

AUTOMATICAL RECONSTRUCTION AND ANALYSIS OF MATHEMATICAL MODEL FOR GENE REGULATORY NETWORKS

**Akberdin I., Kazantsev F., Ree M., Ree N., Timonov V.^{1,2},
Khlebodarova T.M., Likhoshvai V.A.¹**

ICG SB RAS, Lavrentyeva ave.,10, Novosibirsk, Russia, 630090

¹NSU, Pirogova str., 2, Novosibirsk, Russia, 630090

²SSUTIS, Kirova str., 86, Novosibirsk, Russia, 630102

Mathematical models of gene regulatory networks are based on the information about the structural and functional organization of gene networks and their dynamic properties that disseminated over hundreds and thousands of scientific papers. The problem arises of data comparison and analysis of non-uniformed experimental data, analysis of cause-and-effect relations between molecular structure, dynamics and phenotypic features of molecular-genetic system, and software development for automatic generation of mathematical models, storage of creating models in the database and their numerical analysis.

In the context of solving some of the above mentioned problems we have developed an integrated computer system that does not only render automatically the process of mathematical models reconstruction based on the structural and functional organization of gene networks but also implements original approaches and algorithms to modeling and studying molecular-genetic systems. At the same time we have developed the MGSmodelsDB database and implemented the technology for automatical generation of mathematical models in this web-resource.

MGSmodelsDB is a new repository of mathematical models of cell subsystems. The current version of the database includes models of enzymatic reactions and gene expression regulatory processes of *de novo* nucleotide metabolism and anaerobic respiration in *Escherichia coli*. The database contains 110 elementary models, each of which represents an enzymatic reaction or regulatory process rate function. Model parameters were obtained from published data or fitted to the available experimental data. MGSmodelsDB enables to search, select and automatically generate more complex models in SBML and other formats from a subset of elementary models.

The examples of using of these systems are demonstrated on a modeling of the gene regulatory network for auxin metabolism in a plant meristem cell and gene regulatory networks for pyrimidine biosynthesis in *E.coli*.

Availability: http://modelsgroup.bionet.nsc.ru/?page_id=729

Acknowledgements

Funding: This work was supported by the Russian Foundation for Basic Research [10-01-00717-a, 11-04-01748-a], by the Interdisciplinary Integration Projects of the Siberian Branch of the Russian Academy of Sciences [107, 119] and Programs of the Russian Academy of Sciences [A.II.5.26, A.II.6.8, B.26.29]. The development of MGSmodelsDB was partially supported by the "PATHOSYS" grant [260429] of the Seventh Framework Programme.