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 **Abstracts (/osszefoglalok)**

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MODELING THE CITRIC ACID CYCLE, MALATE-ASPARTATE AND CITRATE-PYRUVATE SHUTTLES

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Text of the abstract

Introduction: In the Neurobiochemistry working group, we have taken enzyme kinetic measurements of several mitochondrial enzymes. We have determined oxygen consumption and analyzed interactions between enzymes and various respiratory substrates, but further analysis of the processes is important.

Aims: A suitable qualitative model is constructed which describes the temporal changes in the quantities of citric acid cycle's (CAC) molecules. The modeling goal is to at least qualitatively describe the increased/decreased operation of the catalyzing enzymes as well as the modified operation of the intermediate molecules. We would like to predict whether mitochondria have the ability to adapt to this new metabolic state by activating/inhibiting metabolic pathways.

Method: We modeled the reactions of CAC, malate-aspartate and citrate-pyruvate shuttles. Initially, we constructed 3 individual modules for each process, and later we combined them. The overall model is given

in the form of kinetic ordinary differential equations assuming Michaelis-Menten kinetics with 39 state variables, which was implemented in MATLAB environment. The initial values of the state variables can be provided by the user, depending on the simulated metabolic status.

Results: A dynamical model was constructed and evaluated for describing the quantities in the CAC and its two transport systems. Simulation results are discussed from a biological point of view. Initially, the sub-models of the three subsystems were developed and tested, later these modules were integrated into a unified dynamical model. It is theoretically possible to study the dynamical interplay between all described species.

Conclusion: We introduced a model for describing the dynamics of key quantities in mitochondrial metabolism. Simulations show that the obtained results are qualitatively correct for our expectations. Additional laboratory measurements are in progress to determine kinetic parameters which we have incomplete knowledge about. An important planned application of the model is the dynamical description of pathological processes.

Data of the presenter

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