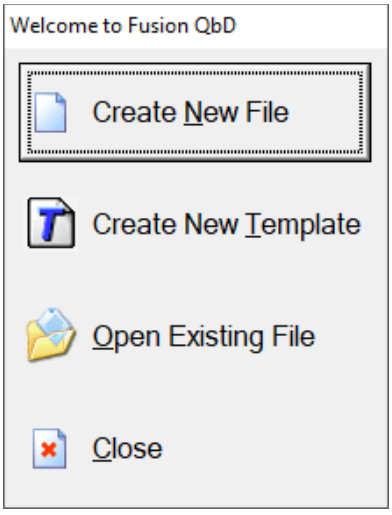
Create the GC Method Development Experiment Design

The Fusion Process 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 Process Development' module.



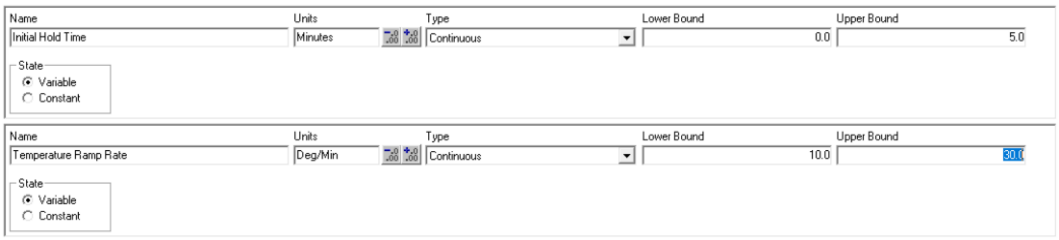
2. Select the 'Create New File' option.



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

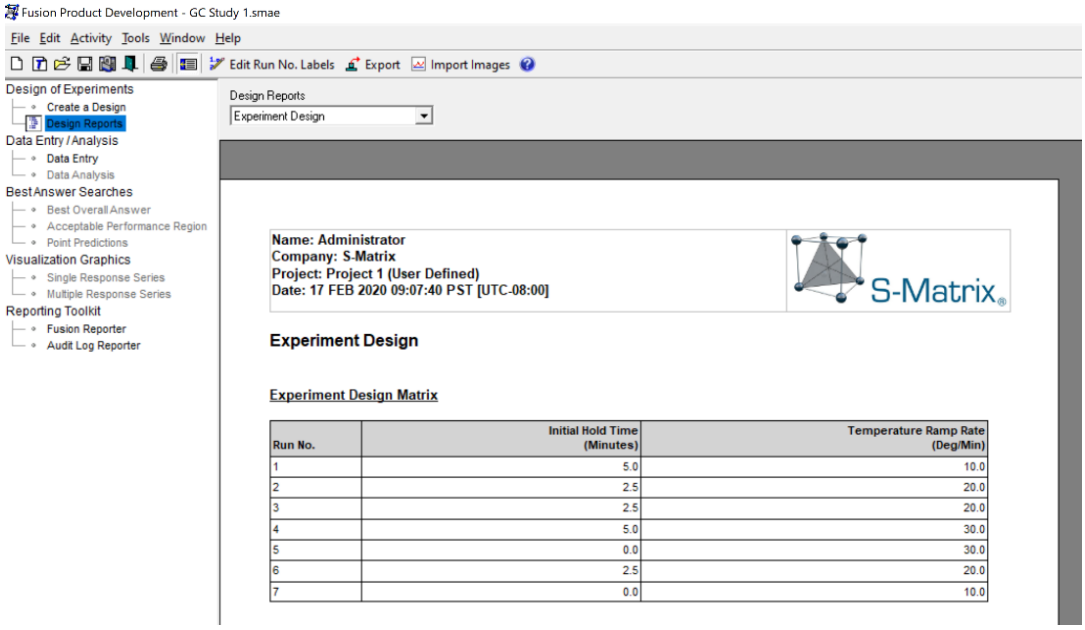
Set the ‘No. of Process Variables’ to your desired number (2 in this example). Enter your variable settings

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



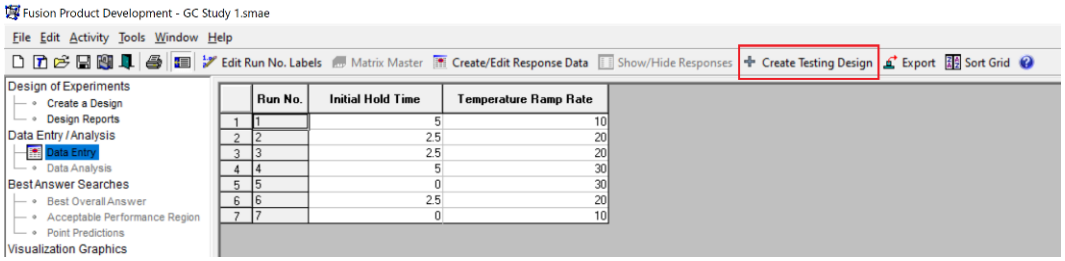
Note – you can add parameters and set them as ‘State=Constant’ if you want to document the constant settings used in the experiment.

4. Generate the Design.



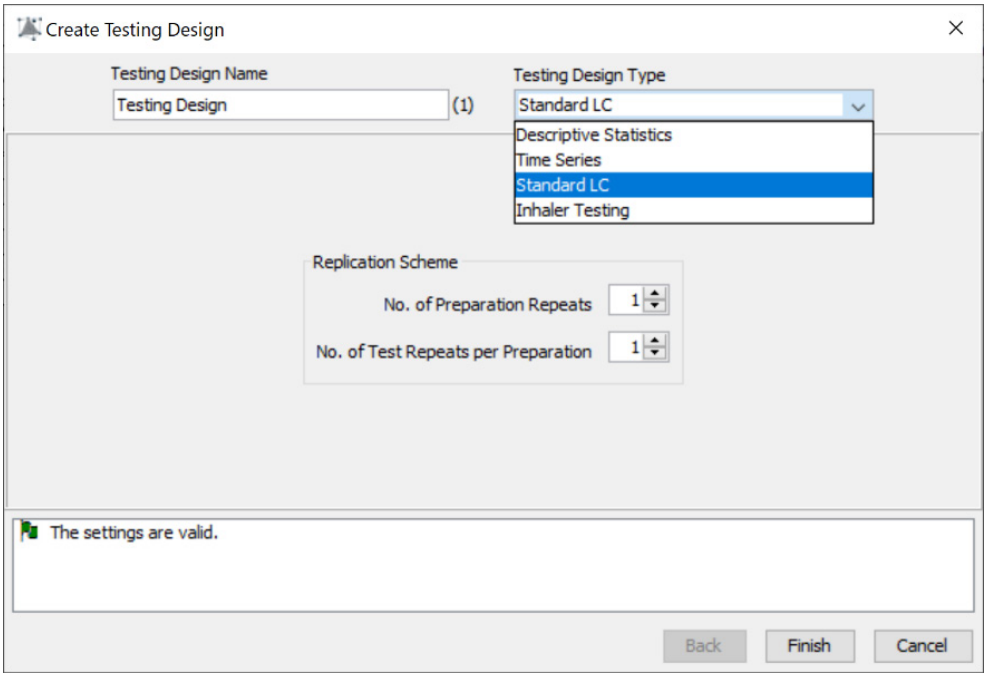
Create the Companion Testing Design

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

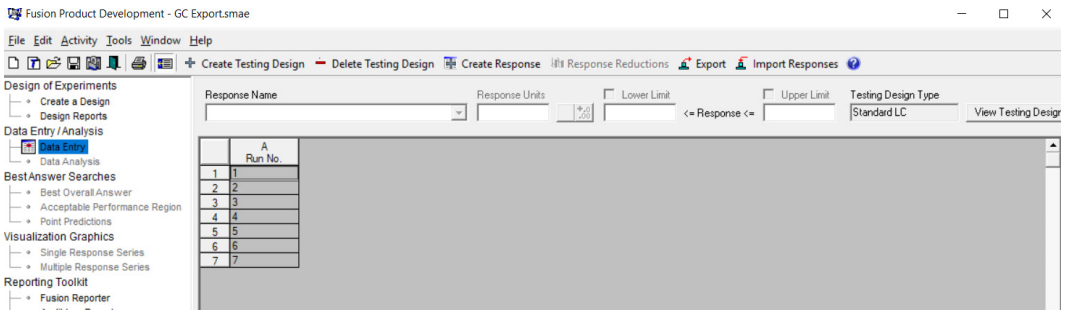


2. Select Standard LC from the 'Testing Design Type' list box.

   Use the settings shown in the image below.



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



Construct a Template GC Method in 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 will export your experiment design.

3. Open an existing GC instrument method (or create a new GC method) which correctly operates the GC on which you will run your experiment design and is consistent with your sample compound mix and general experimental approach.

4. Edit the method to contain the exact level settings for all GC parameters you **did NOT include** in your design so that the constant level settings are correct to the study.

   NOTE – you will use this method as the basis of constructing your experiment methods and linking them to your exported sequence. Therefore, constructing this method with the correct constant level settings will reduce the manual editing required to only the experiment design parameters.

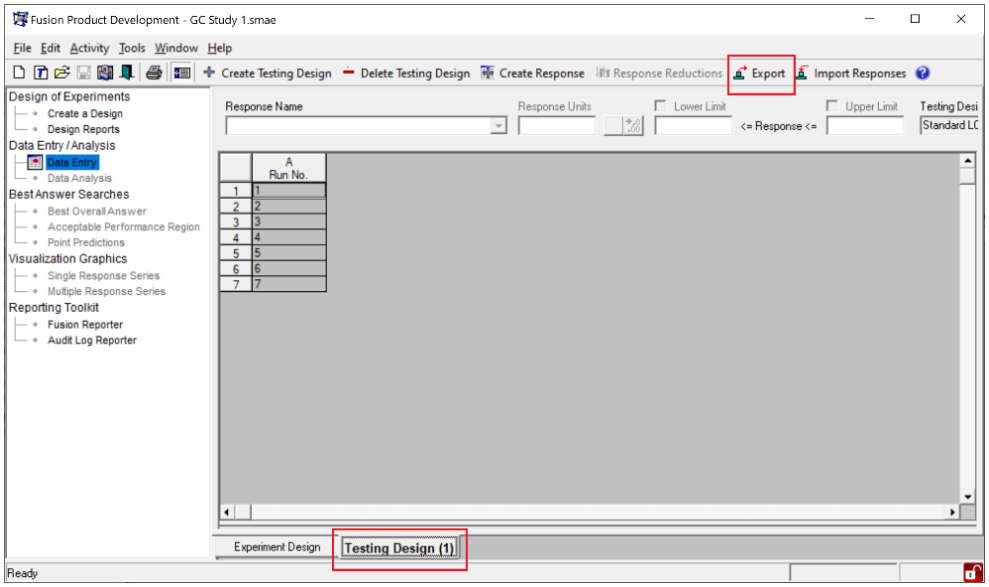
5. Execute the ‘File | Save As…’ operation to save the file with a recognizable name. In this example we will use the name “Fusion_GC_Base_Method” for the instrument method and the associated method set method.

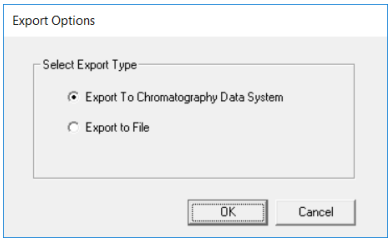
Export the Testing Design to the CDS

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

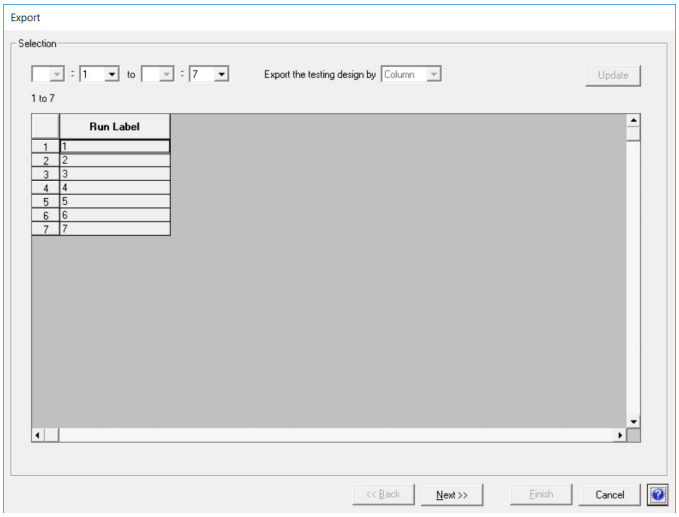
   Click the ‘Export’ button on the main menu bar.

   Select on the ‘Export to CDS’ option on the ‘Export Options’ dialog.

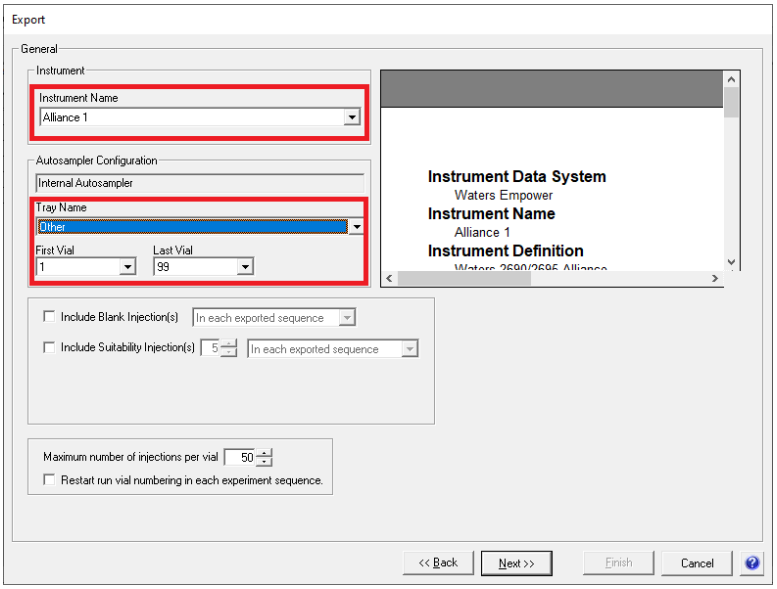




2. Click ‘Next’ on the 1st Export wizard dialog pictured below.



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

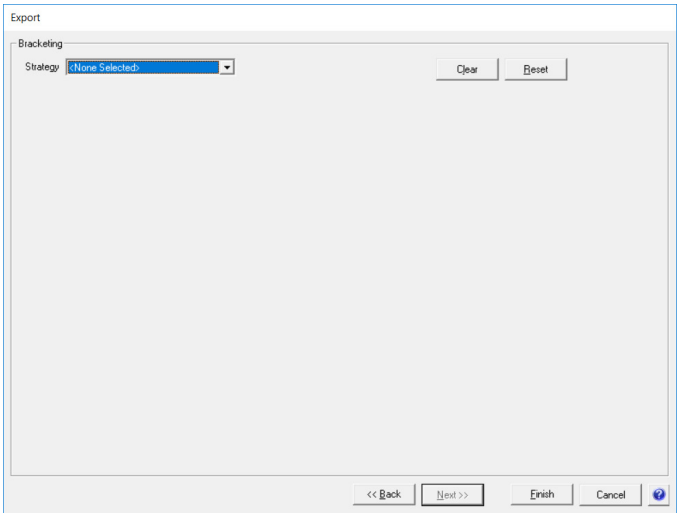


IMPORTANT

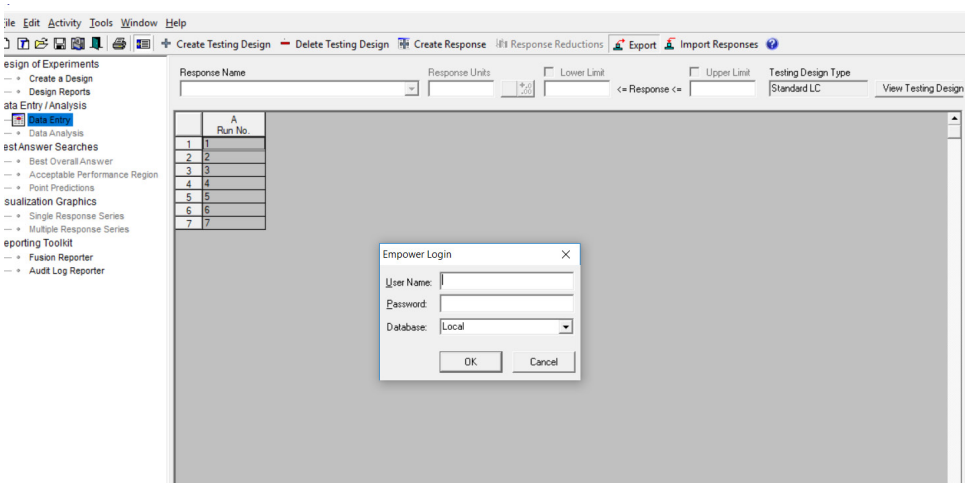
As shown in the image above, you must select an Autosampler Tray with the same Vial Position label designations as your GC instrument autosampler tray.

NOTE – The "**Other**" tray option uses the standard "1, 2, …, 100" vial position designation.

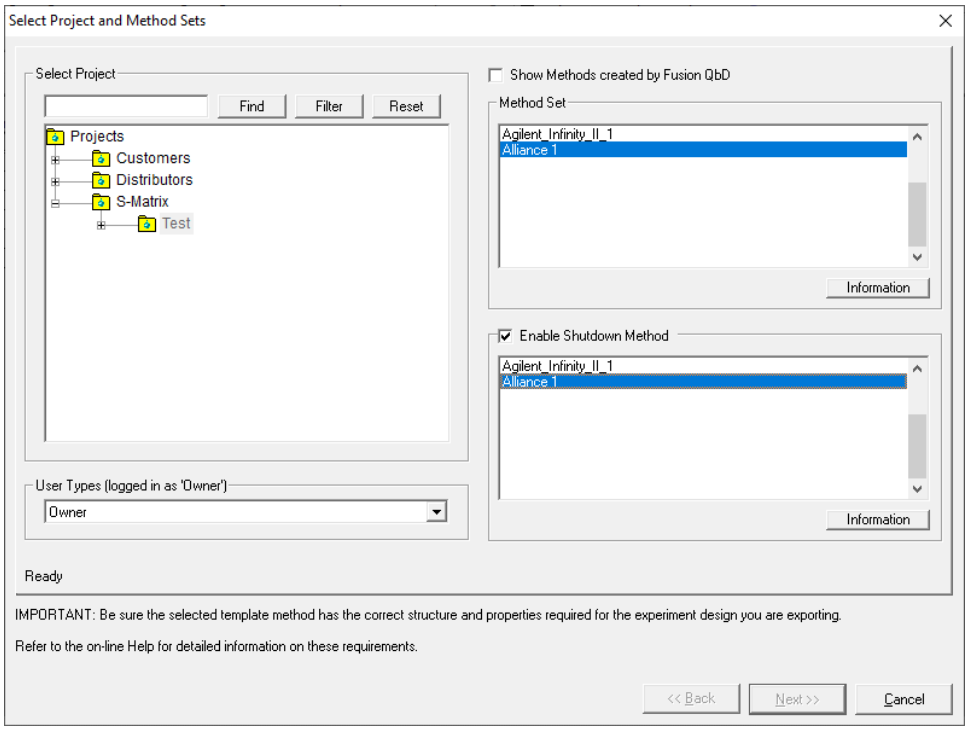
4. Select the 'None Selected' option in the Standards Strategy list box within the 3rd Export wizard dialog pictured below, and click 'Finish'.



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'.

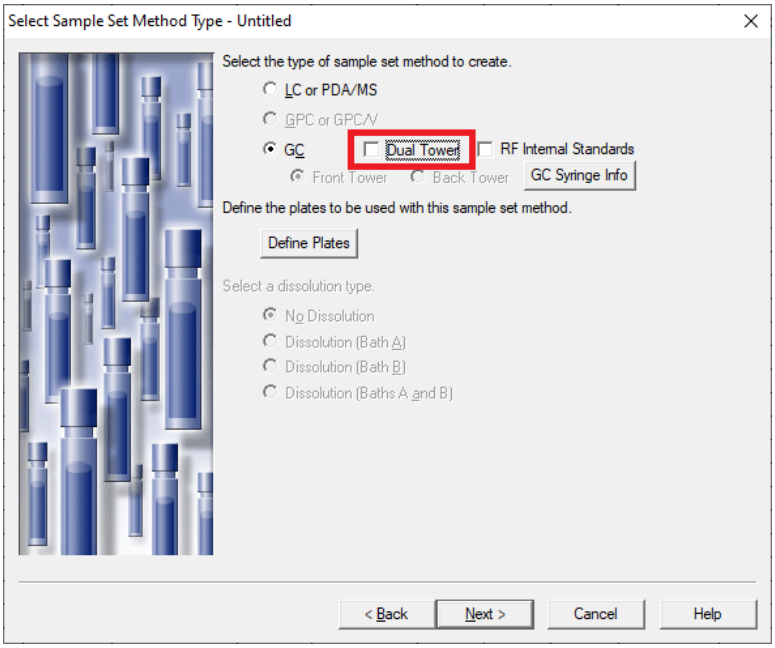


CRITICAL

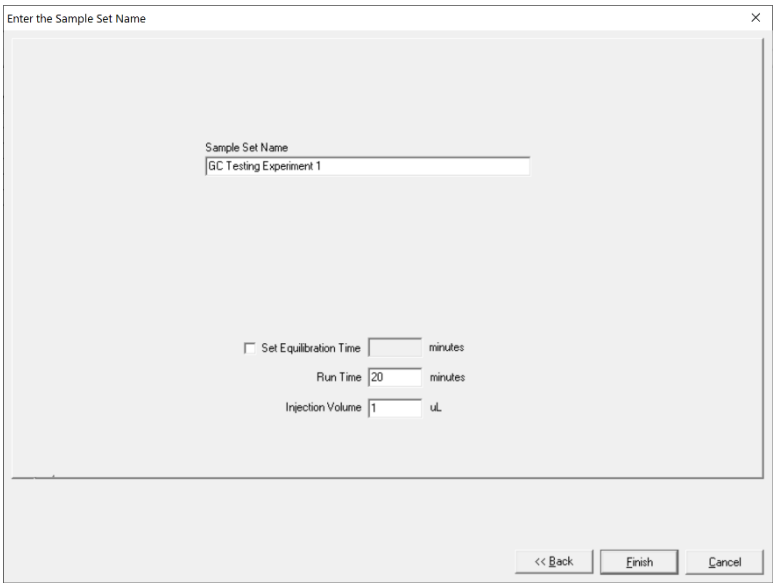
Fusion QbD versions prior to Version 9.9.1 require that you select a Method Set method associated with an Instrument method specific to the **LC** instrument system you selected in Step 3 above.

IMPORTANT

If you build your Sample Set method manually, or using the New Sample Set Method Wizard, make sure that the “Dual Tower” option is UNchecked, as shown below.



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

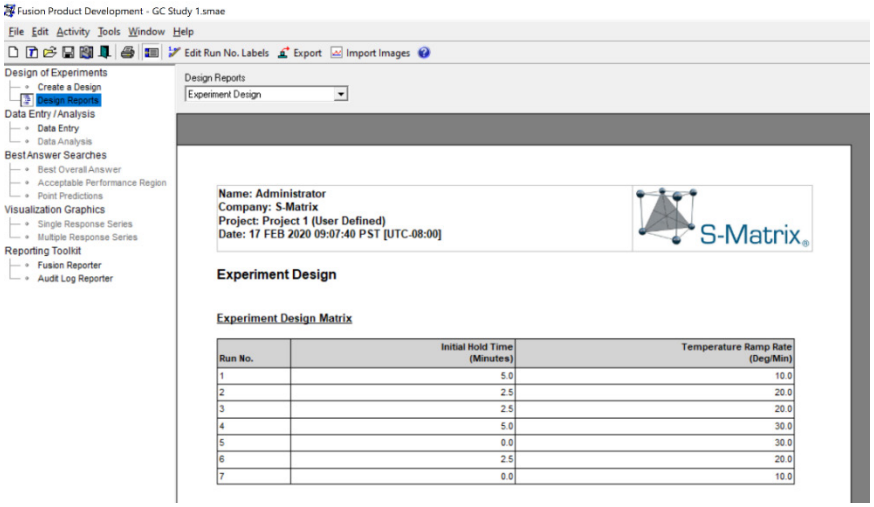
Equilibration Time, **Run Time** and **Injection Volume** – the level settings you enter here will be automatically written to the Sample Set method. You should review and edit these settings as needed in Empower for your experiment run conditions.

Construct the Required GC Methods in 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.

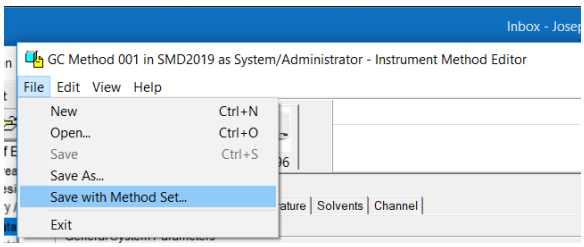
3. With Empower open, launch Fusion QbD, open your GC experiment design file, navigate to the ‘Design Reports’ View, and select the ‘Experiment Design’ report from the ‘Design Reports list box, as pictured below.



4. Open the template (base) **GC** instrument method you created according to the steps in the earlier section titled “**Construct a Template (Base) GC Methods within the CDS**”.

5. Edit the GC method to reflect the level settings of the variables in Experiment Run No. 1 (refer to the Fusion QbD experiment design for the required run settings).

6. 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”.



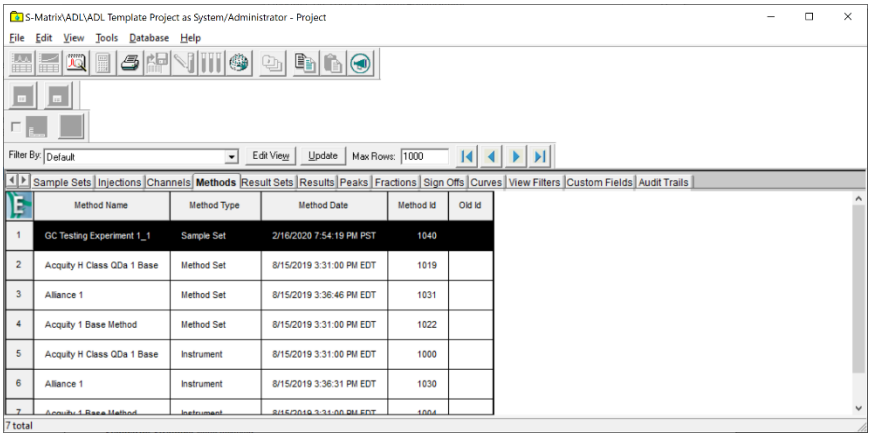
7. Repeat Steps 4 – 6 above to generate the Instrument methods and associated Method Set methods required for 1) all experiment design runs, and 2) all Column Conditioning runs required for correct experiment execution (e.g. to support column baking required prior to executing the next experiment run or runs). It is best to do this in the sequential order of the experiment design – for example:

Fusion_GC_Study_Conditioning_1 (Initial Conditioning)
Fusion_GC_Study_001
Fusion_GC_Study_002
…
Fusion_GC_Study_007

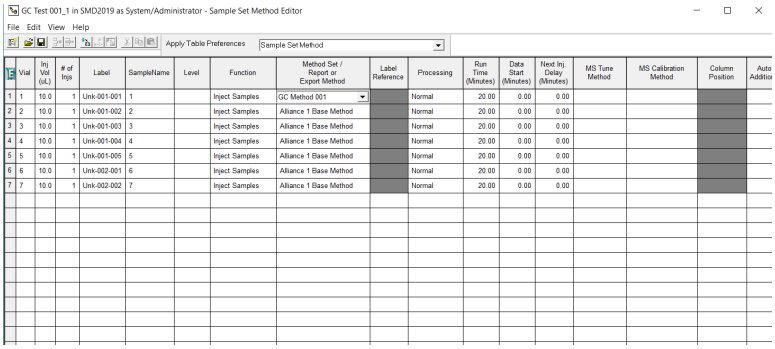
Note – doing this in sequential order minimizes mistakes, and supports ease of association of the methods into the associated Sample Set method constructed at the time of export from Fusion QbD.

Edit the Sample Set Method in the CDS

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



2. Manually insert conditioning rows as needed. For each column conditioning run (row) in the Sample Set method, use the Instrument method list boxes within the 'Method Set / Report or Export Method' column to select the **GC** conditioning method you constructed in the previous section for the conditioning run.



3. Modify the Vial positions in the 'Vial' column of the sequence so that all experiment run injections point to the vial position containing your sample compound mix.

4. Perform a column conditioning run to bake your column – either prior to running the experiment or by adding a new first row to the sequence for the baking method.

5. Confirm that the equilibration times, run times, and injection volumes match the experiment method requirements, and your method times.

6. Save the edited Sample Set method when the exchanges and edits are complete.

Run your Experiment in the CDS and Import Your Results

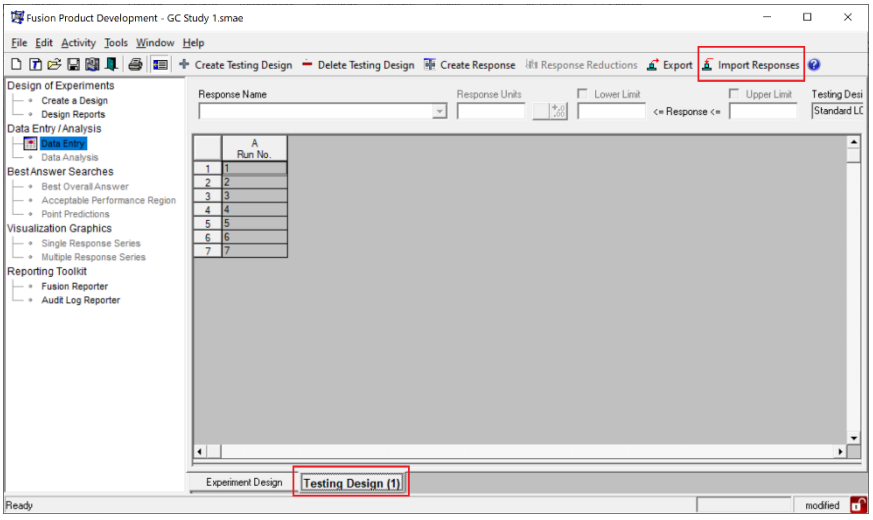
1. Prepare your GC system. Load and execute the Sample Set in Empower.

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.