MGSmodeller – A COMPUTER SYSTEM FOR RECONSTRUCTION, CALCULATION AND ANALYSIS MATHEMATICAL MODELS OF MOLECULAR GENETIC SYSTEM

Kazantsev F.V.[1, 3]*, Akberdin I.R.[1], Bezmaternykh K.D.[1, 2], Lashin S.A.[1], Podkolodnaya N.N.[1], Likhoshvai V.A.[1, 2]

[1] Institute of Cytology and Genetics, SB RAS, Novosibirsk, Russia

[2] Novosibirsk State University, Novosibirsk, Russia

[3] High College of Informatics of the Novosibirsk State University, Novosibirsk, Russia

e-mail: kazfdr@bionet.nsc.ru

[*] Corresponding author

Motivation and Aim: Development of multifunctional analytical computer system that presents resources for modelling and analysis of the functional patterns in molecular genetic systems of eu- and prokaryote cells is one of the current important problems in system biology. In this study the MGSmodeller computer system that intended for reconstruction, calculation and analysis mathematical models of molecular genetic system is presented.

Methods and Algorithms: MGSmodeller as a computer system contains the next set of modules: “model constructor/editor”, “model calculation”, “inverse problem”, “optimal control”. Multifunctionality of the system is based on the facilities of each module. Such module as “model constructor/editor” allows to create and to edit models using original standard SiBML for specification mathematical models of molecular genetic networks. SiBML based on generalized chemical kinetic method [1] and taking into account the structure of their genetic and compartmental levels.. The system also includes: (i) tools for model reconstruction with arbitrary structure of the molecular genetic systems taking into account positional relationship and orientation genes in genomes, polyallel genes, matrix principles of the passing such fundamental processes as replication, transcription and translation, and milticompartmental structure of studying systems, (ii) tools for dynamic calculation, solving of inverse problems and problems of optimal control. MGSmodeller is java-application and is supplied with attributes of the user friendly interfaces. User interface of the MGSmodeller allows to hierarchically represent data, edit them and to clearly represent the calculation results and to perform analysis of molecular genetic models.

Results: The original format of models description SiBML, algorithms and the MGSmodeller system are developed for generation, reconstruction, edition and calculation of molecular genetic networks models. This system was used for reconstruction the auxin metabolism mathematical model [2]. All information relatively MGSmodeller and about authors is available on the web-site http://www.bionet.nsc.ru/labs/modelgroup/indexEng.html

References:

1. V.A. Likhoshvai et al. (2001). Generalized chemokinetic method for gene network simulation, *Mol. Biol.*, **35:**1072-1079.
2. I.R. Akberdin et al, Mathematical model of auxin metabolism in shoots of arabidopsis thaliana L, *this volume*