

## Mapping condition-specific metabolomics data onto network reconstructions generates meaningful dynamic models

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Genome-scale metabolic network reconstructions provide a context within which omics data can be analyzed to understand phenotypic functions. Here, we develop a workflow to integrate three disparate data types (metabolomic, fluxomic, and thermodynamic) within the context of a metabolic reconstruction. First we determine that the data sets are thermodynamically consistent. Then, we use the mass action stoichiometric simulation (MASS) model-building framework to develop three condition-specific kinetic models of *E. coli* core metabolism. The results from this study demonstrate: 1) that the MASS approach, that generates condition-specific rate constants based on *in vivo* data, can generate network-scale dynamic models in a data-driven manner, 2) that the MASS models generated under many conditions have underlying dynamic similarities, and 3) that this structured and integrated omics data analysis yields consistent physiological results from data that otherwise would be treated as a series of independent measurements. The impending onslaught of quantitative *in vivo* metabolomics data can thus be converted into useful dynamic models in a data-driven fashion to generate descriptions of integrated network functions.