Thermodynamic analysis for improving the reliability of flux balance analysis (FBA)

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Flux balance analysis (FBA) is one of the constraints-based modeling techniques for obtaining the flux distributions of complex biochemical networks based on the quasi-steady state assumption and mass balance constraints. However, it may not be guaranteed that the flux distribution is reliable because FBA considers solely quantitative constraints. In this study, thermodynamic constraints which are qualitative constraints were also considered. The flux directions were assessed based on the thermodynamic principles, and the thermodynamic database updated with the most recent data was constructed. Additionally, a systematic approach for estimating biochemical properties was proposed. As a result, the more reasonable solution of E.coli model was obtained by exploiting newly constructed thermodynamic database and thermodynamic constraints.