Design Acceptance Tests

Reaction Setup/Definition

Given	When	Then
No prior work on the platform	A Chemist wants to synthesize a given compound.	The Chemist is able to define and register that compound in Transcriptic by drawing it or entering a SMILES string.
No prior work on the platform	A Chemist wants to complete one of the five pre-determined types of reactions.	The Chemist is able to configure their desired reaction type, including starting compounds, reagents, solvents, and times/temps.
No prior work on the platform.	A Chemist wants to synthesize a compound of interest.	The Chemist is able to define the desired final mass of product produced.
A Chemical route defined for the synthesis of a compound of interest.	A Chemist wants to submit a compound to a bio-assay after synthesis.	The Chemist is able to define the assay (or assays) they want the compound run in following synthesis.
A Chemical route defined for the synthesis of a compound of interest.	A Chemist wants to access the resulting product after synthesis.	The Chemist is able to request the synthesized product be returned to an address of their choosing.
A Chemical route defined for the synthesis of a compound of interest.	A Chemist wants to store the resulting product for later use.	The Chemist is able to indicate the desired storage conditions for the resulting product.
No prior work on the platform.	A Chemist anticipates needing to synthesize a compound using custom intermediates.	The Chemist is able to send these intermediates to the facility and have them placed in storage.

No prior work on the platform	A Chemist wants to synthesize a compound using custom intermediates.	The Chemist can submit them for shipping during configuration of their reaction.
No prior work on the platform.	A Chemist wants to synthesize a compound of interest.	The Chemist is informed if the compound has been synthesized before, and if so, what parameters/route was most effective.
A Chemical structure entered and registered.	A Chemist wants to understand the basic properties of the product they want to synthesize.	The Chemist is able to see the basic properties of the defined chemical, such as solubility.
No prior work on the platform.	A Chemist wants to synthesize a compound of interest.	The Chemist can define custom parameters (time/temp) for their desired route.
Previous submission of custom intermediates/reagents.	A Chemist wants to complete one of the five pre-determines types of reactions.	The Chemist is able to configure the reaction, referencing the stored reagents.
A list of compounds of interest to be synthesized.	A Chemist wants to synthesize all compounds in a list of SMILES strings.	The Chemist is able to import the list of compounds into a single synthesis setup.
A list of compounds of interest to be synthesized.	A Chemist wants to attempt a synthesis for every chemical in the compounds.	The Chemist is able to set the details for each route so that every desired compound can be generated.
A set of analog reactants	A Chemist wants to apply the same/a similar synthesis to every analog in the list	The Chemist is able to import the list to the platform to generate a submission with many syntheses in parallel.
Initial synthesis definition	A Chemist wants to understand the time it will take to synthesize a compound.	The Chemist is able to receive an estimated completion time for the synthesis.

Initial synthesis definition.	A Chemist wants to understand the cost of synthesizing a compound.	The Chemist is able to see the cost of synthesis for the reagents, and final product they have defined.

Reaction Monitoring

Given	When	Then
Prior submission of a synthesis that is still in the queue.	A Chemist wants to know when their synthesis will start.	The Chemist is able to access an estimated start time.
Prior submission of a synthesis that is still in the queue.	A Chemist wants to make changes to the synthesis.	The Chemist is able to edit the parameters and settings of the synthesis and resubmit it to the queue.
Prior submission of a synthesis that is still in the queue.	A Chemist wants to cancel a submitted synthesis.	The Chemist is able to cancel the desired synthesis.
Prior submission of one or more syntheses.	A Chemist wants to understand the queue status of each synthesis.	The Chemist is able to view all syntheses that they have submitted, past, present and future.
A synthesis that has begun.	A Chemist wants to understand what the current status of the synthesis is.	The Chemist is able to see the past steps, present status, and upcoming steps of the synthesis.
A synthesis that has been modified by a laboratory operator.	A Chemist wants to understand what the current status of the synthesis is.	The Chemist is able to see if anything about the synthesis has been changed.
A synthesis that has been modified by a laboratory operator.	A Chemist wants to understand how a synthesis has been changed.	The Chemist is able to see what the initial conditions of the reaction were, how they were modified, and the reasoning for changing them.

A synthesis that has been modified by a laboratory operator.	A Chemist does not agree with the modifications made my L2S2 operators.	The Chemist is able to provide structured feedback indicating what they would have done instead.

Finished Reaction Review

Given	When	Then
A synthesis that has successfully completed	A Chemist wants to know if their synthesis is complete.	The Chemist is able to see all syntheses that have completed, and can narrow in on the synthesis of interest.
A synthesis that has successfully completed	A Chemist reviews the synthesis.	The Chemist is able to understand to what extent the reaction was successful.
A synthesis that has failed to complete.	A chemist reviews the synthesis.	The Chemist is able to understand where the reaction failed to succeed, and what intervening steps were taken to address this.
A synthesis that has completed, either successfully or unsuccessfully.	A Chemist wants to understand the details of how the reaction was completed.	The Chemist is able to see data that illustrates the conditions under which the reactions was completed.