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Research article

Estimation of metabolic fluxes distribution in Saccharomyces cerevisiae during the production of volatile compounds of Tequila

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Supplementary

Table S1. Composition of the biomass.

METABOLITE	Cellular Content (% weight)			
	D = 0.10 h^{-1}	D = 0.20 h^{-1}	D = 0.30 h^{-1}	D = 0.40 h^{-1}
Protein	45	50	55.5	60.1
Glycogen	8.4	4.2	0.6	0
Trehalose	0.8	0.2	0	0
Mannose	13.1	12.9	12	13.3
Other carbohydrates	18.4	15.4	12.6	3.7
RNA	6.3	8.2	10.1	12.1
DNA	0.4	0.4	0.5	0.6
Free amino acids	1.1	1.3	1.1	2
Lipids	2.9	3	3.8	3.4
Ashes	5	5	5	5
Total	101.4	100.6	101.2	100

Source: Nissen et al. (1997)

Table S2. Experimental restrictions specified in the optimization under anaerobic conditions.

Metabolite	Li (mmol/g DW h)	Ls (mmol/g DW h)
Glucose	0	5.917
Oxygen	0	0
Ammonium	0	1000

Table S3. Experimental restrictions specified in optimization under microaerobic conditions.

Metabolite	Li (mmol/g DW h)	Ls (mmol/g DW h)
Glucose	0	14.00
Oxygen	0	1.00
Ammonium	0	1000

Table S4. Experimental restrictions specified in optimization under oxide-fermentative growth.

Metabolite	Li (mmol/g DW h)	Ls (mmol/g DW h)
Glucose	0.00	12.00
Oxygen	0.00	9.00
Ammonium	0.00	1.00

Table S5. Experimental restrictions specified in optimization under Glucose-limited Aerobic Growth.

Metabolite	Li (mmol/g DW h)	Ls (mmol/g DW h)
Glucose	0	2.50
Oxygen	0	8.00
Ammonium	0	1000

Table S6. Fermentation conditions of continuous culture reported in literature.

D[1] (h^-1)	Biomass[1] (g/L)	Ethanol[1] (g/L)	Residual[1] Sugars (g/L)	Rx[1] (g/Lh)	Rp[1] (g/Lh)	Rs[1] (g/Lh)	Sugar flux (mmol/g DW h)	Ethanol flux (mmol/g DW h)	Specific Growth Velocity μ (h^{-1})
0.04	5.83	43.92	3.94	0.23	1.76	3.8	3.671	6.654	0.04
0.08	3.38	29.63	35.34	0.27	2.37	5.08	8.362	15.266	0.08
0.12	3.04	19.76	59.75	0.36	2.37	4.69	8.685	17.174	0.12
0.16	2.75	9.95	79.08	0.44	1.59	2.52	5.092	12.569	0.16

Experimental data from Morán et al. (2011); Rx, Rp, and Rs represent productivity of biomass and sugar of the fermentation process.

Table S7. Volatile compounds fluxes for a dilution rate of D = 0.04 h^{-1} specified as experimental restrictions.

Fluxes	D = 0.04 *Experimental (mmol/g DW h)	*In silico* (mmol/g DW h)	% Variation
Fructose	3.671	3.671	0%
Ethanol	6.654	5.8	-13%
Biomass	0.04	0.04	0%
CO_2	-	7.448	
Nitrogen Source	-	0.274	
Acetaldehyde	0.0036	0.0035	0%
Methanol	0.0373		
n-Propanol	0.0066	0.0066	0%
Isobutanol	0.0017	0.0017	0%
Isoamyl and Amylalcoho	0.0092	0.0092	0%
2-Phenyl-ethanol	0.00059	0.00059	0%
Ethyl acetate	0.00063	0.00063	0%

Table S8. Metabolic fluxes deriving from experimental data of fermentation with agave juice at different Dilution (D) rates.

Ethanol Flux	*Experimental (mmol/g DW h)	In Silico (mmol/g DW h)	% Variation
D = 0.04 h^{-1}	6.6541	5.813	-13%
D = 0.08 h^{-1}	15.266	11.469	-2.4%
D = 0.12 h^{-1}	17.174	13.155	-23%
D = 0.16 h^{-1}	12.569	–	–