

Metabolic Pathway Identification Based on Thermodynamic Properties

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An effective strategy comprising two phases is proposed to determine the thermodynamically dominant pathways in a metabolic network involving a number of metabolic reactions. In the first phase, stoichiometrically feasible metabolic pathways are exhaustively identified through the flux balance analysis and the graph-theoretic method based on P-graphs. In the second phase, thermodynamically dominant pathways are selected from these stoichiometrically feasible metabolic pathways on the basis of the Gibbs free energy change of reaction. The proposed strategy's efficacy is demonstrated by applying it to two E. coli models.

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