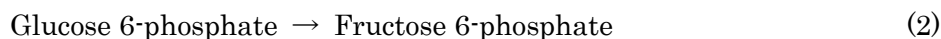


Supplement

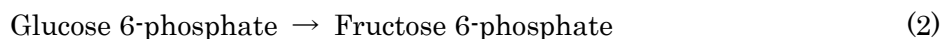
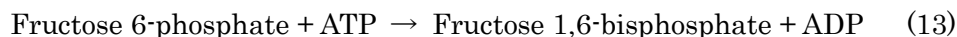
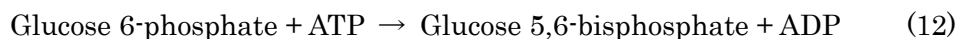
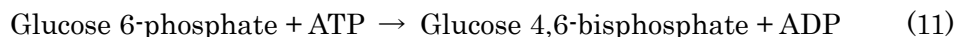
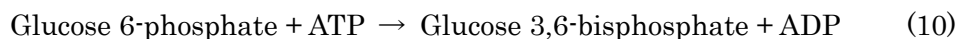
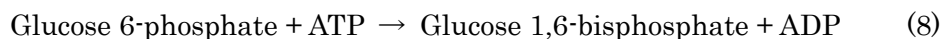
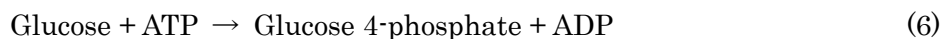
Example of BRP expansion, stoichiometric metabolic network generation, and classification of reactions

The following are hexokinase and glucose 6-phosphate isomerase reactions.

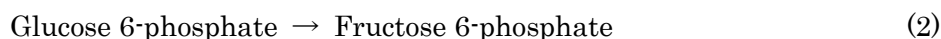
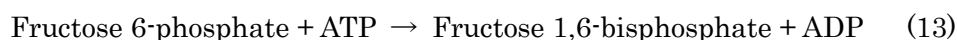


These two reactions are composed of two BRPs for phosphorylation of hydroxyl group attached to carbon atoms and isomerization between aldose and ketose and of five metabolites, glucose, glucose 6-phosphate, fructose 6-phosphate, ATP and ADP.

When one step BRP expansion is conducted to the above BRPs and metabolites as seed compounds, the following reactions are generated.

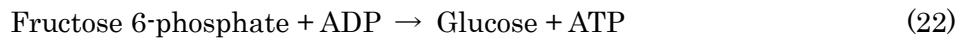
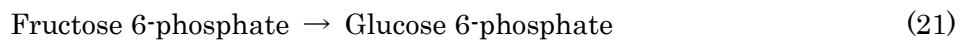
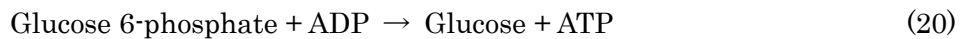
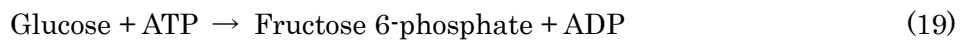
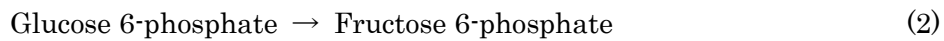
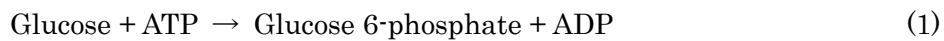


The following of them are given reactions and not given but established reactions.

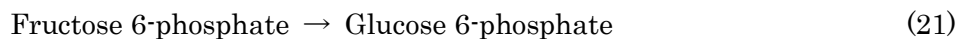
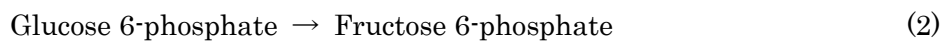
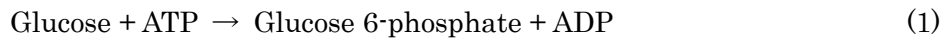


They produce given metabolites, glucose 6-phosphate and fructose 6-phosphate and not given but established metabolites, fructose 1,6-bisphosphate and fructose 2,6-bisphosphate. The other reactions are not established and produce hypothetical metabolites, glucose 2-phosphate, glucose 3-phosphate, glucose 4-phosphate, glucose 5-phosphate, glucose 1,6-bisphosphate, glucose 2,6-bisphosphate, glucose 3,6-bisphosphate, glucose 4,6-bisphosphate, glucose 5,6-bisphosphate, fructose 3,6-bisphosphate, fructose 4,6-bisphosphate, and fructose 5,6-bisphosphate, and not given but established metabolites, glucose 1-phosphate and fructose.

When stoichiometric metabolic network generation is conducted to the above metabolites seen in hexokinase and glucose 6-phosphate isomerase reactions, glucose, glucose 6-phosphate, fructose 6-phosphate, ATP and ADP, the following reactions are generated.



The following of them are given reactions and a not given but established reaction.



They contain given BRPs and a not given but established BRP. The other reactions are not established and give hypothetical BRPs.

Type 1 reactions are reactions 1 and 2. Type 2 reactions are reactions 3 to 18. Type 3 reactions are reactions 19 to 22.