In silico experiments for biochemical production in Escherichia coli

<u>박종명</u>, 김태용, 이상엽* 한국과학기술원 (leesy@kaist.ac.kr*)

In this work, the various gene targeting strategies are presented for the strain improvement on the basis of constraints-based flux analysis. First, we constructed a genome-scale in silico E. coli comprising 764 metabolites and 935 metabolic reactions. Under pseudo-steady state assumption, the unknown internal fluxes within the metabolic reaction network constructed can be evaluated by this flux analysis, subject to the constraints satisfying mass conservation and reaction thermodynamics. Second, the various in silico knock-out method can be developed by fixing the relevant fluxes at zeros among enzyme reactions. In the amplification method, any reactions can be amplified by changing minimum to maximum of flux value. Third, results obtained from the simulation are arranged with the maximum of production and biomass formation. For each strain, the correlation between the biomass formation and biochemcial production was obtained. [This work was supported by the Korean Systems Biology Research Project (M10309020000–03B5002–00000) of the Ministry of Science and Technology, and by the Brain Korea 21 Project. Further supports by the LG Chem Chair Professorship, Microsoft, and IBM SUR program are appreciated.]