Kenichiro Honda, Metabolomics 2014, 4:2
http://dx.doi.org/10.4172/2153-0769.S1.025

OMICS Group Conferences
Accelerating Scientific Discovery

3rd International Conference and Exhibition on
Metabolomics & Systems Biology
March 24-26, 2014 Hilton San Antonio Airport, San Antonio, USA

Evaluation of metabolic systems based on dynamical stability using a model of 1-butanol producing *Escherichia coli*

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One of the goals of systems biology is to simulate and design metabolic pathways based on quantitative predictions with the aid of mathematical models. To construct a dynamic model of metabolic system inside a cell, there are roughly two types of approaches: reductive and holistic. While the former focuses on accurate estimation of reaction parameters of each enzyme to reproduce detail time evolution of some specific chemical species, the later evaluates global behavior of the entire metabolic systems such as robustness against external perturbations. And for applications in metabolic engineering, understanding of long-term behavior of the whole cell will be more important. In this study, we developed a dynamic model of the entire central metabolic system of *Escherichia coli* for understanding the behavior of metabolic pathway around the steady state.

The Flux Balance Analysis is a useful approach that estimates the flux profiles of the whole metabolic network under the steadily growing state. However, in order to evaluate dynamical behavior, we need to estimate not only flux profiles but also reaction coefficients and absolute concentration of related metabolites. However, comprehensive measurements of metabolite concentration using qualitative methods such as mass spectrometry are still difficult. Not all the metabolites can be measured simultaneously, and we also cannot evaluate absolute quantity but relative values. To address this problem, in evaluation of stability of the metabolic system at the steady state, we searched probable profiles of metabolite concentrations using an evolutionary algorithm under the physico-chemical constraint, and optimized the linear stability of the dynamic system.

Using this model, we evaluated the metabolic system of *Escherichia coli*, which produces 1-butanol. We estimated plausible ranges of metabolite concentration where a cell can stay in a stable steady state. We also examine the importance of each metabolic reaction for the production of 1-butanol by sensitivity analysis of this dynamic model to improve its productivity.

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