Supporting Information

Antioxidant green-factories: Towards sustainable production of vitamin E in plant *in vitro* cultures

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Table 1. Plant metabolic model reconstructions and their applications

Species	Reconstructed model	Objective function (Modeling approach)	Applications
Arabidopsis thaliana	Heterotrophic cell culture[1,2,3]	Minimize total reaction flux (FBA)	Predicting metabolic capabilities under heterotrophy, elevated temperature and hyperosmosis
	AraGEM[4]	Minimize uptake of photon/sucrose (FBA)	Predicting metabolic capabilities under photosynthesis, photorespiration and heterotrophy
	Improved AraGEM and C4GEM[5]	Maximize (separately) CO_2 fixation and biomass synthesis (FBA)	Comparative analysis of the effect of gene knockouts, light intensity and CO_2 concentration between C3 and C4 plants
	Compartmentalized and photosynthetic / heterotrophic tissue-specific models [6]	Minimization of flux difference (MoMA/ROOM)	Assessment of metabolic behavior of various tissue types with integration of omics data, predicting flux distribution following gene knockout, Metabolic engineering strategies (knockout targets) for vitamin E biosynthesis
	Bottom-up metabolic reconstruction- AraCore [7]	Maximize biomass and energy efficiency (FBA)	Carbon utilization under normal, carbon-and nitrogen-limiting conditions, estimation of metabolic cost for enzyme production
Oryza sativa (**Rice**)	Photoautotrophic model based on RiceCyc [8]	Minimize total reaction flux (FBA)	Predicting flux distributions in response to varying light intensity
	Central metabolic/regulatory network model representing germinating seeds and photorespiring leaves [9]	Maximize biomass (FBA) followed by Flux variability analysis (FVA)	Predicting phenotypic and metabolic states of cells under anaerobic conditions and photorespiration (simulating flooding and drought stress)
	Improved genome-scale model iOS2164 [10]	Maximize biomass (FBA) followed by random sampling	Understanding metabolic and regulatory states in response to light by integrating multi-omics data with constraint-based analysis
Solanum lycopersicum (**Tomato**)	Medium-scale central metabolic flux model of tomato fruit, constrained with experimental data [11]	Minimization of sum of the fluxes (FBA)	Understanding metabolic changes in developing tomato fruit
	Genome-scale metabolic model of tomato leaf-iHY3410 [12]	Minimize total reaction flux (FBA) followed by max/min of individual reactions (FVA)	Investigating the photorespiratory metabolism (metabolic response to drought stress) and reaction essentiality analysis.

C4GEM	Multi-tissue models of maize, sugarcane and wheat [13]	Minimize photon uptake (FBA)	Capturing interaction between mesophyll and bundle sheath cells in C4 photosynthesis.
Zea mays (**Maize**)	iRS1563 [14]	Maximize biomass (FBA)	Predicting metabolic capabilities under photosynthesis, photorespiration and respiration
	Compartmentalized leaf genome-scale model a. Maize [15] b. Mazie [16]	a. Flux-sum analysis (FBA) followed by FVA b. Maximum rate of sucrose export (FBA)	Constraint-based analysis of GSM integrated with a. Transcriptome and proteome data under nitrogen-limitation b. Metabolomics and enzyme activity data to investigate yield of kernels
Hordeum vulgare (**Barley**)	Central metabolic network of developing endosperm [17]	Maximization of growth (FBA) followed by minimization of overall flux (Quadratic programming)	Metabolic flux distribution under anoxic, hypoxic, aerobic and enzyme deletion conditions
	Multiscale metabolic modeling by integrating static organ-specific models with dynamic whole-plant model [18]	Minimize carbon source uptake followed by minimization of overall flux (FBA-static part)	Dynamic FBA (dFBA) to analyze source-sink interactions during barley seed development
Brassica napus (**Rapeseed**)	Compartmentalized model of central metabolism [19]	Maximize biomass (FBA)	Simulation of seed growth at various oil accumulation stages and insights into network plasticity by FBA, principal component analysis and reaction deletion studies.
	Metabolic network model of seed storage metabolism in developing embryos- bna572[20]	Allowable range of fluxes (FVA)	Quantitative analysis of reaction contributions during storage metabolism using flux variabilities

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