

Application of Computational Systems Biology in Drug Discovery

Maryam Mohammadi*, Seddigeh Mohammadi

Department of Engineering, Islamic Azad University of Lamerd, Lamerd, Iran

*e-mail: m.mohammadi@modares.ac.ir

Abstract: Computational systems biology is a new method for biological simulation that constructs intercellular model or simulate genomic, proteomic or metabolomics datasets to predict cell functions. Genomic, proteomics, metabolomics and biochemical datasets have presented valuable information regarding the molecular basis of cell function. In most of disease disorders, proteins play an important role. By systems biology analysis, we can comfort the connection between disorder and its target gene [1]. Systems biology by using integrated approach, investigate the function of biological systems and perturbations that occur in them, for example the administration of a therapeutic drug, affect their function. The biological system simulation can be at the level of cell, organ, tissue or organism. Systems biology by integrating huge datasets of experimental genomic, proteomic or metabolomic data, construct predictive models by using computers, and then correcting these simulation models by comparing the predicted data with experimental data [2,3]. If these models developed well, then it is not hard to see how computational systems biology could help for identification of novel drug targets or dosing of drug compounds. For example, by using advanced modeling, novel drug targets discover by identifying the key protein in a disease-related pathway. drug toxicity could be evaluated by modeling organ specific metabolic stress responses. Furthermore, drug distribution and metabolism could be modeled through multi-organ, multi-tissue methods, and drug dosing regimes could be assessed by modeling tumor responses to different drug concentrations or doses [4-6].

Keywords: Computational Systems Biology; Drug Discovery; Metabolomic and Proteomic Integration; Biological System.

References

- [1] EJ Davidov, JM Holland, EW Marple, S Naylor, (2003) Advancing drug discovery through systems biology, Drug discovery today,
- [2] Hood, L. (2003) Systems biology: integrating technology, biology, and computation. Mech. Ageing Dev. 124, 9–16
- [3] Ideker, T. et al. (2001) A new approach to decoding life: systems biology. Annu. Rev. Genomics Hum. Genet. 2, 343–372
- [4] Bugrim, A. et al. (2004) Early prediction of drug metabolism and toxicity: systems biology approach and modeling. Drug Discov. Today 9, 127–135
- [5] Cho, C.R. et al. (2006) The application of systems biology to drug discovery. Curr. Opin. Chem. Biol. 10, 294–302
- [6] Kumar, N. et al. (2006) Applying computational modeling to drug discovery and development. Drug Discov. Today 11, 806–811