

## Quantitative metabolic modeling at the Joint BioEnergy Institute (JBEI)

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<https://www.jbei.org>

### Project Goals:

The Quantitative Metabolic Modeling (QMM) directorate at the Fuels Synthesis Division is devoted to developing models of metabolism which are both quantitative and predictive, in order to improve biofuel production in a rationally directed fashion. Here, we present our work in three different thrusts: machine learning modeling, mechanistic modeling, and software development. Machine learning modeling is used to systematically improve biofuel production without a detailed understanding of pathway dynamics and, separately, is combined with kinetic modeling in order to predict time-dependent metabolomic data from measured protein levels. Mechanistic models involving <sup>13</sup>C Metabolic Flux Analysis for genome-scale models are used to produce actionable items for metabolic engineering that have improved fatty acid production by 70%. All these methods are supported by a suite of software tools that improve productivity: the Experiment Data Depot (EDD) stores data and metadata for a variety of metabolic engineering experiments. EDD allows easy visualization of these data and its access in a standardized manner for use with modelling approaches. Arrowland (<https://public-arrowland.jbei.org/>) provides an intuitive and interactive tool to explore -omics data and make predictions on possible metabolic engineering approaches. The JBEI QMM library is a python open source library that provides the tools for all the aforementioned capabilities.

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