Metabolic flux analysis with grouping reaction constraint based on genomic context and flux-converging pattern analyses

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Flux balance analysis (FBA) of a genome-scale metabolic model allows calculation of intracellular metabolic fluxes by optimizing an objective function. However, FBA simulation without additional information has some limitations, such the inaccurate prediction of fluxes and existence of multiple solutions for an optimal objective value. Here, we report a strategy to accurately predict metabolic fluxes based on grouping reaction constraints that restrict the achievable flux ranges of grouped reactions by genomic context and flux-converging pattern analyses. FBA of *Escherichia coli* genome-scale metabolic model was carried under several genotypic and environmental conditions by applying these constraints, resulted in flux values that were in good agreement with the experimentally measured ^{13}C-based fluxes. [This work was supported by the Korean Systems Biology Research Project (20110002149) of the Ministry of Education, Science and Technology (MEST) through the National Research Foundation (NRF) of Korea. Further support by the WCU Program (R32-2009-000-10142-0) through the NRF of Korea funded by the MEST is appreciated.]