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Constrictor: Flux Balance Analysis Constraint Modification Provides Insight for Design of Biochemical Networks KEESHA ERICKSON, ANUSHREE CHATTERJEE, University of Colorado - Boulder — The use of in silico methods has become standard practice to correlate the structure of a biochemical network to the expression of a desired phenotype. Flux balance analysis (FBA) is one of the most prevalent techniques for modeling metabolism. FBA models have been successfully applied to obtain growth predictions, theoretical product yields from heterologous pathways, and genome engineering targets. We take inspiration from high-throughput recombineering techniques, which show that combinatorial exploration can reveal optimal mutants, and apply the advantages of computational techniques to analyze these combinations. We introduce Constrictor, an in silico tool for FBA that allows gene mutations to be analyzed in a combinatorial fashion, by applying simulated constraints accounting for regulation of gene expression. We apply this algorithm to study ethylene production in E. coli through the addition of the heterologous ethylene-forming enzyme from P. syringae. Targeting individual reactions as well as sets of reactions results in theoretical ethylene yields that are as much 65% greater than yields calculated using typical FBA. Constrictor is an adaptable technique that can be used to generate and analyze disparate populations of in silico mutants & select gene expression levels.

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