

Supplementary Table 3. Absolute metabolite concentrations that were constrained by thermodynamics.

Metabolite[compartment] \ Concentration(M)	BIGG ID	KEGG ID	Brenda ID	Mammalian	IBMK	L.B.	U.B.	Yeast	L.B.	U.B.	<i>E. coli</i>	L.B.	U.B.
1,3-bisphosphoglycerate[c]*	13dpg[c]	C00236	18032	2.24E-6	-	6.77E-7	3.28E-6	4.91E-6	3.26E-7	6.47E-5	1.65E-5	1.07E-5	2.97E-5
2-phosphoglycerate[c]**	2pg[c]	C00631	17976	9.49E-6	-	1.37E-6	9.18E-5	2.38E-5	4.39E-6	1.60E-4	9.18E-5	3.81E-5	3.22E-4
carbon dioxide[c]**	co2[c]	C00011	28651	7.63E-3	-	6.37E-3	9.55E-3	8.16E-5	6.01E-5	9.01E-5	7.52E-5	5.02E-5	7.54E-5
carbon dioxide[m]**	co2[m]	C00011	28651	6.53E-3	-	6.37E-3	9.55E-3	7.71E-5	6.01E-5	9.01E-5	-	-	-
coenzyme-A[m]**	coa[m]	C00010	11741	4.04E-3	-	4.00E-3	6.00E-3	4.90E-3	4.00E-3	6.00E-3	-	-	-
dihydroxyacetonephosphate [directly measured]	dhap	C00111	89172	-	-	-	-	8.07E-4	7.01E-4	9.13E-4	3.06E-3	2.90E-3	3.22E-3
dihydroxyacetonephosphate[c]*	dhap[c]	C00111	89172	1.63E-3	-	1.47E-3	1.75E-3	8.23E-4	7.46E-4	9.10E-4	-	-	-
erythrose-4-phosphate[c]*	e4p[c]	C00279	59851	1.03E-5	-	7.54E-6	1.58E-5	1.46E-5	6.92E-6	1.95E-5	4.90E-5	4.19E-5	5.64E-5
fructose-6-phosphate[c]*	f6p[c]	C00085	56501	9.69E-5	-	8.18E-5	1.27E-4	2.37E-3	1.53E-3	2.92E-3	2.52E-3	2.16E-3	2.89E-3
fumarate [directly measured]	fum	C00122	19266	3.87E-4	-	2.83E-4	4.90E-4	1.21E-4	8.05E-5	1.61E-4	1.15E-4	3.00E-6	4.42E-3
fumarate[c]	fum[c]	C00122	19266	-	-	-	-	-	-	-	2.88E-4	2.85E-4	2.93E-4
fumarate[m]*	fum[m]	C00122	19266	-	-	-	-	1.24E-4	8.88E-5	1.54E-4	-	-	-
glucose-6-phosphate[c]*	g6p[c]	C00092	22626	6.75E-4	-	6.74E-4	1.05E-3	5.31E-3	4.36E-3	6.18E-3	7.88E-3	7.59E-3	8.17E-3
glyceraldehyde-3-phosphate[c]*	g3p[c]	C00661	59	1.41E-4	-	1.28E-4	1.52E-4	1.18E-4	1.07E-4	1.30E-4	2.71E-4	2.56E-4	2.89E-4
isocitrate[c]*	icit[c]	C00311	23698	-	-	-	-	-	-	-	3.67E-5	4.68E-6	4.29E-5
isocitrate[m]*	icit[m]	C00311	23698	3.21E-5	-	2.10E-5	3.38E-5	5.79E-6	1.90E-6	9.79E-6	-	-	-
oxaloacetate[c]*	oaa[c]	C00036	19271	-	-	-	-	-	-	-	4.87E-7	2.81E-7	8.55E-7
oxaloacetate[m]*	oaa[m]	C00036	19271	2.01E-6	-	1.18E-6	3.31E-6	5.01E-7	1.32E-7	9.86E-7	-	-	-
phosphate [orthophosphate][c]**	pi[c]	C00009	92038	5.83E-3	-	4.00E-3	6.00E-3	4.93E-2	4.00E-2	6.00E-2	2.39E-2	1.60E-2	2.40E-2
ribose-5-phosphate [directly measured]	r5p	C00117	34575	7.83E-5	-	2.84E-5	1.28E-4	1.52E-4	1.14E-4	1.90E-4	-	-	-
ribose-5-phosphate[c]*	r5p[c]	C00117	34575	2.84E-5	-	2.84E-5	4.01E-5	-	-	-	7.87E-4	7.86E-4	8.36E-4
ribulose-5-phosphate[c]*	ru5p-D[c]	C00199	20587	5.27E-6	-	4.10E-6	5.85E-6	1.22E-4	7.73E-5	1.95E-4	1.12E-4	1.12E-4	1.27E-4
sedoheptulose-7-phosphate [directly measured]	s7p	C05382	24563	1.51E-5	-	1.21E-5	1.81E-5	3.61E-4	3.29E-4	3.92E-4	8.82E-4	8.40E-4	9.24E-4
sedoheptulose-7-phosphate[c]*	s7p[c]	C05382	24563	1.81E-5	-	1.28E-5	1.81E-5	-	-	-	-	-	-
succinyl-CoA [directly measured]	succoa	C00091	55439	-	-	-	-	-	-	-	2.33E-4	1.42E-4	3.83E-4
succinyl-CoA[m]*	succoa[m]	C00091	55439	6.80E-6	-	3.49E-7	3.16E-3	-	-	-	-	-	-
xylulose-5-phosphate [directly measured]	xu5p-D	C00231	29847	3.15E-5	-	2.33E-5	3.95E-5	-	-	-	-	-	-
xylulose-5-phosphate[c]*	xu5p-D[c]	C00231	29847	2.99E-5	-	2.34E-5	3.31E-5	2.46E-4	1.59E-4	3.93E-4	1.81E-4	1.80E-4	2.03E-4

* Concentrations satisfy directly measured 95% confidence intervals of both ΔG and concentrations. [c] and [m] denote values consistent with reaction free energies in cytosol and mitochondria, respectively.

** CO2 concentration was calculated using Henry's law at the respective culture conditions. Coenzyme A and phosphate concentrations were taken from literature.