A Novel Genome Scale Metabolic Model of *Clostridium thermocellum* DSM 1313 Implementing an Adjustable Cellulosome for Examining Complex Cellular Phenotypes and Model-Guided Strain Design

Supplementary File S2

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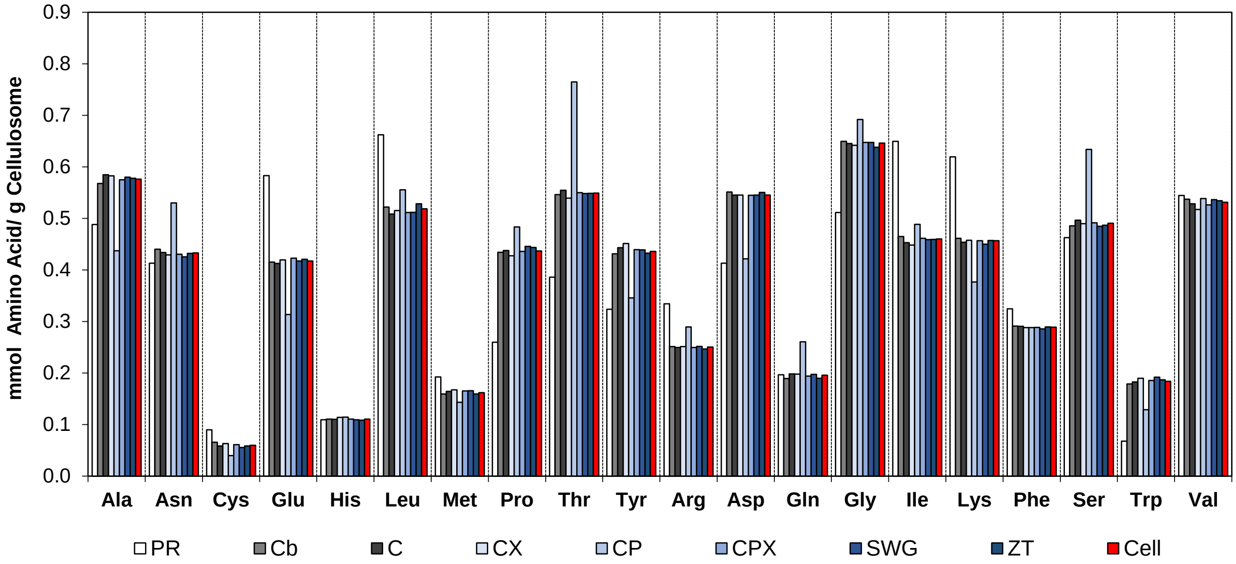
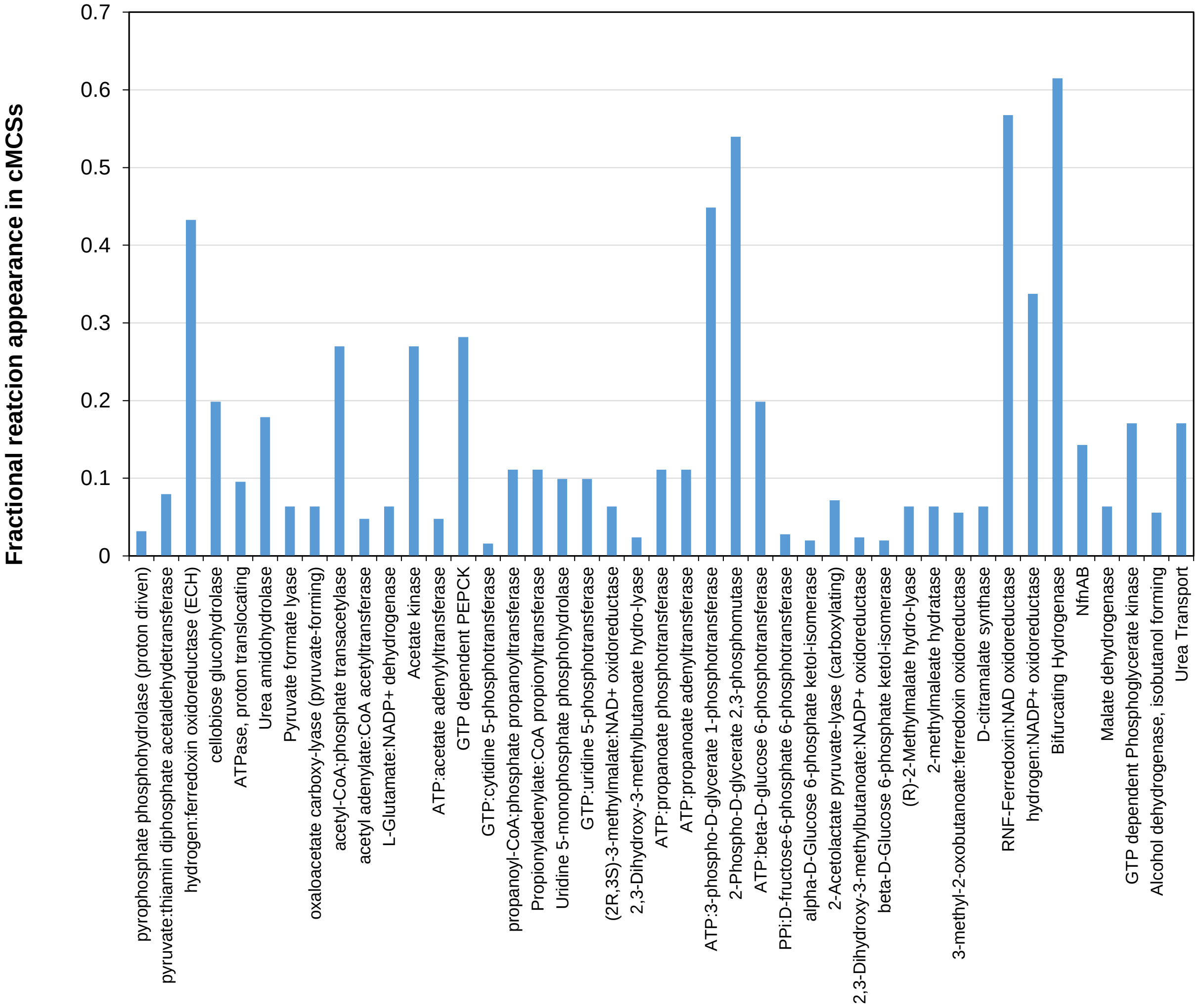
Supplementary Table S1. Comparison of *i*AT601 predictions of mutant strain growth using the calculated GAM parameter. Fermentation product fluxes were constrained using experimental values presented in Thompson et al, *Met. Eng.*, 2015, **32**:207-219. Gene deletions were implemented by constraining appropriate reaction bounds to zero.

	Specific growth rate μ (hr^{-1})	
Strain	**Experiment**	**Simulation**
Parent	0.33	0.33
Δ*hydG*	0.24	0.26
Δ*hydG* Δ*ech*	0.22	0.25
Δ*hydG* Δ*pta-ack*	0.16	0.18

Supplementary Figure S1. Distribution of amino acids per unit cellulosome for growth of *C. thermocellum* on various cellulosic substrates. Abbreviations: Cb, cellobiose; C, crystalline cellulose (Avicel); CX, cellulose + xylan; CP, cellulose + pectin; CPX, cellulose + pectin + xylan; SWG, pretreated switchgrass; ZT, amorphous cellulose (Z-Trim®); and Cell, median values across all other amino acid distributions and the values used in our cellulosome term. Data adapted from Raman et al, *PLoS ONE*, 2009, **4**:e5271.



Supplementary Figure S2. Fractional reaction appearance in ethanol constrained Minimal Cut Set strategies for reactions with a fraction above 1%. Fractional appearance calculated by summing the times a reaction is present in an MCS divided by the total cMCS count.



Supplementary Figure S3. Predicted averaged fluxes of major fermentation products for growth of *C. thermocellum* on cellobiose (**A-C**) and cellulose (**D-F**). These fluxes were presented for low growth phase (**A, D**), moderate growth phase (**B, E**), and high growth phase (**C, F**).