Protein constraints in genome-scale metabolic models: data integration, parameter estimation, and prediction of metabolic phenotypes

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Abstract

Genome-scale metabolic models provide a valuable resource to study metabolism and cell physiology. These models are employed with approaches from the constraint-based modelling framework to predict metabolic and physiological phenotypes. The prediction performance of genome-scale metabolic models can be improved by including protein constraints. The resulting protein-constrained models consider data on turnover numbers (k_{cat}) and facilitate the integration of protein abundances. In this systematic review, we present and discuss the current state-of-the-art regarding the estimation of kinetic parameters used in protein-constrained models. We also highlight how data-driven and constraint-based approaches can aid the estimation of turnover numbers and their usage in improving predictions of cellular phenotypes. Lastly, we identify standing challenges in protein-constraint metabolic models and provide a perspective regarding future approaches to improve the predictive performance.

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