Prediction of metabolic fluxes based on genomic context and flux-converging pattern analyses for genome-scale simulation

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Constraints-based flux analysis including flux balance analysis (FBA) has found numerous applications in the field of systems biology and biotechnology. However, the FBA simulation without additional information has some limitations such as inaccurate prediction of fluxes and existence of multiple solutions for an optimal objective value. Here, we report a strategy based on FBA combined with 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 performed to validate the strategy under different genotypic and environmental conditions. The predictions with the constraints agreed well with experimentally measured fluxes. [This work was supported by the Korean Systems Biology Research Project (20100002164) of the Ministry of Education, Science and Technology (MEST) through the National Research Foundation of Korea. Further support by the World Class University Program (R32-2009-000-10142-0) through the National Research Foundation of Korea funded by the MEST is appreciated.]