Framework for Elucidating the Causal Relationship of Metabolic Fluxes

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Metabolic fluxes, an ultimate phenotype of the cell, are condition-specific, so that it is very difficult to predict their distribution patterns under conditions of interest. To provide insight into this problem, we developed a framework that employes constraint-based flux analysis and Bayesian network analysis. This framework first performs constraint-based flux analysis with constraints adopted from 13C isotope-labelling experiments. Information from 13C isotope-labelling experiments is used in order to calculate more accurate genome-scale metabolic flux distributions. Also, least absolute deviation method is used to account for infeasibility of the system due to a large number of constraints. The calculated metabolic flux profiles are then categorized into functional sub-metabolisms, and each of these is subjected to Bayesian network analysis in oder to infer the causal relationship among metabolic fluxes.