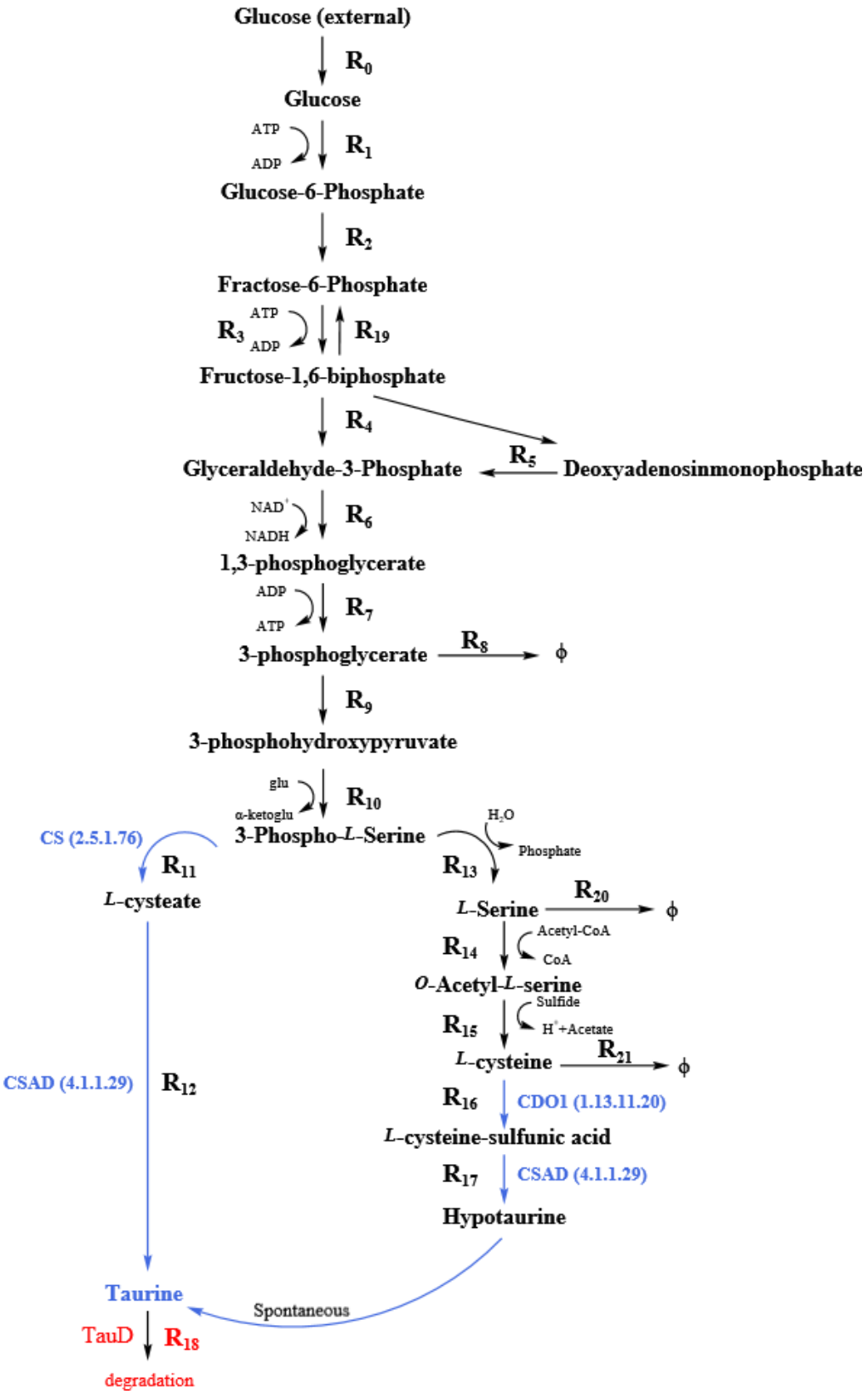
Supplementary Information of Model 1


Glucose (external)
R0
Glucose
ATP
ADP
R1
Glucose-6-Phosphate
R2
Fractose-6-Phosphate
R3
ATP
ADP
R19
Fructose-1,6-biphosphate
R4
R5
Glyceraldehyde-3-Phosphate
Deoxyadenosinmonophosphate
NAD+
NADH
R6
1,3-phosphoglycerate
ADP
ATP
R7
3-phosphoglycerate
R8
ϕ
R9
3-phosphohydroxypyruvate
glu
α-ketoglu
R10
3-Phospho-L-Serine
H2O
Phosphate
CS (2.5.1.76)
R11
L-cysteate
R13
L-Serine
R20
ϕ
Acetyl-CoA
CoA
R14
O-Acetyl-L-serine
Sulfide
H+Acetate
R15
L-cysteine
R21
ϕ
CSAD (4.1.1.29)
R12
R16
CDO1 (1.13.11.20)
L-cysteine-sulfunic acid
R17
CSAD (4.1.1.29)
Hypotaurine
Taurine
Spontaneous
TauD
R18
degradation

Supplementary Table S1: Differential equations of the kinetic model

Equations
$\frac{dC_{Glu}}{dt} = -r_1$
$\frac{dC_{G6P}}{dt} = r_1 - r_2$
$\frac{dC_{F6P}}{dt} = r_2 - r_3 + r_{19}$
$\frac{dC_{FBP}}{dt} = r_3 - r_{19} - r_4$
$\frac{dC_{DHAP}}{dt} = r_4 - r_5$
$\frac{dC_{GAP}}{dt} = r_4 + r_5 - r_6$
$\frac{dC_{PGP}}{dt} = r_6 - r_7$
$\frac{dC_{3PG}}{dt} = r_7 - r_8 - r_9$
$\frac{dC_{PHP}}{dt} = r_9 - r_{10}$
$\frac{dC_{PSer}}{dt} = r_{10} - r_{11} - r_{13}$
$\frac{dC_{Ser}}{dt} = r_{13} - r_{14} - r_{20}$
$\frac{dC_{OAS}}{dt} = r_{14} - r_{15}$
$\frac{dC_{Cys}}{dt} = r_{15} - r_{16} - r_{21}$
$\frac{dC_{Cystate}}{dt} = r_{11} - r_{12}$
$\frac{dC_{CSD}}{dt} = r_{16} - r_{17}$
$\frac{dC_{Taurine}}{dt} = r_{12} + r_{17} - r_{18}\ (optional)$

The C represents the concentration (mM) of each metabolite shown as subscript. The *r* represents the rate (mmol/mg/min) of each reaction shown as subscript.

Supplementary Table S2: Rate equations of the kinetic model

Reaction	Rate equation	Reference
PTS (R1)	$r_{\mathrm{PTS}} = \frac{V_{\mathrm{max\_PTS}} \cdot C_{GLC}^{extracellular} \cdot \frac{C_{PEP}}{C_{PYR}}}{\left(K_{\mathrm{m\_PTS}\_a1} + K_{\mathrm{m\_PTS}\_a2} \cdot \frac{C_{PEP}}{C_{PYR}} + K_{\mathrm{m\_PTS}\_a3} \cdot C_{GLC}^{extracellular} + C_{GLC}^{extracellular} \cdot \frac{C_{PEP}}{C_{PYR}}\right) \cdot \left(1 + \frac{C_{G6P}^{n_{PTS}}}{K_{\mathrm{m\_PTS}\_G6P}}\right)}$	[1]
PGI (R2)	$r_{\mathrm{PGI}} = \frac{V_{\mathrm{max\_PGI}} \cdot \left(C_{G6P} - \frac{C_{F6P}}{K_{\mathrm{eq\_PGI}}}\right)}{K_{\mathrm{m\_PGI}\_G6P} \cdot \left(1 + \frac{C_{F6P}}{K_{\mathrm{m\_PGI}\_F6P} \cdot \left(1 + \frac{C_{6PG}}{K_{\mathrm{m\_PGI\_F6P\_6PGinh}}}\right)} + \frac{C_{6PG}}{K_{\mathrm{m\_PGI\_G6P\_6PGinh}}}\right) + C_{G6P}}$	[1]
PFK (R3)	$r_{\mathrm{PFK}} = \frac{V_{\mathrm{max\_PFK}} \cdot {C_{F6P}}^{n_{\mathrm{PFK}}} \cdot C_{ATP}}{\left({K_{\mathrm{m\_PFK}\_F6P}}^{n_{\mathrm{PFK}}} + {C_{F6P}}^{n_{\mathrm{PFK}}}\right) \cdot \left(K_{\mathrm{m\_PFK}\_ATP} + C_{ATP}\right)}$	[2]
FBA (R4)	$r_{\mathrm{FBA}} = \frac{V_{\mathrm{max\_FBA}} \cdot \left(C_{FBP} - \frac{C_{GAP} \cdot C_{DHAP}}{K_{\mathrm{eq\_FBA}}}\right)}{K_{\mathrm{m\_FBA}\_FBP} + C_{FBP} + \frac{K_{\mathrm{m\_FBA}\_GAP} \cdot C_{DHAP}}{K_{\mathrm{eq\_FBA}} \cdot V_{blf}} + \frac{K_{\mathrm{m\_FBA}\_DHAP} \cdot C_{GAP}}{K_{\mathrm{eq\_FBA}} \cdot V_{blf}} + \frac{C_{FBP} \cdot C_{GAP}}{K_{\mathrm{m\_FBA}\_GAP\_inh}} + \frac{C_{DHAP} \cdot C_{GAP}}{K_{\mathrm{eq\_FBA}} \cdot V_{blf}}}$	[1,2]

Supplementary Table S2: ***Continued***

TPI (R5)	$$r_{\mathrm{TPI}} = \frac{V_{\mathrm{max\_TPI}} \cdot \left(C_{DHAP} - \frac{C_{GAP}}{K_{\mathrm{eq\_TPI}}}\right)}{K_{\mathrm{m\_TPI}\_DHAP} \cdot \left(1 + \frac{C_{GAP}}{K_{\mathrm{m\_TPI}\_GAP}}\right) + C_{DHAP}}$$	[1,2]
GAPDH (R6)	$$r_{\mathrm{GAPDH}} = \frac{V_{\mathrm{max\_GAPDH}} \cdot \left(C_{GAP} \cdot C_{NAD} - \frac{C_{PGP} \cdot C_{NADH}}{K_{\mathrm{eq\_GAPDH}}}\right)}{\left(K_{\mathrm{m\_GAPDH}\_GAP} \cdot \left(1 + \frac{C_{PGP}}{K_{\mathrm{m\_GAPDH}\_PGP}}\right) + C_{GAP}\right) \cdot \left(K_{\mathrm{m\_GAPDH}\_NAD} \cdot \left(1 + \frac{C_{NADH}}{K_{\mathrm{m\_GAPDH}\_NADH}}\right) + C_{NAD}\right)}$$	[1,2]
PGK (R7)	$$r_{\mathrm{PGK}} = \frac{V_{\mathrm{max\_PGK}} \cdot \left(C_{ADP} \cdot C_{DGP} - \frac{C_{ATP} \cdot C_{3PG}}{K_{\mathrm{eq\_PGK}}}\right)}{\left(K_{\mathrm{m\_PGK}\_ADP} \cdot \left(1 + \frac{C_{ATP}}{K_{\mathrm{m\_PGK}\_ATP}}\right) + C_{ADP}\right) \cdot \left(K_{\mathrm{m\_PGK}\_DGP} \cdot \left(1 + \frac{C_{3PG}}{K_{\mathrm{m\_PGK}\_3PG}}\right) + C_{DGP}\right)}$$	[1,2]

Supplementary Table S2: ***Continued***

Reaction	Rate equation and its parameters	Reference
PGDH (R9)	$r_{PGDH} = \frac{k_{cat\_PGDH} \cdot E_{t\_PGDH} \cdot \frac{C_{3PG}}{K_{m\_PGDH\_3PG}}}{\left(1 + \frac{C_{Ser}}{K_{i\_PGDH\_ser}}\right) \cdot \left(1 + \frac{C_{3PG}}{K_{m\_PGDH\_3PG}} + \frac{C_{PHP}}{K_{m\_PGDH\_PHP}}\right)}$	[3]
PSAT (R10)	$r_{PSAT} = \frac{k_{cat\_PSAT} \cdot E_{t\_PSAT} \cdot \frac{C_{PHP}}{K_{m\_PSAT\_PHP}}}{\left(1 + \frac{C_{PSER}}{K_{m\_PSAT\_PSER}} + \frac{C_{PHP}}{K_{m\_PSAT\_PHP}}\right)}$	[3]
CS (R11)	$r_{\mathrm{CS}} = \frac{V_{\mathrm{max\_CS}} \cdot C_{PSER}}{K_{\mathrm{m\_CS}\_PSER} + C_{PSER}}$	M-M equation
CSAD_1 (R12)	$r_{\mathrm{CSAD\_1}} = \frac{V_{\mathrm{max\_CSAD\_1}} \cdot C_{cystate}}{K_{\mathrm{m\_CSAD}\_cystate} \cdot \left(1 + \frac{C_{CSA}}{K_{i\_CSAD\_CSA}}\right) + C_{cystate}}$	M-M equation

Supplementary Table S2: ***Continued***

PSP (R13)	$$r_{PSP} = \frac{k_{cat\_PSP} \cdot E_{t\_PSP} \cdot \frac{C_{PSer}}{K_{m\_PSP\_PSer}}}{\left(1 + \frac{C_{PSer}}{K_{m\_PSP\_PSer}} + \frac{C_{Ser}}{K_{m\_PSP\_Ser}}\right)}$$	[3]
SAT (R14)	$$r_{\mathrm{SAT}} = \frac{V_{\mathrm{max\_SAT}} \cdot C_{Ser} \cdot C_{AcCoA}}{K_{\mathrm{m\_SAT}\_AcCoA} \cdot C_{Ser} \cdot \left(1 + \frac{C_{Cys}}{K_{i\_SAT\_Cys1}}\right) + K_{\mathrm{m\_SAT}\_Ser} \cdot C_{AcCoA} \cdot \left(1 + \frac{C_{Cys}}{K_{i\_SAT\_Cys2}}\right) + C_{Ser} \cdot C_{AcCoA}}$$	[4]
OASS (R15)	$$r_{\mathrm{OASS}} = \frac{V_{\mathrm{max\_OASS}} \cdot C_{OAS}}{K_{\mathrm{m\_OASS}\_OAS} \cdot \left(1 + \frac{C_{Cys}}{K_{i\_OASS\_Cys}} + \frac{K_{i\_OASS\_sulfide} \cdot C_{Cys}}{K_{i\_OASS\_Cys} \cdot C_{sulfide}}\right) + C_{OAS} \cdot \left(1 + \frac{K_{\mathrm{m\_OASS}\_sulfide}}{C_{sulfide}}\right)}$$	[4]
CDO1 (R16)	$$r_{\mathrm{CDO1}} = \frac{V_{\mathrm{max\_CDO1}} \cdot C_{Cys}}{K_{\mathrm{m\_CDO1}\_Cys} + C_{Cys}}$$	M-M equation
CSAD_2 (R17)	$$r_{\mathrm{CSAD\_2}} = \frac{V_{\mathrm{max\_CSAD\_2}} \cdot C_{CSA}}{K_{\mathrm{m\_CSAD}\_CSA} \cdot \left(1 + \frac{C_{cystate}}{K_{i\_CSAD\_cystate}}\right) + C_{CSA}}$$	M-M equation

Supplementary Table S2: ***Continued***

Reaction	Rate equation and its parameters	Reference
FBPase (R19)	$r_{\mathrm{FBPase}} = \dfrac{V_{\mathrm{max\_FBPase}} \cdot \dfrac{C_{FBP}}{K_{\mathrm{m\_FBPase}\_FBP}} \cdot \left(1 + \dfrac{C_{FBP}}{K_{\mathrm{m\_FBPase}\_FBP}}\right)^{n_{\mathrm{FBPase}}-1}}{\left(1 + \dfrac{C_{FBP}}{K_{\mathrm{m\_FBPase}\_FBP}}\right)^{n_{\mathrm{FBPase}}} + \dfrac{L_{\mathrm{FBPase}}}{\left(1 + \dfrac{C_{PEP}}{K_{\mathrm{m\_FBPase}\_PEP}}\right)^{n_{\mathrm{FBPase}}}}}$	2
Taurine Dioxygenase (R18)	$r_{TauD} = \dfrac{V_{\mathrm{max\_TauD}} \cdot C_{Tau}}{K_{\mathrm{m\_TauD}} + C_{Tau}}$	5
R8	$r_8 = 4 \cdot r_{PGDH}$	Estimate
R20	$r_{20} = \dfrac{1}{2} \cdot r_{SAT}$	Estimate
R21	$r_{21} = r_{\mathrm{CDO1}}$	Estimate

Supplementary Table S3: Parameters of the Rate equations

Reaction	Equation	Parameter	Value	Unit	Source
PTS	Glu→G6P	$K_{m\_PTS\_a1}$	3082.3	mM	[1]
		$K_{m\_PTS\_a2}$	0.01	mM	[1]
		$K_{m\_PTS\_a3}$	245.3		[1]
		$K_{m\_PTS\_G6P}$	2.15	mM	[1]
		n_{PTS}	3.66	1	[1]
		V_{max_PTS}	60000	mM /h	Estimated
		$C_{GLC}^{extracellular}$	optional	mM	
		C_{PEP}	2.67	mM	[1]
		C_{PYR}	2.67	mM	[1]
		C_{G6P}	0 / 3.48 *	mM	[1]
PGI	G6P→F6P	K_{eq_PGI}	0.1725	1	[1]
		$K_{m\_PGI\_G6P}$	2.9	mM	[1]
		$K_{m\_PGI\_F6P}$	0.266	mM	[1]
		$K_{m\_PGI\_F6P\_6PGinh}$	0.2	mM	[1]
		$K_{m\_PGI\_G6P\_6PGinh}$	0.2	mM	[1]
		V_{max_PGI}	8352	mM /h	[6]
		C_{G6P}	0 / 3.48 *	mM	[1]
		C_{F6P}	0 / 0.60 *	mM	[1]
		C_{6PG}	0.808	mM	[1]
PFK	F6P→FBP	$K_{m\_PFK\_F6P}$	0.13	mM	[2]
		$K_{m\_PFK\_ATP}$	0.12	mM	[2]
		n_{PFK}	3.0	1	[2]
		V_{max_PFK}	666	mM /h	[6]
		C_{F6P}	0 / 0.60 *	mM	[1]
		C_{ATP}	4.27	mM	[1]

*: initial concentration/ steady-state concentration in physiological state

Supplementary Table S3: Continued

Reaction	Equation	Parameter	Value	Unit	Source
FBA	FBP→GAP+DHAP	$K_{\text{eq\_FBA}}$	0.144	1	[1,2]
		$K_{\text{m\_FBA\_}FBP}$	0.133	mM	[1,2]
		$K_{\text{m\_FBA\_}GAP}$	0.088	mM	[1,2]
		$K_{\text{m\_FBA\_}DHAP}$	0.088	mM	[1,2]
		$K_{\text{m\_FBA\_}GAP\_inh}$	0.6	mM	[1,2]
		V_{blf}	2	1	[1,2]
		$V_{\text{max\_FBA}}$	7728	mM/h	[2]
		C_{FBP}	0 / 0.272 *	mM	[1]
		C_{GAP}	0 / 0.218 *	mM	[1]
		C_{DHAP}	0 / 0.167 *	mM	[1]
TPI	DHAP→GAP	$K_{\text{eq\_TPI}}$	1.39	1	[1,2]
		$K_{\text{m\_TPI\_}DHAP}$	2.8	mM	[1,2]
		$K_{\text{m\_TPI\_}GAP}$	0.3	mM	[1,2]
		$V_{\text{max\_TPI}}$	1680	mM/h	[6]
		C_{DHAP}	0 / 0.167 *	mM	[1]
		C_{GAP}	0 / 0.218 *	mM	[1]
GAPDH	GAP→PGP	$K_{\text{eq\_GAPDH}}$	0.63	1	[1,2]
		$K_{\text{m\_GAPDH\_}GAP}$	0.683	mM	[1,2]
		$K_{\text{m\_GAPDH\_}PGP}$	$1.04 * 10^{-5}$	mM	[1,2]
		$K_{\text{m\_GAPDH\_}NAD}$	0.252	mM	[1,2]
		$K_{\text{m\_GAPDH\_}NADH}$	1.09	mM	[1,2]
		$V_{\text{max\_GAPDH}}$	31212	mM/h	[6]
		C_{GAP}	0 / 0.218 *	mM	[1]
		C_{NAD}	1.47	mM	[1]
		C_{PGP}	0 / 0.008 *	mM	[1]
		C_{NADH}	0.1	mM	[1]

Supplementary Table S3: Continued

Reaction	Equation	Parameter	Value	Unit	Source
PGK	PGP→3PG	$K_{\text{eq\_PGK}}$	1934.4	1	[1,2]
		$K_{\text{m\_PGK\_}ADP}$	0.185	mM	[1,2]
		$K_{\text{m\_PGK\_}ATP}$	0.653	mM	[1,2]
		$K_{\text{m\_PGK\_}DGP}$	0.0468	mM	[1,2]
		$K_{\text{m\_PGK\_}3PG}$	0.473	mM	[1,2]
		$V_{\text{max\_PGK}}$	57960	mM/h	[6]
		C_{ADP}	0.595	mM	[1]
		C_{DGP}	0 / 0.008 *	mM	[1]
		C_{ATP}	4.27	mM	[1]
		C_{3PG}	0 / 2.13 *	mM	[1]
PGM	3PG→2PG	$K_{\text{eq\_PGM}}$	0.188	1	[1,2]
		$K_{\text{m\_PGM\_}3PG}$	0.2	mM	[1,2]
		$K_{\text{m\_PGM\_}2PG}$	0.369	mM	[1,2]
		$V_{\text{max\_PGM}}$	39600	mM/h	[6]
		C_{3PG}	0 / 2.13 *	mM	[1]
		C_{2PG}	0.399	mM	[1]
PGDH	3PG→PHP	k_{cat_PGDH}	1980	$1/h$	[3]
		E_{t_PGDH}	1.15	mM	[3]
		$K_{m\_PGDH\_3PG}$	1.2	mM	[3]
		$K_{i\_PGDH\_Ser}$	0.0038	mM	[3]
		$K_{m\_PGDH\_PHP}$	0.0032	mM	[3]
		C_{3PG}	0 / 2.13 *	mM	[1]
		C_{Ser}	0 / 4.9 *	mM	[3]
		C_{PHP}	0 / 0.6 *	mM	[3]
PSAT	PHP→PSer	k_{cat_PSAT}	6300	$1/h$	[3]
		E_{t_PSAT}	0.1	mM	[3]
		$K_{m\_PSAT\_PHP}$	0.0015	mM	[3]
		$K_{m\_PSAT\_PSER}$	0.0017	mM	[3]
		C_{PHP}	0 / 0.6 *	mM	[3]
		C_{PSer}	0 / 0.09 *	mM	[3]
CS	PSer→cystate	$K_{\text{m\_CS\_}PSER}$	6.2	mM	Estimated
		$V_{\text{max\_CS}}$	6.144	mM/h	Estimated
		C_{PSer}	0/ 0.09 *	mM	[3]

Supplementary Table S3: Continued

Reaction	Equation	Parameter	Value	Unit	Source
CSAD_1	Cystate→Tau	$K_{\mathrm{m\_CSAD\_}cystate}$	11.2	mM	Estimated
		$K_{i\_CSAD\_CSA}$	3.6	mM	Estimated
		$V_{\mathrm{max\_CSAD\_1}}$	14.94	mM/h	Estimated
		$C_{cystate}$	0	mM	
		C_{CSA}	0	mM	
PSP	PSer→Ser	k_{cat_PSP}	5148	$1/h$	[3]
		E_{t_PSP}	0.25	mM	[3]
		$K_{m\_PSP\_PSer}$	0.0015	mM	[3]
		$K_{m\_PSP\_Ser}$	0.15	mM	[3]
		C_{PSer}	0 / 0.09 *	mM	[3]
		C_{Ser}	0 / 4.9 *	mM	[3]
SAT	Ser→OAS	$K_{\mathrm{m\_SAT\_}AcCoA}$	0.58	mM	[4]
		$K_{i\_SAT\_Cys1}$	0.85	mM	[4]
		$K_{\mathrm{m\_SAT\_}Ser}$	1.9	mM	[4]
		$K_{i\_SAT\_Cys2}$	1.5	mM	[4]
		$V_{\mathrm{max\_SAT}}$	72.2	mM/h	Estimated
		C_{Ser}	0 / 4.9 *	mM	[3]
		C_{AcCoA}	0.61	mM	[7]
		C_{Cys}	0 / 1.7 *	mM	Estimated
OASS	OAS→Cys	$K_{\mathrm{m\_OASS\_}OAS}$	4.8	mM	[4]
		$K_{i\_OASS\_Cys}$	8.6	mM	[4]
		$K_{i\_OASS\_sulfide}$	0.011	mM	[4]
		$K_{\mathrm{m\_OASS\_}sulfide}$	0.006	mM	[4]
		$V_{\mathrm{max\_OASS}}$	8660	mM/h	[6]
		C_{OAS}	0 / 7 *	mM	[8]
		C_{Cys}	0 / 1.7 *	mM	Estimated
		$C_{sulfide}$	0.005	mM	[9]
CDO1	Cys→CSD	$K_{\mathrm{m\_CDO1\_}Cys}$	13.6	mM	Estimated
		$V_{\mathrm{max\_CDO1}}$	20.28	mM/h	Estimated
		$V_{\mathrm{max\_CDO1}}$	20.28	mM/h	Estimated
		C_{Cys}	0 / 1.7 *	mM	Estimated

Supplementary Table S3: Continued

Reaction	Equation	Parameter	Value	Unit	Source
CSAD_2	CSD→hypoTau	$K_{\mathrm{m\_CSAD\_}CSA}$	3.6	mM	Estimated
		$K_{i\_CSAD\_cystate}$	11.2	mM	Estimated
		$V_{\mathrm{max\_CSAD\_2}}$	30.42	mM/h	Estimated
		C_{CSA}	0	mM	
FBPase	FBP→F6P	$K_{\mathrm{m\_\_FBPase\_}FBP}$	0.00892	mM	[2]
		n_{FBPase}	4	1	[2]
		L_{FBPase}	4000000	1	[2]
		$K_{\mathrm{m\_FBPase\_}PEP}$	0.49	mM	[2]
		$V_{\mathrm{max\_FBPase}}$	777.6	mM/h	[6]
		C_{FBP}	0 / 0.272 *	mM	[1]
		C_{PEP}	2.67	mM	[1]
Taurine Dioxygenase		$V_{\mathrm{max\_TauD}}$	2.61	mM/h	Estimated
		$K_{\mathrm{m\_TauD}}$	0.058	mM	[10]

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