

Prediction of the maximum yields of metabolites by metabolic flux analysis

홍순호, 문수연, 이상엽

한국과학기술원 생명화학공학과 및 생물공정연구센터

전화 (042)869-3930, FAX (042)869-8800

The intracellular metabolic fluxes can be calculated by metabolic flux analysis, which uses a stoichiometric model for the intracellular reactions along with mass balances around the intracellular metabolites (1, 2, 3). In this study, metabolic flux analyses were carried out to estimate flux distributions for the maximum in silico yields of various metabolites in *Escherichia coli*. The maximum in silico yields of acetic acid and lactic acid were identical to their theoretical yields. On the other hand, the in silico yields of succinic acid and ethanol were only 83% and 6.5% of their theoretical yields, respectively. The lower in silico yield of succinic acid was found to be due to the insufficient reducing power, which could be increased to its theoretical yield by supplying more reducing power. The maximum theoretical yield of ethanol could be achieved when a reaction catalyzed by pyruvate decarboxylase was added in the metabolic network. Furthermore, the optimal metabolic pathways for the production of various metabolites could be proposed based on the results of metabolic flux analyses. In the case of succinic acid production, it was found that pyruvate carboxylation pathway should be used rather than phosphoenolpyruvate carboxylation pathway for its optimal production in *E. coli*.

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