

SUPPLEMENTARY MATERIAL

to the article by F.V. Kazantsev, S.A. Lashin, Yu.G. Matushkin

“Frame-based mathematical models – a tool for the study of molecular genetic systems”

Model with non-competitive regulation mechanism

In the paper we have shown the repressilator model in which the regulation was given in a form of competitive mechanism. To address the question does it change the model behavior with another regulation mechanism, we performed the model variation changing the mechanism to a non-competitive one. For that purpose, we modified only equations. The model structure remains the same. The model as a file for Copasi tool with the all variants of parameter sets one can find in the supplementary materials. The model structure, equations and simulation results are shown at a Figure S1.

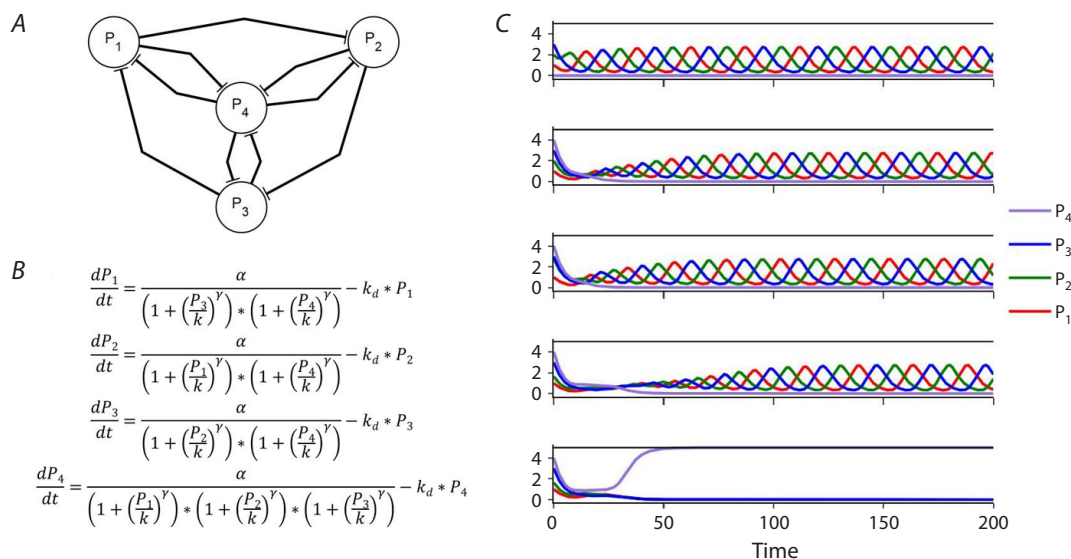


Fig. S1. A four-node model of HGS and its characteristic behavior. *A*, Structural model, where arcs define the conditions of biosynthesis inhibition. *B*, Model equations that correspond to the structure. They provides non-competitive regulation mechanism. *C*, Characteristic plots of concentration vs time obtained for the presented model from Figure *B*.

The dynamics are obtained at parameters $\gamma = 3$, $\alpha = 1$, $k_b = 0.5$, $k_d = 0.2$ and starting points $[P_1, P_2, P_3, P_4]$: (1) [1.0, 2.0, 3.0, 0.0]; (2) [1.0, 2.0, 3.0, 4.0]; (3) [1.0, 2.8, 3.0, 4.0]; (4) [1.0, **1.64**, 3.0, 4.0]; (5) [1.0, **1.65**, 3.0, 4.0]. Plots 1–3 obtained for the same starting points at Figure 3 in a main text.

In a series of simulations, we have shown that within condition of same parameters and starting concentration points the solutions (Fig. S1, 1–3) are differ from the case of model with competitive regulation mechanism (Fig. 3D). At the same time model mode of behavior remains the same. One can find the starting concentration points or the additional stimulus at concentrations that leads to similar stationary regimes and their switching. Hence, the selected model structure shows similar regimes of functioning in dynamic and switching behavior between them (by the concentration changes) independently of regulation mechanism underlie it.