

BT4110: Computational Biology Laboratory

Constraint-Based Modeling - Assignment

Note: Present your results in the form of a spreadsheet and document. Submit your Script and Result files in Moodle before 1st October, 2:00 pm.

Section A

1. Referring to scientific literature summarize the principle and scope of Genome-Scale Metabolic Modelling (Less than 300 words).

Section B

2.

R1: \rightarrow Glucose

V1: $\text{Glucose} + 2 \text{ ADP} + 2 \text{ NAD} \rightarrow 2 \text{ Pyruvate} + 2 \text{ ATP} + 2 \text{ NADH} + 2 \text{ H}_2\text{O}$

V2: $\text{Pyruvate} + \text{NADH} \leftrightarrow \text{Lactate} + \text{NAD}$

V3: $\text{Pyruvate} + \text{CoA} + \text{NAD} \rightarrow \text{Acetyl CoA} + \text{CO}_2 + \text{NADH}$

V4: $\text{Pyruvate} + \text{CoA} \rightarrow \text{Formate} + \text{Acetyl CoA}$

V5: $\text{Acetyl CoA} + \text{ADP} \rightarrow \text{Acetate} + \text{CoA} + \text{ATP}$

V6: $\text{Acetyl CoA} + 2 \text{ NADH} \rightarrow \text{Ethanol} + \text{CoA} + 2 \text{ NAD}$

V7: $\text{ATP} \rightarrow \text{ADP}$

R2: $\text{Lactate} \rightarrow$

R3: $\text{Ethanol} \rightarrow$

R4: $\text{Acetate} \rightarrow$

Constructing a Stoichiometric Matrix and write down the Bounds for each reaction

Section C

3. Download the [Oryza sativa](#) model. Refer to the research article by Lakshmanan et al., 2013 (PMID: [23753178](#)). Perform FBA simulation following the methodology described in the paper for the following conditions. Present your results in a spreadsheet and add your interpretation in comparison with the discussions in the paper.

- a. Seed-derived cells in Aerobic and Anaerobic conditions (at an oxygen uptake rate of 1, 2, 3, 3.35, and 4 mmol/gDCW.d).
- b. Seed-derived cells in Sucrose and Glucose batch culture at Aerobic (Oxygen uptake rate of 3.35 mmol/gDCW . d) and Anaerobic Conditions.

Note: Use the following formula to calculate sucrose, glucose, and fructose rates for the shaded time interval in the Concentration profile (Fig 1)

$$\text{Rate of reaction} = \frac{\Delta \text{ sugar conc. (mmol/L)}}{\Delta \text{ Biomass conc. (gDCW/L)} \times \Delta \text{ time (d)}}$$

Where,

Δ sugar conc. = Final sugar concentration - Initial sugar concentration

Δ Biomass conc. = Final biomass concentration - Initial biomass concentration

Δ time = Final time - Initial time

- c. Photorespiring Rice Leaf Cells for the below 7 conditions.

| | | | | | | | |
|------------------------------|---|---|---|---|---|---|----|
| O₂ Uptake | 0 | 1 | 1 | 1 | 1 | 1 | 1 |
| CO₂ Uptake | 1 | 1 | 2 | 4 | 6 | 8 | 10 |

4. For the following Conditions and growth rates perform FVA. Present your results in the form of a spreadsheet.

| Condition | Growth Rate |
|---|--------------------|
| Seed Derived cells at Aerobic Condition | 0.3750 |
| Seed Derived cells at Anaerobic Condition | 0.1133 |
| Leaf Derived cells at Aerobic Condition | 0.174 |