

MGSgenerator – THE TOOL FOR AUTOMATICAL GENERATION OF MOLECULAR GENETIC SYSTEM MATHEMATICAL MODELS ON BASIS OF GENE NETWORKS STRUCTURE

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Motivation and Aim: One of the topical and interesting challenge in the system biology is creating automatic tool for generation of the mathematical models on basis of reconstructed gene networks with further analysis of this complex models and visualization of model results. Since reach this aim we have developed special software that allow to convert information about gene network structure to the mathematical model. We called this system as MGSgenerator.

Methods and Algorithms: MGSgenerator is based on Eclipse (www.eclipse.org) plug-in architecture. The developed converter support following types of plug-ins. First is the data source modules and second is the data export modules. Thus, this tool can be extended for conversion from different systems such as KEGG data base and for generation models in different modeling systems such as *Mathematica*. The reaction rate is described on basis of Hill functions, that allow to represent different types of the molecular-genetic regulation. It's computer system could be used for generation mathematical models only for correct described subset of patterns that could be representing in gene networks. Anyway it might be networks where are complex processes, which couldn't be described by pre-set rules. In this case user can manually set the necessary reaction rate equation.

Results: This software tool MGSgenerator could be and is used to generate math models of gene network patterns subset. Today we have few plug-in modules that allow us to convert format XML of the GeneNet computer system [1] into SiBML format of the MGSmodeller [2]. MGSmodeller is the complex software which allows to reconstruct models and, of course, to analyze and calculate mathematical models. The gene network that we used for MGSgenerator testing didn't allow us to describe for less then 20% of molecular-genetic processes by the mathematical models, but after gene network annotations modification we converted all processes in this gene network in the SiBML. All information relatively MGSgenerator and about authors is available on the web-site <http://www.bionet.nsc.ru/labs/modelgroup/indexEng.html>.

References:

1. Ananko E.A., Podkolodny N.L., Stepanenko I.L., Podkolodnaya O.A., Rasskazov D.A., Miginsky D.S., Likhoshvai V.A., Ratushny A.V., Podkolodnaya N.N., Kolchanov N.A. (2005) GeneNet in 2005. *Nucleic Acids Res.*, 33: 425-427.
2. Kazantsev F.V. et al. MGSmodeller – a computer system for reconstruction, calculation and analysis mathematical models of molecular genetic system, *this volume*