In Silico Modeling and Simulation Environment For Metabolic Flux Analysis

Hongseok Yun, Sang Yup Lee
Department of Chemical & Biomolecular Engineering
Korea Advanced Institute of Science and Technology
373-1 Guseong-dong, Yuseong-gu, Daejeon 305-701, Korea
TEL: +82-42-869-3930, FAX: +82-42-869-8800

Abstract

The rapid increase of the number of annotated genomes accelerates systematical study of variety of organisms. Genome-scale modeling and simulation have been regarded as one of the most challengeable research fields which requires both of broad range of biological information and validate methods to construct and analyze complex metabolic networks which come from whole genome sequence. Here we present *in silico* modeling and simulation environment to support for building up metabolic models from whole annotated genomes and analyzing them for practical uses. It consists of three software tools: Biosilico for retrieving the relevant information on genes, enzymes, compounds, reactions and pathways; Metabolic Flux Analysis Markup Language (MFAML) for representing metabolic system with environmental/genetic conditions as well as basic information on metabolites and reactions; and MetaFluxNet for quantitatively analyzing metabolic networks. This environment allows users to efficiently build, validate and analyze the complex metabolic models. [This work was supported by the Korean Systems Biology Research Grant Program from the MOST. Further supports by the BK21 program, LG Chemicals Chair Professorship, Microsoft and IBM SUR program are appreciated.]

References

1. Lee, D.Y., et al. MetaFluxNet: the management of metabolic reaction information and quantitative metabolic flux analysis (2003), Bioinformatics, 19(16), 2144-2146.
2. Hou, B.K., et al, BioSilico: an integrated metabolic database system (2004), Bioinformatics, 20(17), 3270-3272.
3. Yun, H., et al, MFAML: a standard data structure for representing and exchanging metabolic flux models, Bioinformatics, 21(15),3329-3330.