Combined Graph-theoretic and Energy Balance Approach for Identifying Most Plausible Pathway of Metabolic Networks

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There are two well-known approaches for identifying independent pathways of complex biological system. They include elementary mode analysis and extreme pathways analysis which are basically derived from convex analysis. While both approaches are applicable to and good for relatively simple systems, the computational loads increase immensely with the addition of even a few components. To deal with such a "combinatorial explosion" problem, we developed the graph-theoretic approach for pathway identification based on process graph in which a set of axioms express obvious and inherent properties for feasible pathways (Lee et al., 2005). P-graph saves an enormous number of redundant pathways, producing combinatorially feasible pathways. When identifying the most likely pathway among the feasible ones, further estimation criteria based on some other principles are desirable. In this work, thermodynamic properties are exploited in search for the dominant pathways among the feasible pathways.