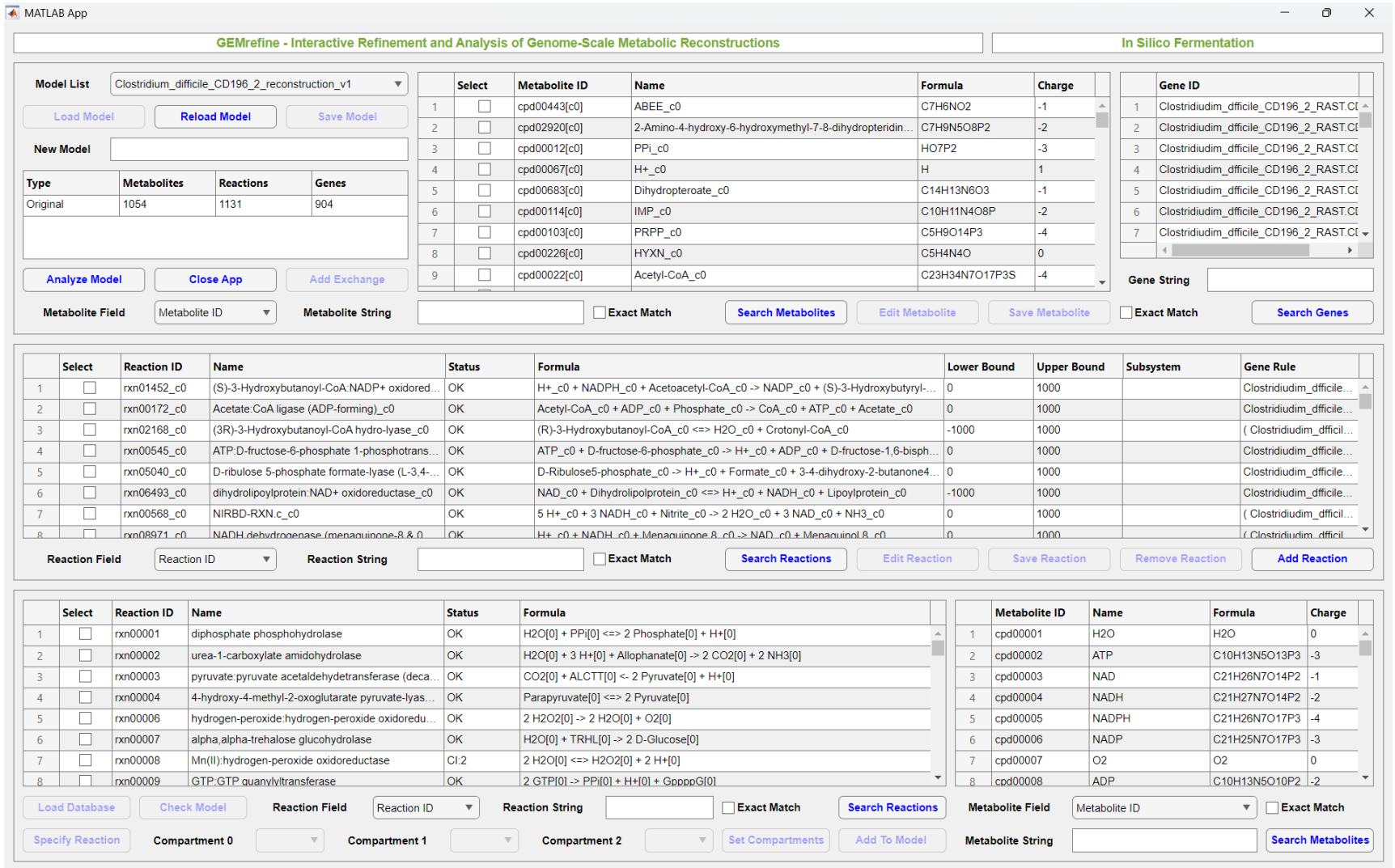
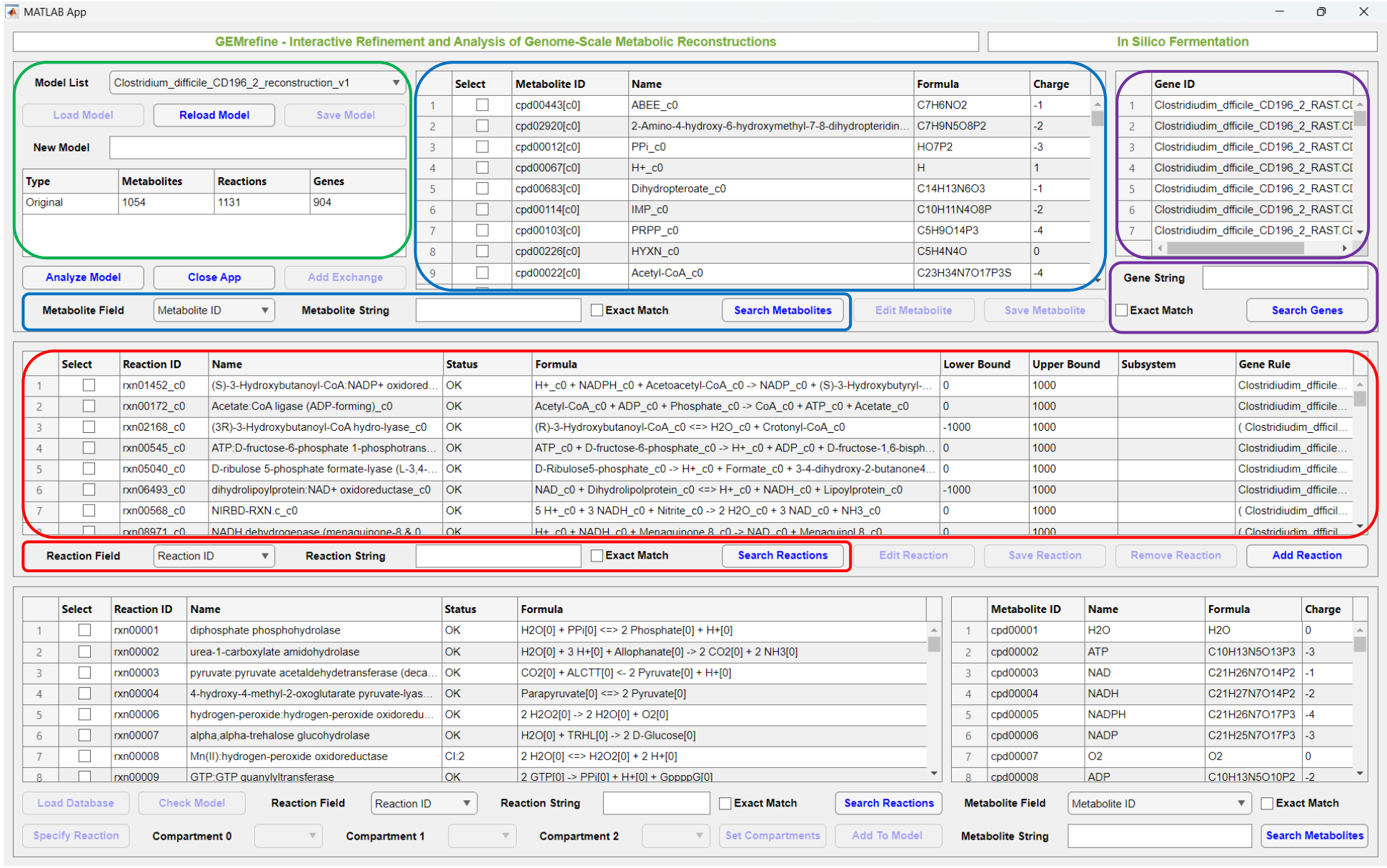
GEMrefine – A MATLAB Application for Refinement and Analysis of Metabolic Reconstructions

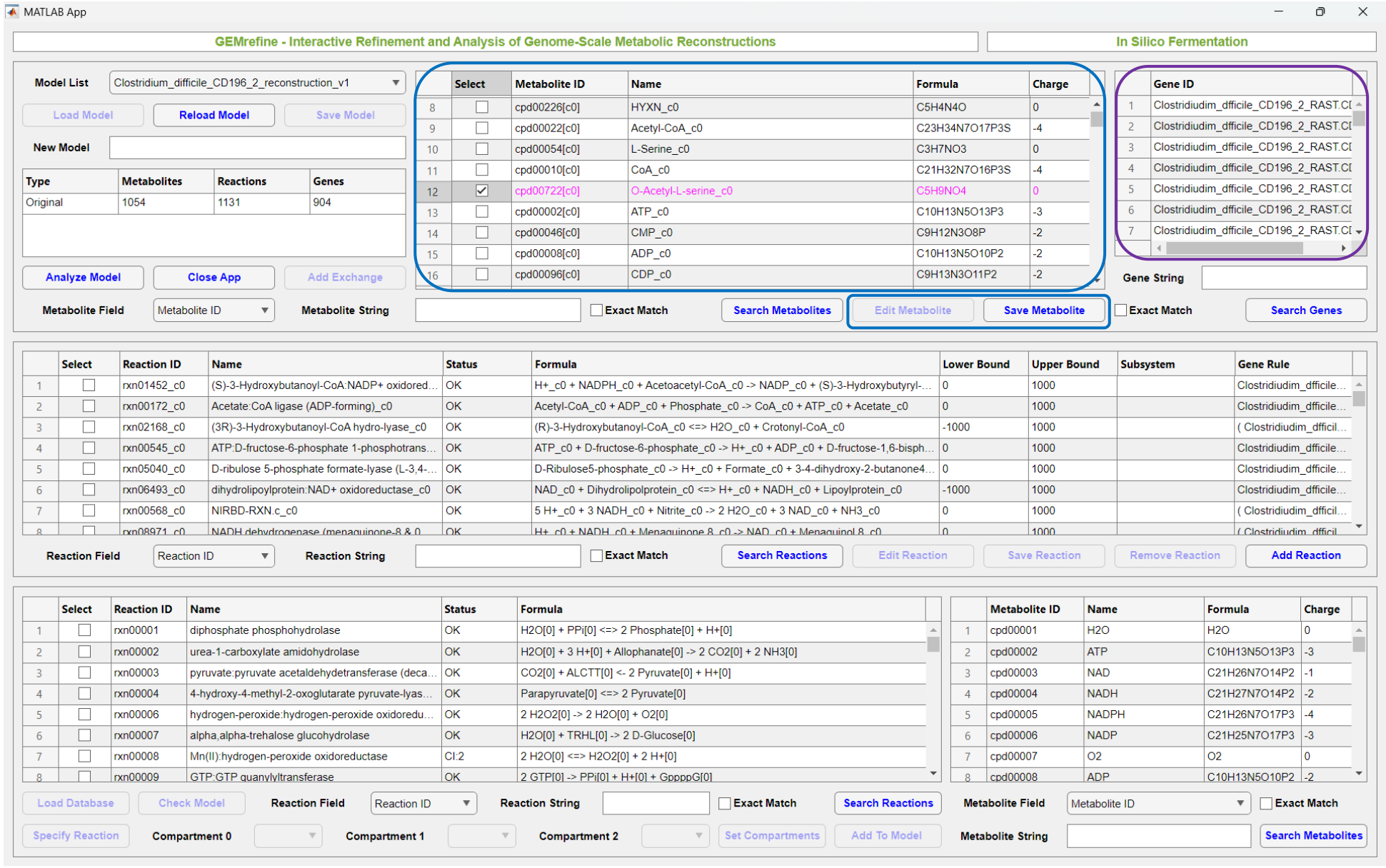


Overview of GEMrefine workflow and capabilities

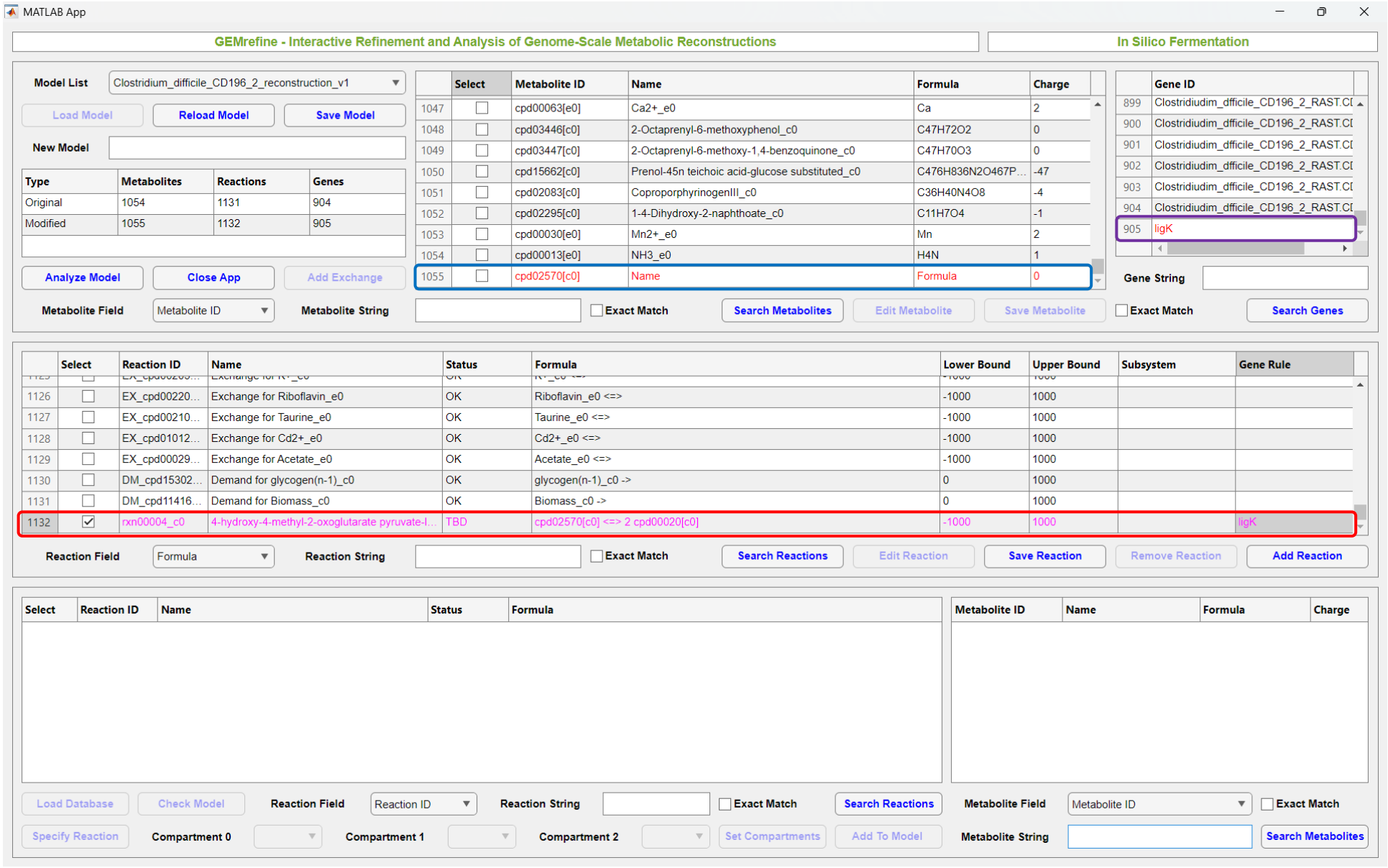
- The desired metabolic model is loaded and proton balancing of any imbalanced reactions is attempted.
- The metabolite table, gene table and reaction table are populated.
- Each table can be independently searched using any column contained in the table.



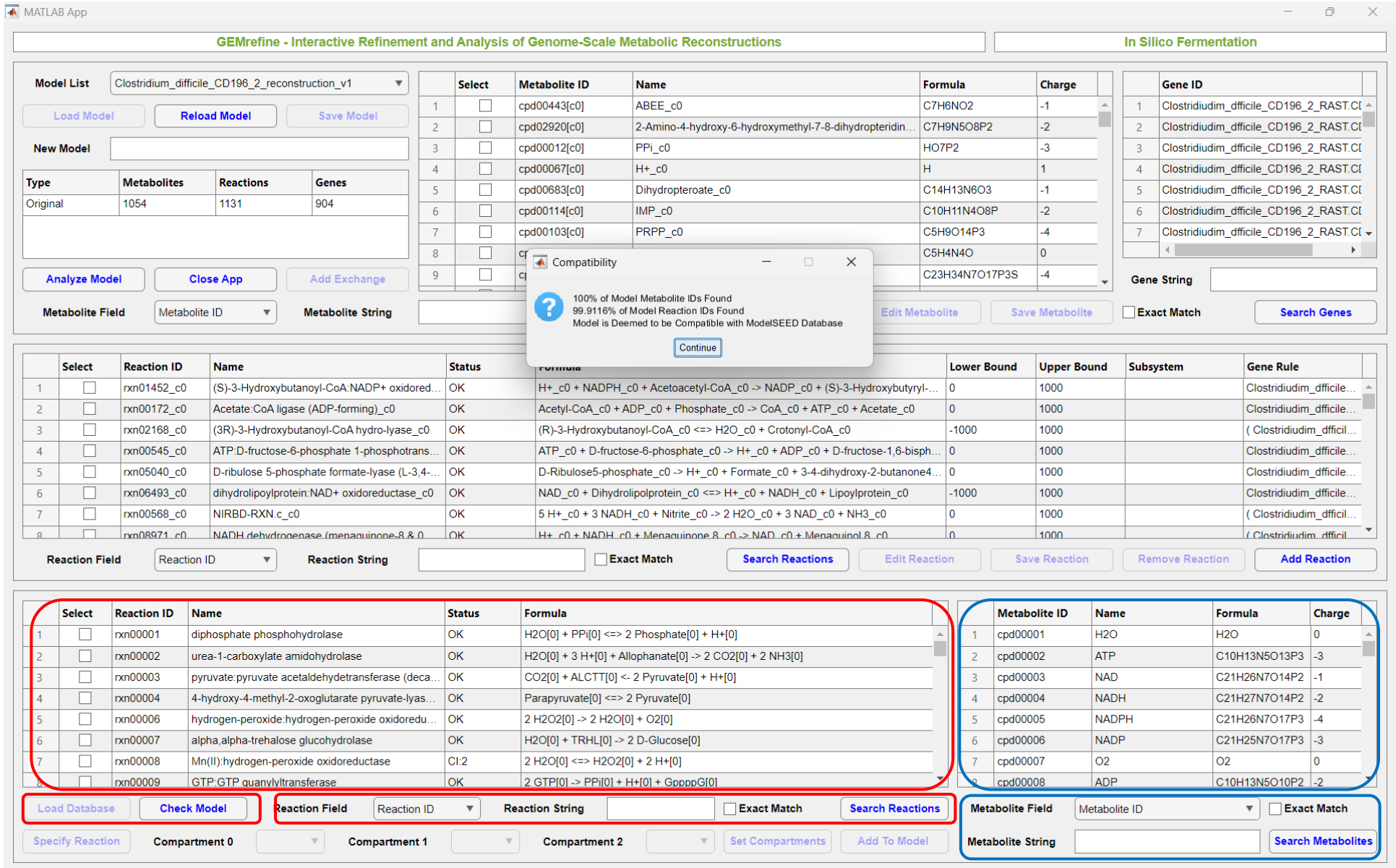
- An existing metabolite in the metabolite table can be selected, edited and saved to change the name, formula and/or charge.
- New metabolites and genes can be added/removed through reaction editing or addition.



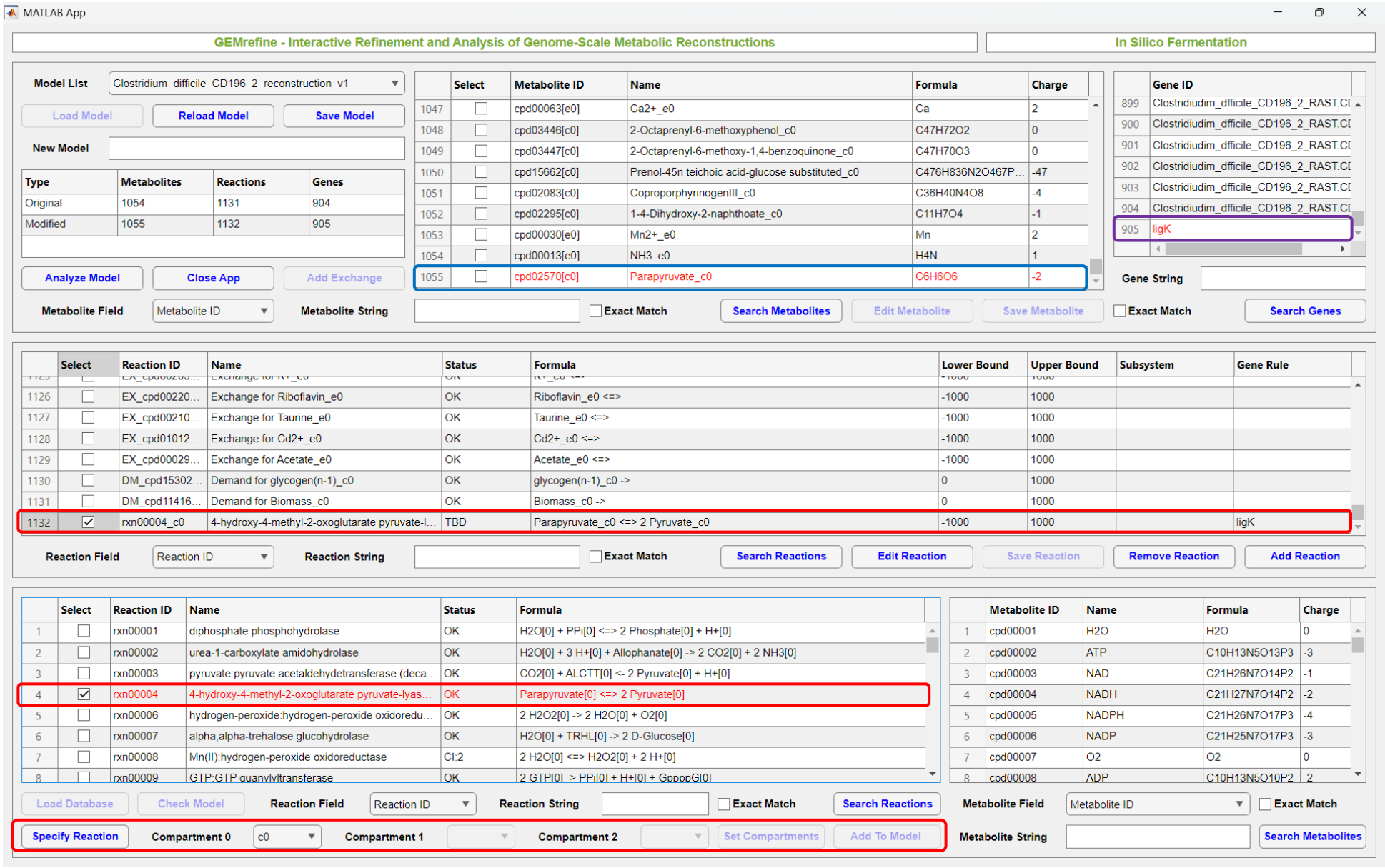
- An existing reaction in the reaction table can be selected, edited and saved to change all fields except the reaction ID.
- Existing reactions can be removed, and new reactions can be manually added and saved.
- The metabolite and gene tables are automatically updated when reactions are edited, added or removed.



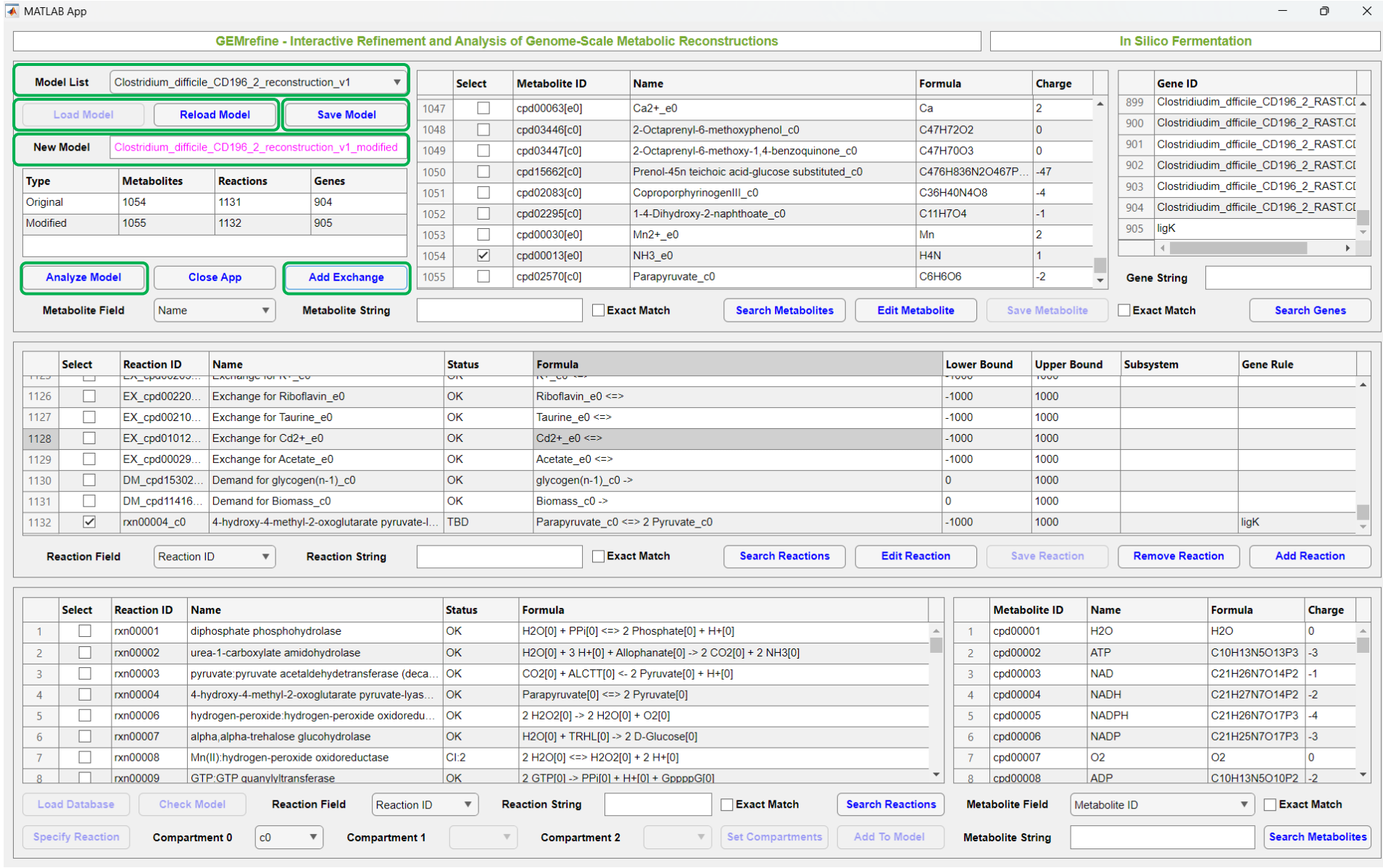
- The ModelSEED biochemistry database can be loaded to populate the database reaction and metabolite tables.
- Each table can be independently searched using any column contained in the table.
- Model compatibility with the database must be checked prior to database reaction and metabolite addition.



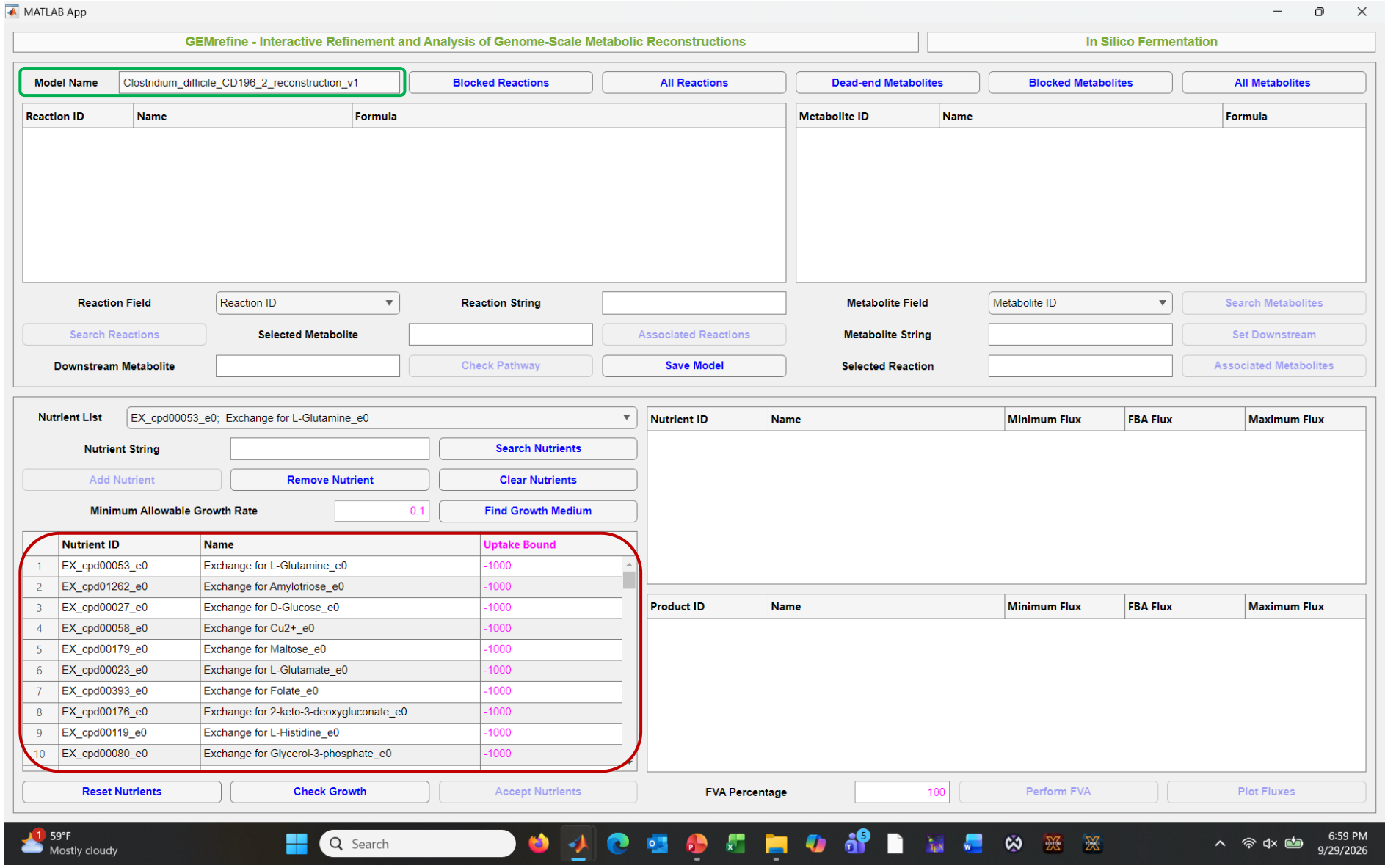
- Any database reaction can be selected, specified and added to a compatible model.
- The database reaction is added to the reaction table with all information except the subsystem and gene rule.
- The metabolite and gene tables are automatically updated when the added reaction is saved.



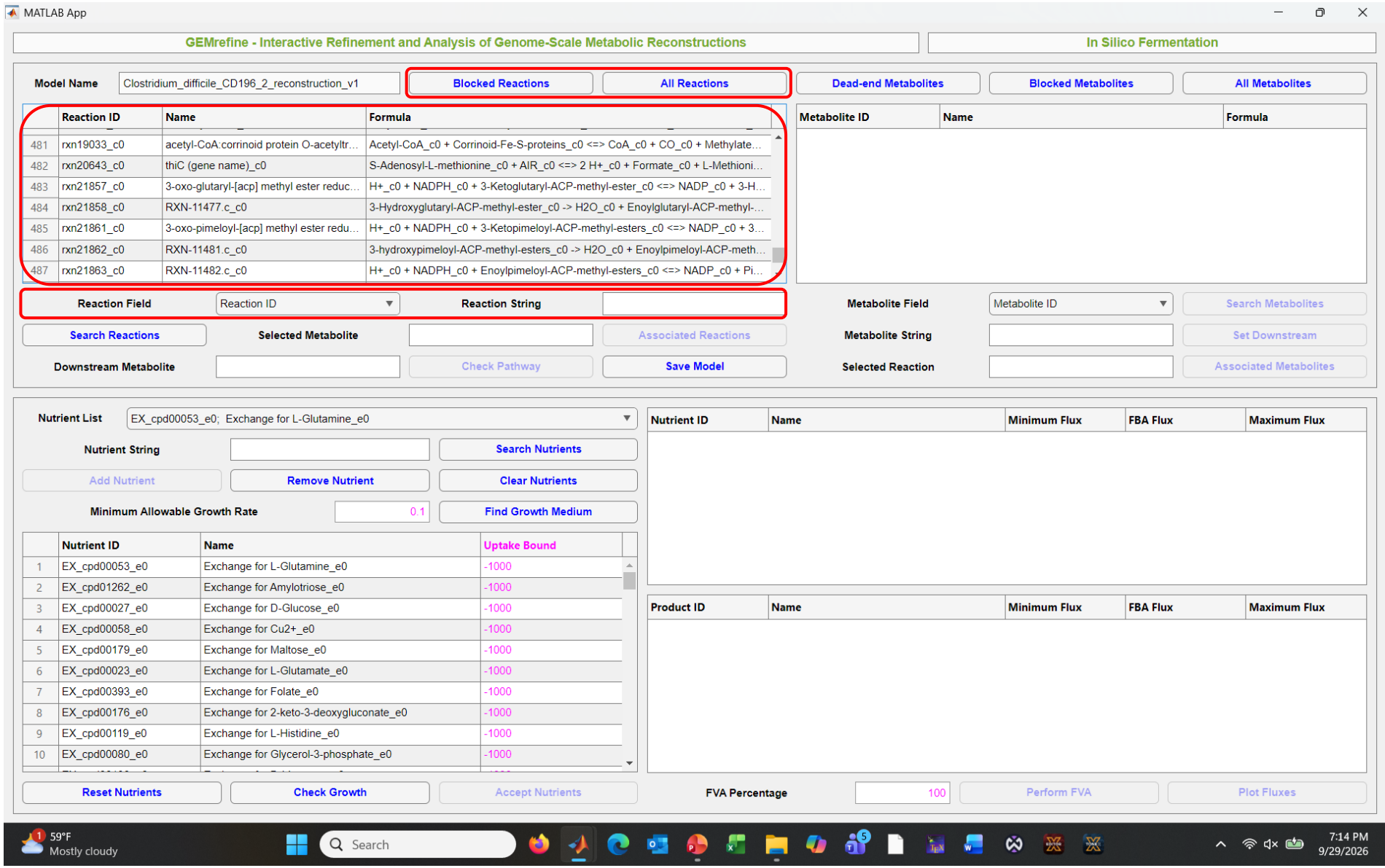
- An exchange reaction can be added for a selected extracellular metabolite.
- The modified model can be saved as a new model in the current directory.
- The original model can be reloaded or another model from the model list can be loaded.
- The current model can be structurally and functionally analyzed using the companion analysis app.



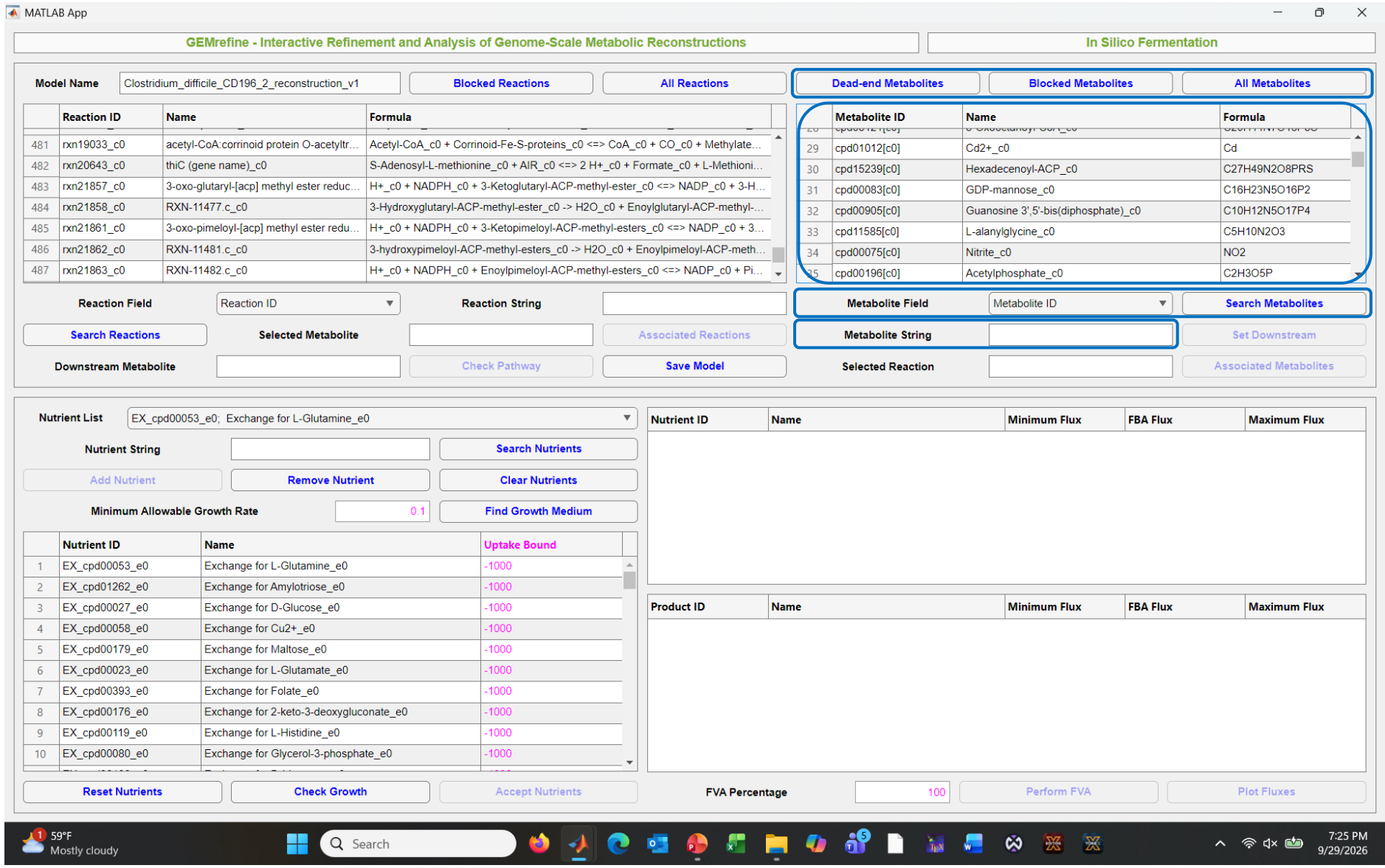
- The analysis app attempts to proton balance any new reactions added to the current version of the model.
- The nutrient table is initialized with nutrient update bounds extracted from the model.
- The current nutrient table is used to perform structural model analysis and FBA/FVA calculations.



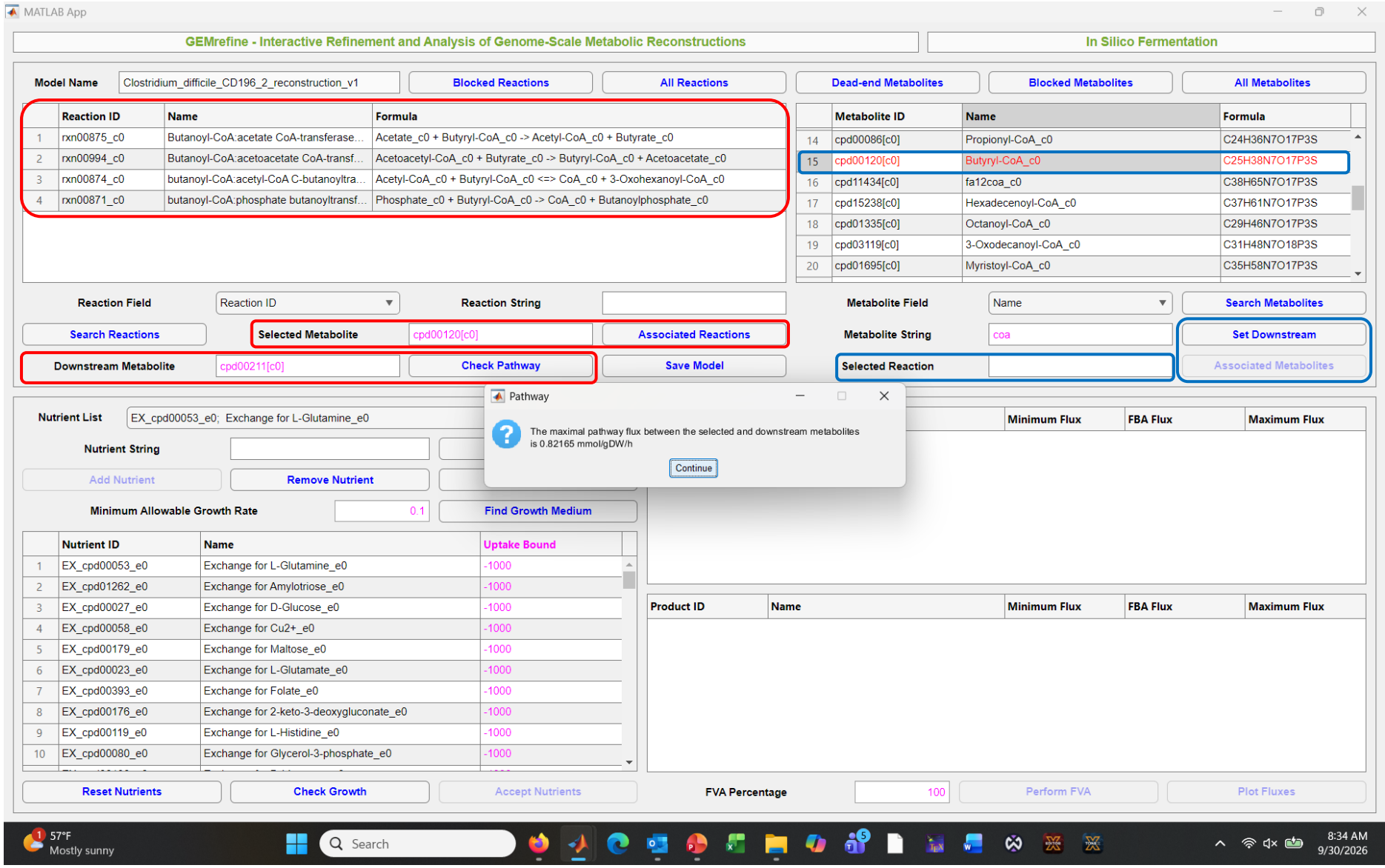
- The reaction table can be populated with the blocked reactions or all model reactions.
- A blocked reaction is incapable of carrying flux given the current nutrients.
- The reaction table can be searched using any column contained in the table.



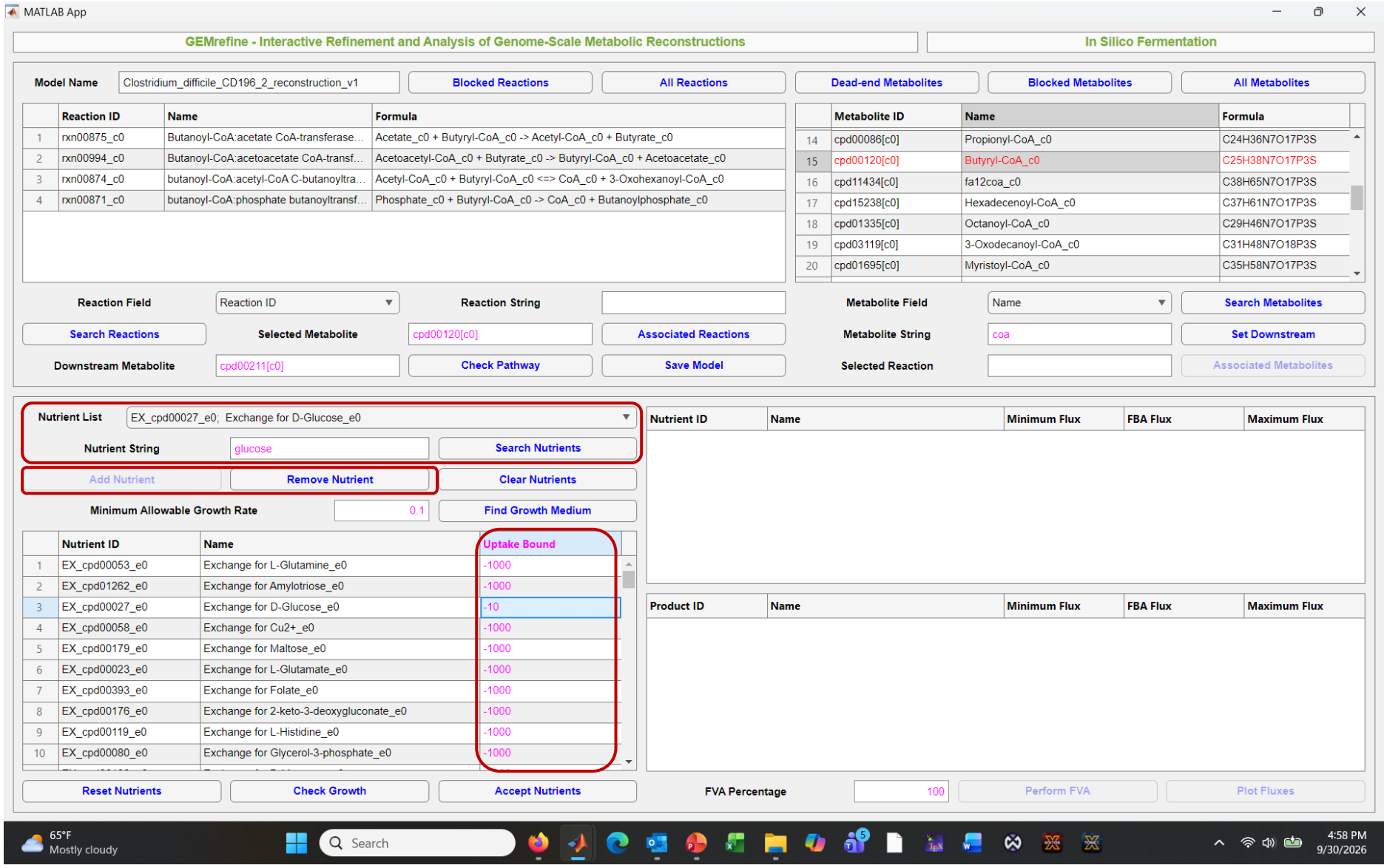
- The metabolite table can be populated with the dead-end metabolites, blocked metabolites or all model metabolites.
- A dead-end metabolite lacks reactions either for its production or its consumption.
- A blocked metabolite cannot be produced or cannot be consumed given the current nutrients.
- The metabolite table can be searched using any column contained in the table.



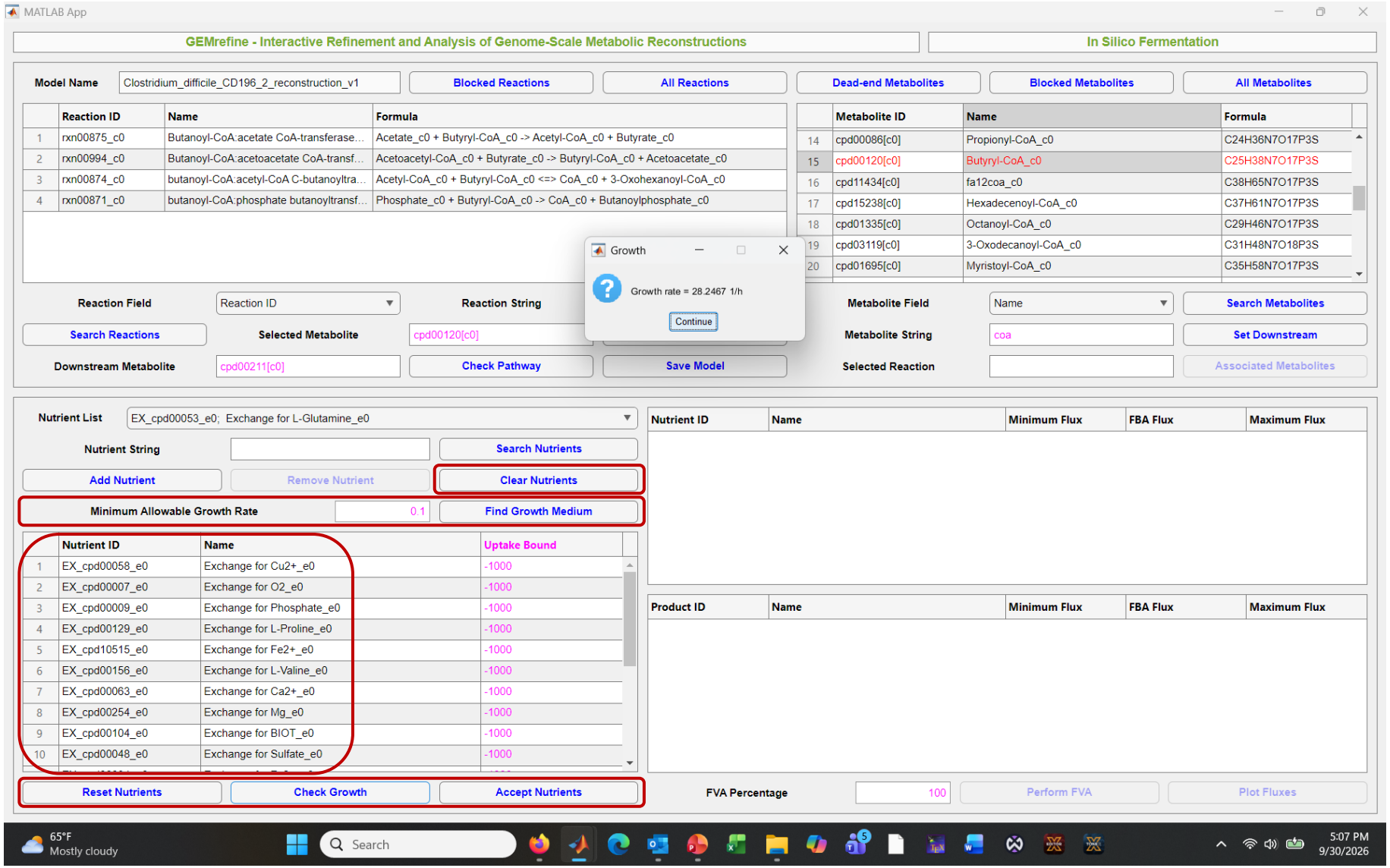
- Any metabolite from the metabolite table can be selected to find all associated reactions.
- Any reaction from the reaction table can be selected to find all associated metabolites.
- Any two metabolites in the metabolite table can be defined as selected and downstream metabolites to calculate the maximal pathway flux between the metabolites.



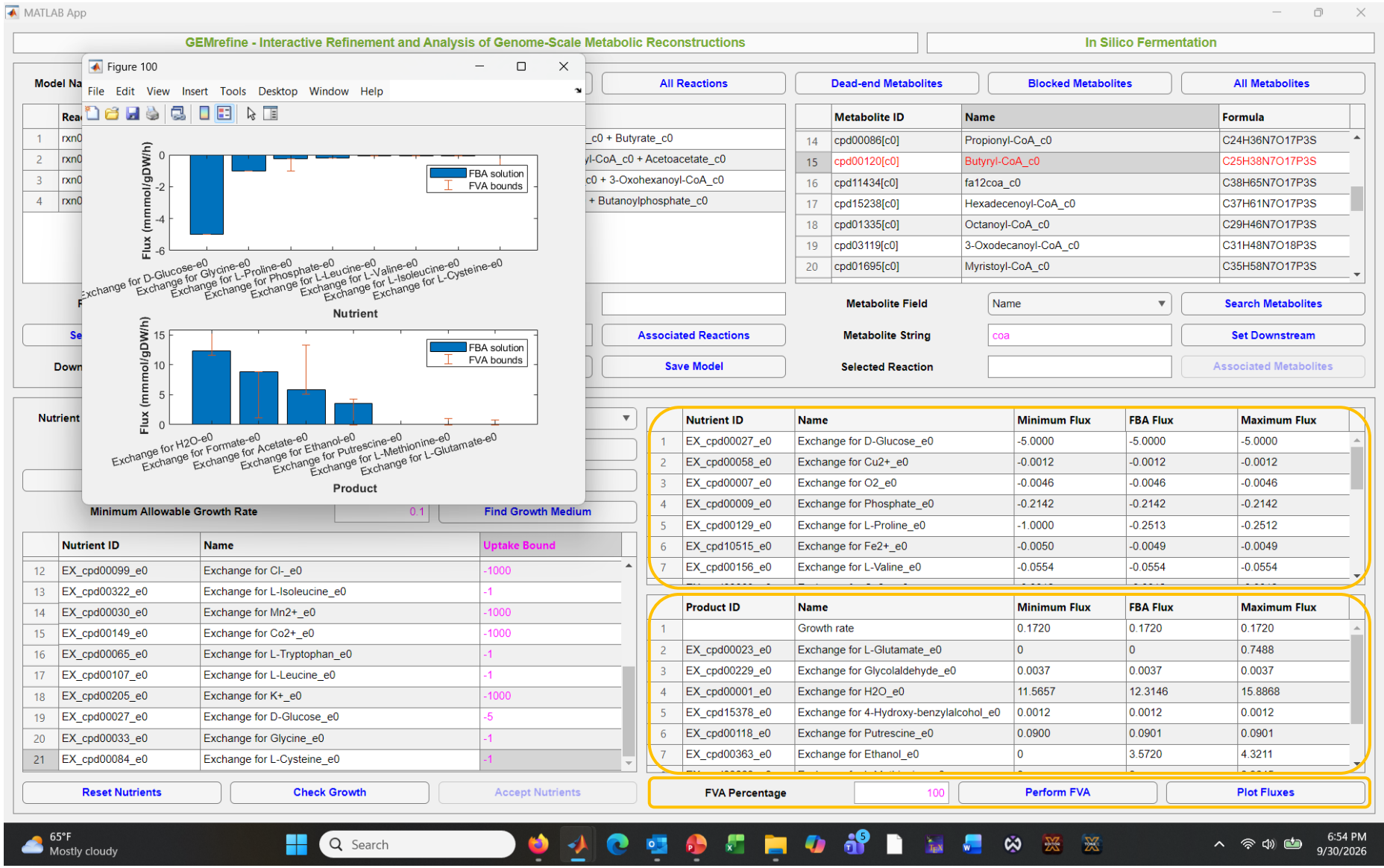
- The nutrient list contains all metabolites with exchange reactions and can be searched.
- Nutrients can be added to or removed from the nutrient table.
- The update bound of any nutrient in the nutrient table can be changed.



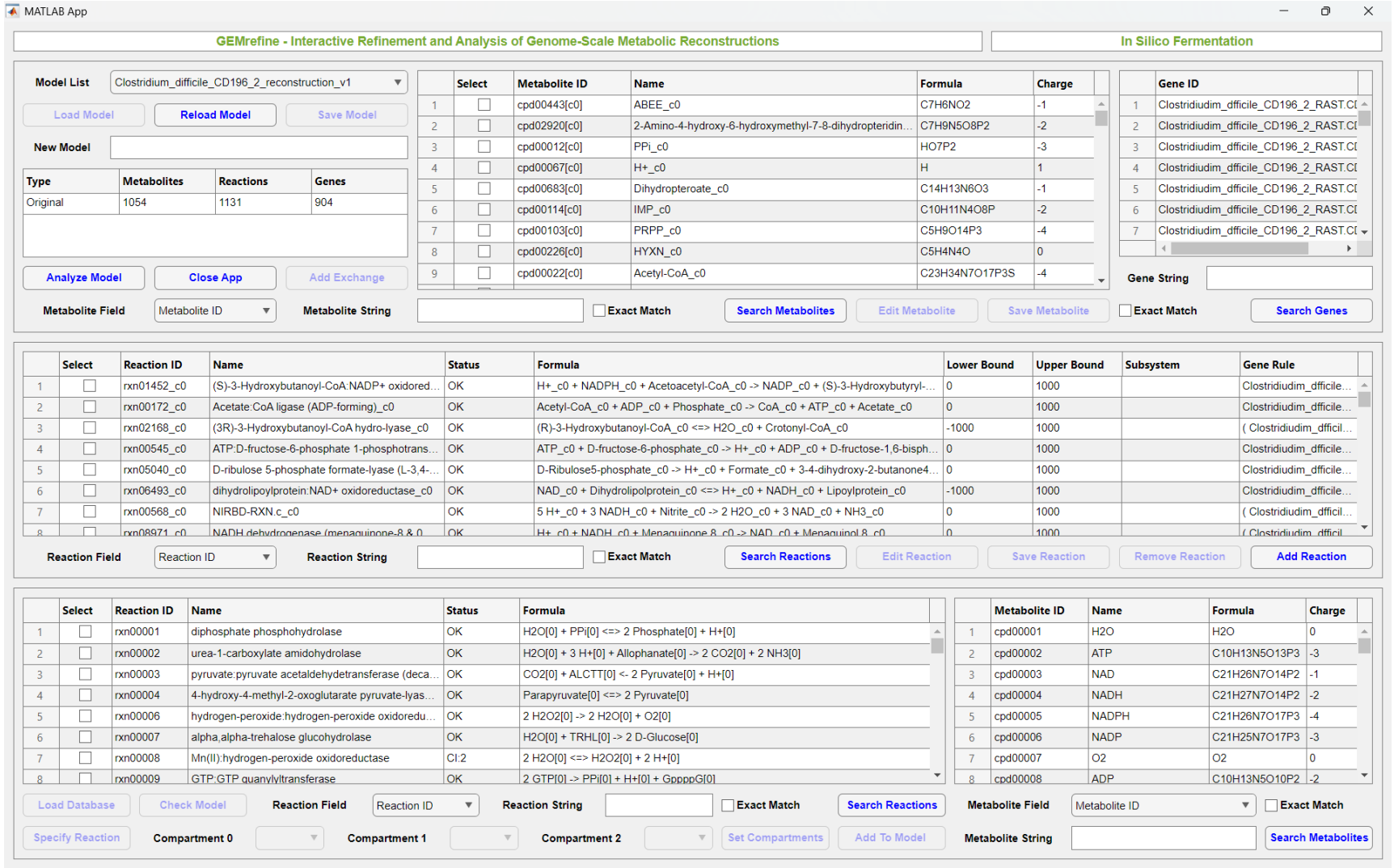
- The growth rate for the current nutrient table can be calculated.
- The nutrient table can be cleared and a search for a minimal growth medium attempted.
- The minimal medium must generate a growth rate exceeding the minimum value.
- The nutrient table can be reset to the original table.
- Once accepted, the current nutrient table is used for all calculations.



- FBA/FVA can be performed using the current nutrient uptake bounds to produce a nutrient uptake table and a product secretion table.
- The percentage of the maximal growth rate used for FVA calculations can be changed.
- The nutrient uptake and product secretion fluxes can be plotted.



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Visit insilicofermentation.com for more information about GEMrefine and instructions for downloading the app