

Answers to exercises of Chapter 10 (Metabolic Networks)

1.

(a): There are different ways to extract the reaction equation from the text file by using different program languages. One of the easy ways is to copy the contents of the files to an excel worksheet and then using VBA to get the reactions in glycolysis pathway. The excel file (including the VBA program) can be downloaded.

(b): In graph representation of the metabolic network, we consider two metabolites are connected if they are in the two sides of one reaction. Therefore by checking the reaction equation, we can get a list of connected metabolite pairs. To visualize the file in pajek, we need to give a number id for each compound and write the connection to a pajek net file format (Glycolysis.net). See excel file for the VBA program.

(c): we need manually identify the currency metabolites and removed the links including them. The list of such metabolites can be seen in the excel file and the removed links are marked. The pajek net file is Glynocurrency.net. Both net files are with layout information.

(d): glucose is v17 and pyruvate is v7 in the graph. In glycolysis.net, the path length is 2 and it is 9 in the graph without currency metabolites. From pajek, select net/paths between 2 vertices/one shortest to calculate the path length.

(e): results in the Pajek project file(ch10-solutions-1.paj). calculated by net/partition/degree/all.

(f): This should be done in a similar way as the steps from (a) to (e).

(g): Centrality can be calculated in pajek by selecting net/vector/centrality. Connectivity can be analyzed by net/components.