

Web Supplements

Table S1. Concentrations of Substances.

Abbreviation	Metabolite name	Initial concentration (M)	Concentration after 100,000 sec in the zone model (M)	Reference/Notes
Substances in Cytoplasm				
SAM	<i>S</i> -adenosyl methionine	4.600E-05	Fix	[8]
AKG	α -ketoglutarate	2.000E-03	Fix	[8]
AMP	AMP	2.180E-04	Fix	[8]
Arg	Arginine	5.000E-05	4.997E-05	[8]
ASA	Arginosuccinate	3.400E-05	3.398E-05	[8]
Asp	Aspartate	1.200E-03	1.199E-03	[8]
Cit	Citrulline	8.500E-05	8.496E-05	[8]
Cre	Creatine	1.000E-03	8.518E-01 (*1)	[8]
Fum	Fumarate	1.000E-03	Fix	[8]
Gln	Glutamine	2.960E-03	2.960E-03	[10]
Glu	Glutamate	1.060E-02	1.059E-02	[8]
Gly	Glycine	6.000E-03	6.000E-03	Assumed
GAA	Guanidinoacetate	1.400E-05	1.398E-05	Assumed
His	Histidine	4.100E-04	Fix	[10]

ATP	MgATP	4.540E-03	Fix	[8]
Na ⁺	Sodium	3.420E-02	Fix	[10]
NH ₄ ⁺	Ammonia	8.900E-05	8.901E-05	Assumed (*2)
OAc	Oxaloacetate	1.500E-05	Fix	[8]
Orn	Ornithine	5.100E-04	5.101E-04	[8]
Pi	Inorganic phosphate	7.400E-03	Fix	[8]
Trp	Tryptophan	2.000E-04	Fix	[10]
urea	Urea	6.000E-03	6.000E-03	[8]

Substances in Mitochondria

AcCoA	Acetyl coenzyme A	2.400E-04	Fix	[8]
NAG	<i>N</i> -acetyl glutamate	6.800E-04	6.798E-04	[8]
	α -Ketoglutarate	3.100E-04	3.100E-04	[8]
	AMP	2.600E-03	Fix	[8]
	Arginine	5.000E-05	4.997E-05	[8]
	Aspartate	4.000E-04	3.999E-04	[8]
	Citrulline	1.500E-04	1.500E-04	[8]
CoA	Coenzyme A	3.800E-04	3.799E-04	[8]
CP	Carbamoylphosphate	8.500E-05	8.497E-05	[8]
	Glutamine	2.000E-02	2.000E-02	[10]
	Glutamate	2.570E-03	2.569E-03	[8]
HCO ₃ ⁻	Bicarbonate	7.000E-03	Fix	[8]
Mg ²⁺	Magnesium ion	8.300E-04	Fix	Assumed (*3)

	MgATP	1.800E-03	Fix	[8]
NAD ⁺	NAD ⁺	1.580E-03	Fix	[8]
NADH	NADH	3.600E-04	Fix	[8]
	Ammonia	8.900E-05	8.900E-05	[8]
OAA	Oxaloacetate	7.000E-05	Fix	[8]
	Ornithine	4.200E-04	4.200E-04	[8]
	Inorganic phosphate	4.100E-03	4.100E-03	[8]
P5C	Pyrroline-5-carboxylate	2.000E-05	Fix	[8]
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Substances in Sinusoid				
	Glutamine	5.000E-04	Fix (*4)	[10]
	Glutamate	1.600E-04	Fix (*4)	Assumed
	Histidine	1.250E-04	Fix	[10]
	Sodium	1.435E-01	Fix	[10]
	Ammonia	2.000E-04	Fix (*4)	Assumed
	Tryptophan	2.500E-04	Fix	[10]
	Urea	6.000E-03	6.660E-01 (*1)	Assumed (*5)

All metabolites exhibited quasi steady-state: the volatilities of metabolites concentrations in the model were within 0.17% after 100,000 seconds of simulation except the end products in the model, *i.e.* creatine in the cytoplasm and urea in sinusoid (*1). “Fix” means fixed values in the model.

*2 Assumed same as the ammonia concentration in cytoplasm.

*3 Assumed same as the K_m for carbamoylphosphate synthetase.

*4 Glutamine, glutamate and ammonia in sinusoid were fixed in the one compartment model, but not fixed in the lobule model with multi compartments.

*5 Assumed same as the urea concentrations in cytoplasm.