Assignment 3: Systems Biology

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1 Exercise 1: Non-essential Enzymes

In this work, I wrote a Python program named "task_1.py" to identify all non-essential enzymes in glycolysis.

1.1 Methods

1. Generate a data frame to describe the glycolysis schematic.
2. For each unique enzyme in the dataset, remove all links related to this enzyme.
3. Use breadth-first search(BSF) to check if we could still get to the endpoint.

1.2 Results

Identified non-essential enzymes are shown in Figure 1.

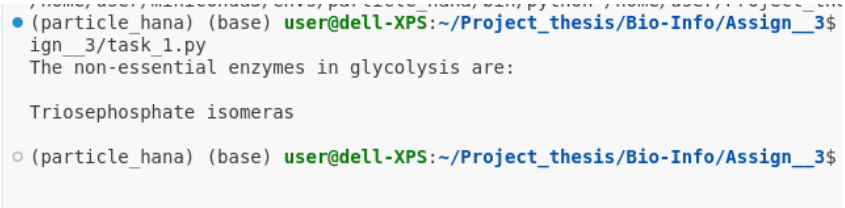

Figure 1: Non-essential enzymes in glycolysis

2 Exercise 2: Essential Enzymes

2.1 Methods

1. Load the dataset and define the set of nodes labeled as "Biological Endpoints" as the terminal nodes of the network.
2. Find unique enzymes in the network.
3. For each unique enzyme, remove all links related to this enzyme. Subsequently, apply a BFS algorithm to check if any of the endpoints is reachable.
4. Mark the enzyme as "Essential" if the removal of links affects endpoints reachability.

2.2 Results

Identified essential enzymes are shown in Figure 2.

```
gn__3/task_2.py
The essential enzymes in central carbon metabolism are:

Enzyme1

Enzyme6

Enzyme8

Enzyme9

Enzyme10

Enzyme16

PseudoEnzymes
```

Figure 2: Essential enzymes in central carbon metabolism.

3 Exercise 3: Suitable Enzymes for killing cancer cells

3.1 Methods

1. Load the edge-list file and determine enzymes existed in healthy cells and cancer cells respectively. Here we assume that cells only contain enzymes with non-zero RNA counts.
2. Identify essential enzymes for cancer cells by removing them from the network and checking if any endpoints become unreachable.
3. Identify non-essential enzymes for healthy cells by removing them and verifying that all endpoints remain reachable.
4. Enzymes that are essential in cancer cells but non-essential or absent in healthy cells are identified as potential targets.

3.2 Results

Identified essential enzymes are shown in Figure 3.

```
ign__3/task_3.py
The enzymes suitable to kill cancer-cells are:

Enzyme21

Transporter1

Enzyme22

Enzyme23

Enzyme24

Transporter2
```

Figure 3: Suitable Enzymes for killing cancer cells.