

Data used in the computation of the results

Table A. Stoichiometric equations and thermodynamic information (per mole glucose) of the four remaining elementary modes. The reaction enthalpy (ΔH) and reaction free energy (ΔG) were computed using the enthalpy and free energies of combustion given in Table D. dF is the dissipation function defined as $(\Delta S - \Delta H/T)$.

Family	Reaction stoichiometry	ΔH [kJ/mol]	ΔG [kJ/mol]	ΔS [kJ/K-mol]	dF [kJ/K-mol]
1	Glucose \rightarrow 2 Ethanol + 2 CO ₂ + 2 ATP	1253.8	1074.5	0.547	-3.28
2	Glucose \rightarrow 2 Ethanol + 2 CO ₂	-69.0	-234.0	0.503	0.71
3	Glucose + 0.70 NH ₃ \rightarrow 2.88 Biomass + 0.11 H ₂ + 1.10 Ethanol + 1.18 CO ₂	-1409.6	-1564.8	0.473	4.77
4	Glucose + 0.70 NH ₃ \rightarrow 2.88 Biomass + 0.11 Formate + 1.10 Ethanol + 1.07 CO ₂	-1426.5	-1575.0	0.453	4.80

Table B. Probabilities of family modes and thermodynamic information for a fully evolved cell metabolism. The thermodynamic information is determined from the weighted sum of the probabilities and the thermodynamic information of individual modes.

Family	Asymptotic p_{Fi}	Predicted p_{Fi}
1	0.214	0.214
2	0.233	0.242
3	0.273	0.264
4	0.298	0.279
ΔS_{TOT} (kJ/K-mole)	0.50	0.49
ΔH_{TOT} (kJ/mole)	-557.7	-518.5
ΔG_{TOT} (kJ/mole)	-721.1	-679.2
dF (kJ/K-mole)	2.20	2.07

Table C. Change in probabilities of family modes and biomass yield during metabolic evolution. The biomass yield is determined from the weighted sum of the probabilities and the yield of biomass of individual modes.

Family	p_{Fi} (at 0 gen)	p_{Fi} (at 280 gen)	p_{Fi} (at ∞ gen)
1	0.411	0.337	0.214
2	0.411	0.337	0.233
3	0.078	0.162	0.273
4	0.078	0.162	0.298
Y_x (g/g)	0.064	0.132	0.234

Table D. Enthalpy and Gibbs free energies of combustion for metabolites. The energy values were obtained from Sandler and Orbey (1991).

Metabolite	Enthalpy of Combustion [kJ/mol]	Free Energy of Combustion [kJ/mol]
glucose	2807.0	2872.0
xylose	2180.8	2204.6
ethanol	1369.0	1319.0
acetate	876.0	894.0
ammonia	348.1	391.9
lactate	1308.4	1322.6
formate	127.5	140.5
hydrogen	285.9	237.2
propionic acid	1529.0	1533.0
biomass	1388056.8	1403173.2
ATP	661.4	654.2

Table E. The biomass growth rate, the glucose consumption rate and the ethanol secretion rates (C-mole/hr) during adaptive evolution. The rate of each metabolite was determined from the slope of the linear regression of time plots of the metabolite concentration.

	unevolved (at 0 gen)	evolved (at 75 gen)	evolved (at 159 gen)	evolved (at 251 gen)	evolved (at 280 gen)
R_{Glucose}	0.64	3.00	4.03	4.27	4.28
R_{Ethanol}	0.27	1.42	1.75	1.78	1.83
R_{Biomass}	0.20	0.40	0.53	0.63	0.62