

Dynamical modeling of the most important pathways in cellular metabolism

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Keywords: dynamical modeling, metabolism, molecular networks, computer simulation

Recently, the study of cell metabolism has been in the focus of biological research, since most of the changes in cell function cause metabolic changes. Observation of these changes is usually difficult, but there are promising possibilities in metabolic pathway modeling. There is a clear need for cellular models which can predict the metabolic states and modified enzyme activity in modified states. Mitochondria which are cell organelles with prokaryotic origins have a key role in cell metabolism. Degradation of carbohydrates, fats and proteins takes place in the mitochondria, and the intermediers formed may partake in anabolic processes.

In our previous works we examined the intermediers of the citric acid cycle. These metabolites can transform to each other according to the actual metabolic state in mitochondria. The key elements in the regulation of citric acid cycle are the concentrations of intermediers and the changes in redox potential. The initial model was extended by adding mitochondrial transporters which connect cellular and mitochondrial metabolic networks. The model can describe the mechanism of competitive inhibition and the function of multifunctional enzymes which play an important role in the metabolism of several different substrates.

In this work we present the model complemented with several mitochondrial transporters and cellular degradation pathways. For example, glycolysis pathway contains the metabolism of glucose and fructose and leads to pyruvate. Several amino acid metabolic pathways are included, which leads to ammonia, which is then used in the urea cycle. Using the constructed model, we analyze the temporal changes of the metabolite concentrations with a quantitative mathematical description.

Acknowledgments

The research was partially supported by the grant K115694 of the National Research, Development and Innovation Office - NKFIH. The project has also been supported by the European Union, co-financed by the European Social Fund through the grants EFOP-3.6.2-16-2017-00013 and EFOP-3.6.3-VEKOP-16-2017-00009.

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