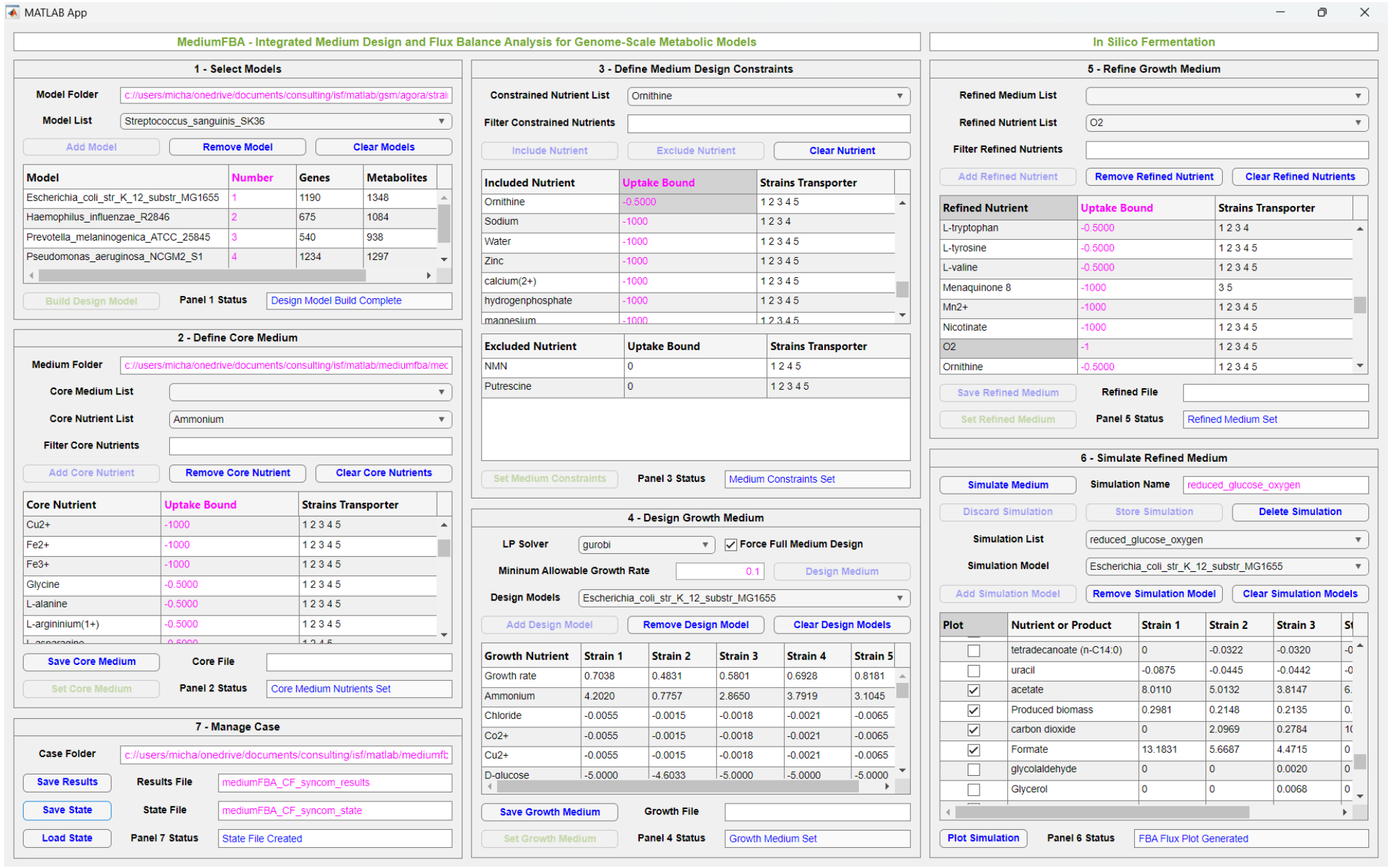
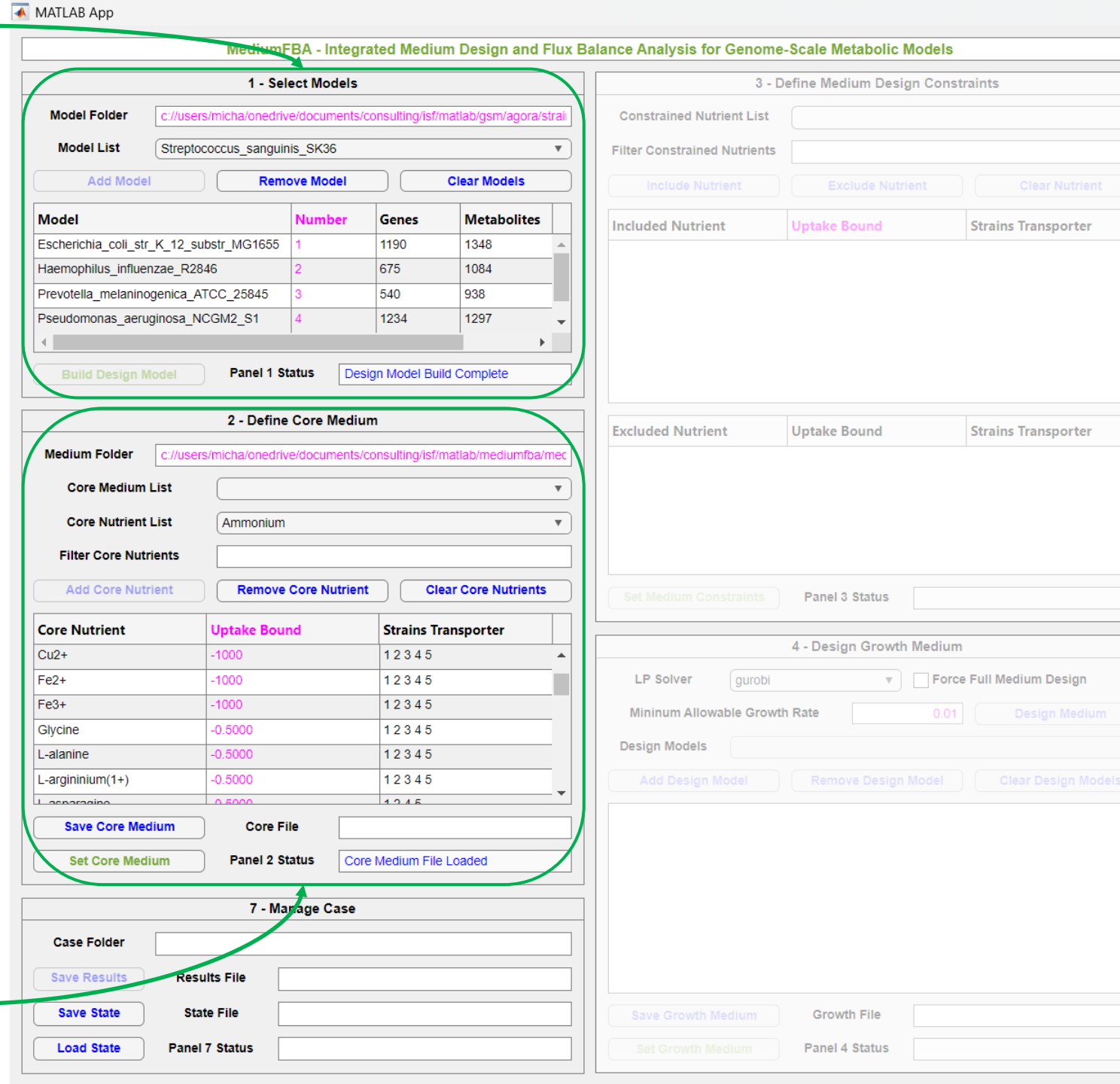
MediumFBA – A MATLAB Application for Integrated Medium Design and Flux Balance Analysis



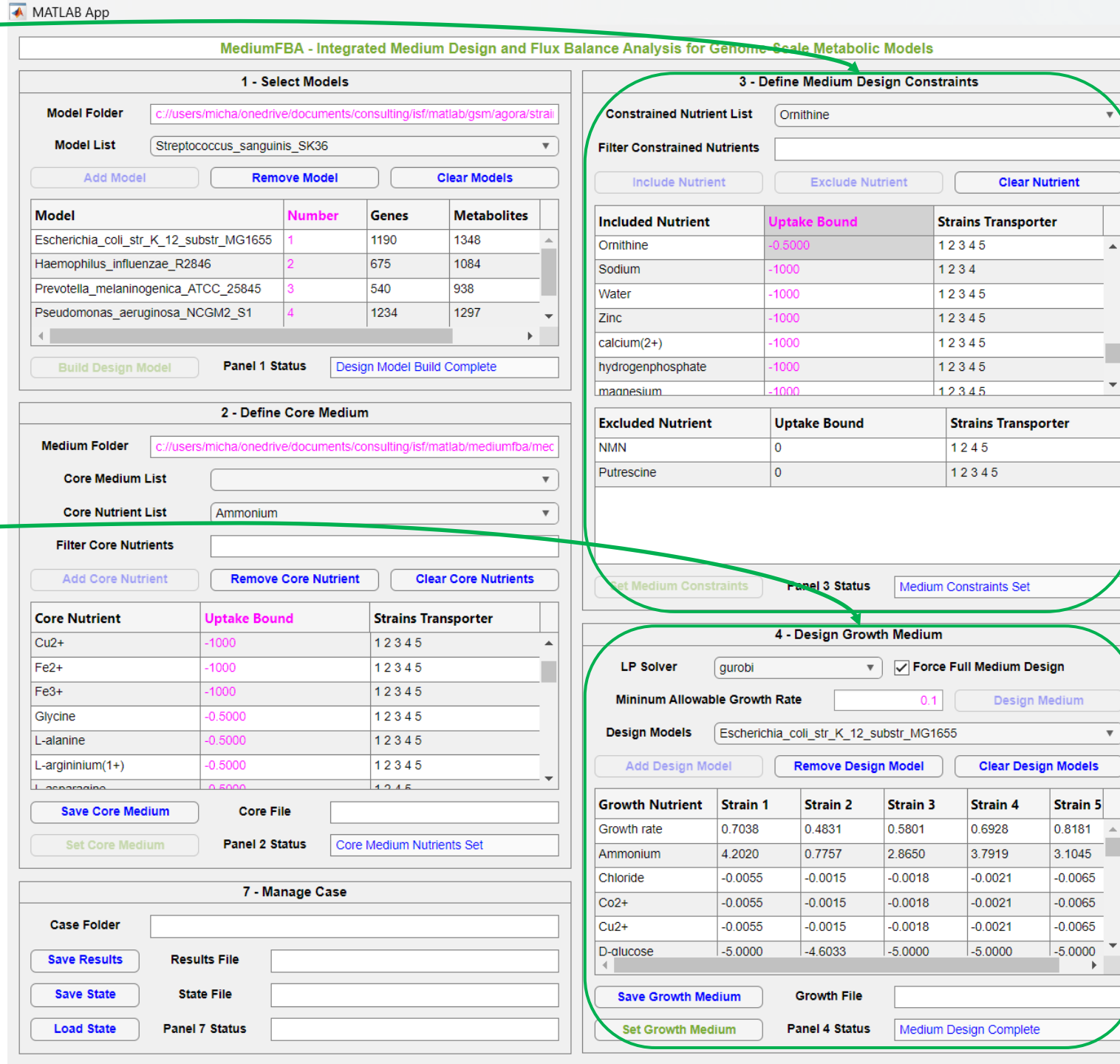
1. Select metabolic models for strains of interest. The designed medium will ensure monoculture growth of all selected strains. Here we selected five bacteria commonly associated with cystic fibrosis airway infections.

2. Define core nutrients contained in the desired medium. The core nutrients are common components included in a putative in vitro medium. Here we included common inorganic salt ions and all 20 amino acids.



3. Impose constraints on the medium design solution. Nutrients can be included with specified uptake bounds or excluded entirely. Here we included glucose and oxygen and excluded unusual nutrients identified by the design algorithm so they can be replaced.

4. Design growth medium by ensuring monoculture growth of all strains. The minimum growth rate and full/partial medium design can be specified. Here the constraints were altered in an iterative manner to generate a desirable set of growth nutrients.



Core Nutrients Specified

Ammonium
Chloride
Co2+
Cu2+
Fe2+
Fe3+
Mn2+
Sodium
Water
Zinc
Calcium(2+)
Hydrogenphosphate
Magnesium
Potassium
Proton
Sulfate

Bounded Nutrients Included

Specified

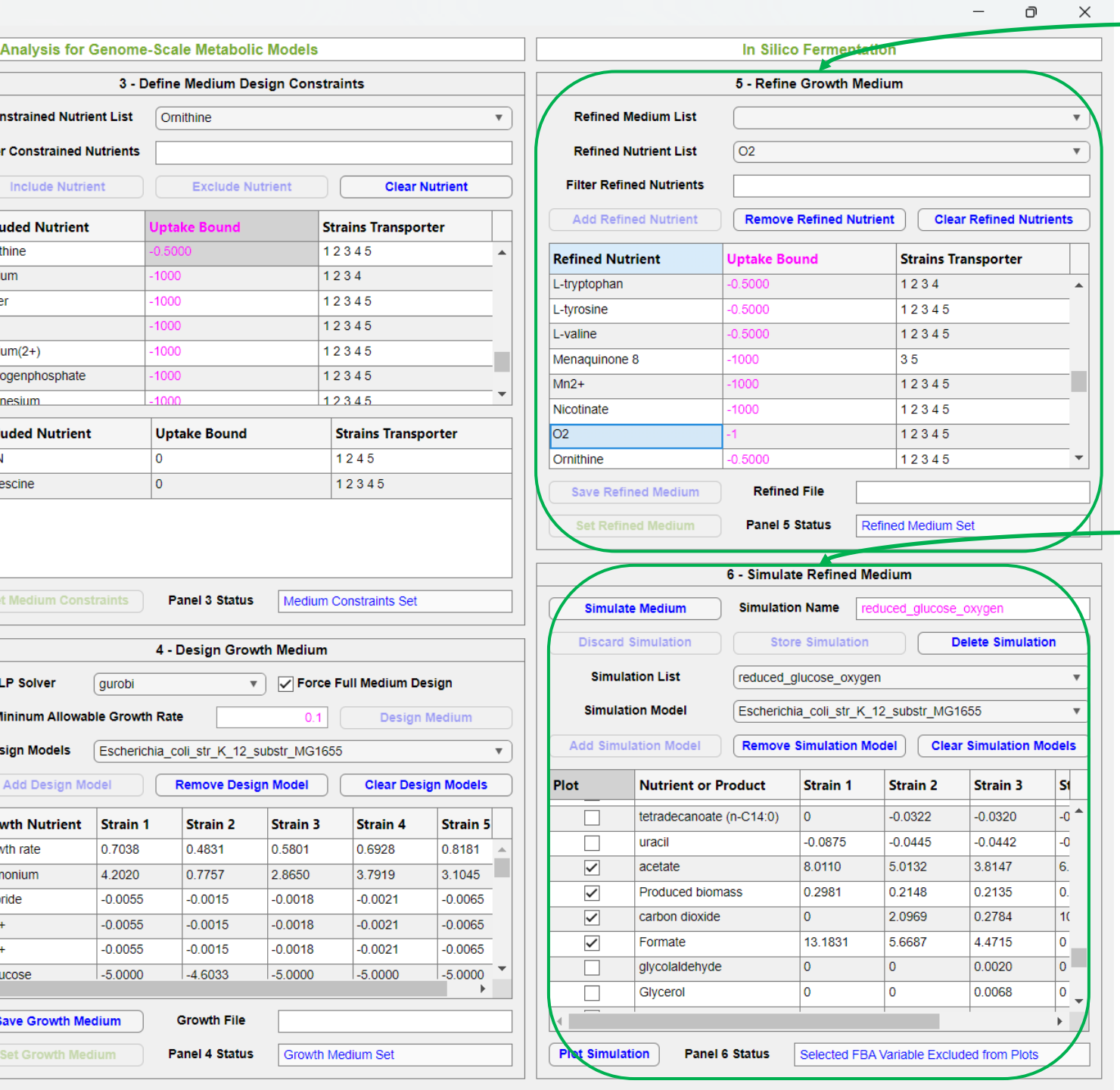
Glucose
Oxygen
All 20 amino acids

Identified

L-cysteinylglycine
Ornithine
Uracil

Unbounded Nutrients Identified

(R)-Pantothenate
2-Demethylmenaquinone 8
4-hydroxybenzoate
Folate
Menaquinone 8
Nicotinate
Oxidized glutathione
Protoheme
Pyridoxine
Riboflavin
Siroheme
Spermidine
Thiamin
Ubiquinone-8
Meso-2,6-Diaminoheptanedioate
Octadecanoate (n-C18:0)
Tetradecanoate (n-C14:0)



5. Refine growth medium by changing uptake bounds of essential nutrients and adding non-essential nutrients. Multiple refined media can be formulated and simulated. Here we modify the designed medium by reducing glucose and oxygen uptakes.

6. Simulate monoculture growth for current refined medium. Multiple FBA solutions can be stored, plotted and later recalled. Here we simulate and plot selected fluxes for reduced glucose and oxygen uptakes.

Figure 100

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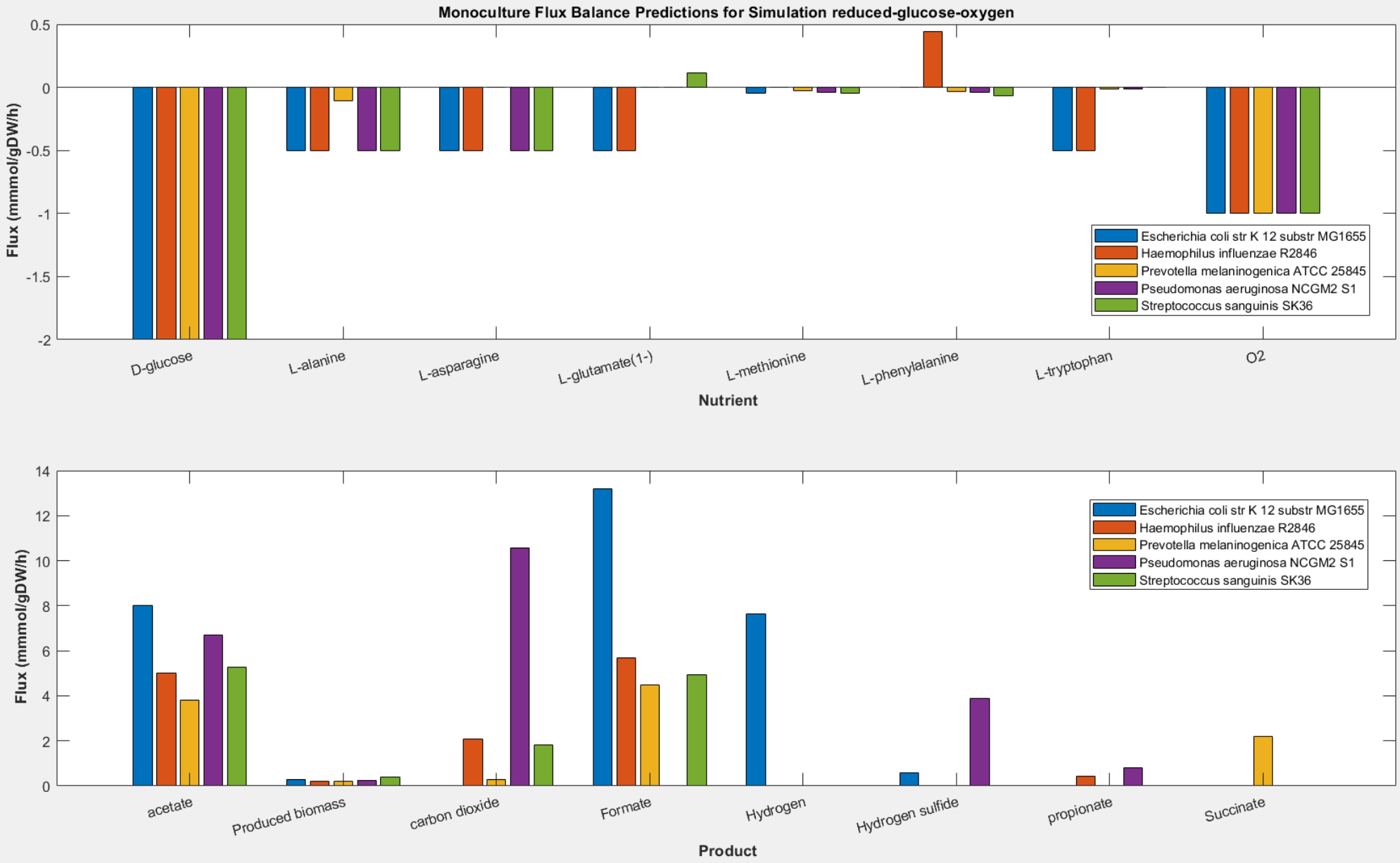

7. Manage case by saving FBA simulation results and saving App states for later loading. The saved results can used outside the App for additional MATLAB analysis. Here we save the current results and App state containing FBA simulations for the designed growth medium and one refined medium.