SBML Model Report

Model name: “Machado2014 - Curcumin production pathway in Escherichia coli”

January 16, 2015

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Daniel Machado[1] and Vijayalakshmi Chelliah[2] at January twelveth 2015 at 12:35 a. m. and last time modified at January twelveth 2015 at 2:14 p. m. Table 1 gives an overview of the quantities of all components of this model.

Table 1: Number of components in this model, which are described in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	2
species types	0	species	26
events	0	constraints	0
reactions	64	function definitions	0
global parameters	8	unit definitions	5
rules	0	initial assignments	0

Model Notes

Machado2014 - Curcumin production pathway inEscherichia coli

This model is described in the article:A kinetic model for curcumin production in Escherichia coli.Machado D, Rodrigues LR, Rocha I.BioSystems 2014 Nov; 125: 16-21

Abstract:

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Curcumin is a natural compound obtained from turmeric, and is well known for its pharmacological effects. In this work, we design a heterologous pathway for industrial production of curcumin in Escherichia coli. A kinetic model of the pathway is then developed and connected to a kinetic model of the central carbon metabolism of E. coli. This model is used for optimization of the mutant strain through a rational design approach, and two manipulation targets are identified for overexpression. Dynamic simulations are then performed to compare the curcumin production profiles of the different mutant strains. Our results show that it is possible to obtain a significant improvement in the curcumin production rates with the proposed mutants. The kinetic model here developed can be an important framework to optimize curcumin production at an industrial scale and add value to its biomedical potential.

This model is hosted on BioModels Database and identified by: BIOMD0000000565.

To cite BioModels Database, please use: BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models.

2 Unit Definitions

This is an overview of nine unit definitions of which four are predefined by SBML and not mentioned in the model.

2.1 Unit `substance`

Name millimole

Definition mmol

2.2 Unit `mM`

Name milli Molar

Definition $\mathrm{mmol} \cdot \mathrm{l}^{-1}$

2.3 Unit `second_inverse`

Name second inverse

Definition s^{-1}

2.4 Unit `mM_per_second`

Name mM per second

Definition $\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot \mathrm{s}^{-1}$

2.5 Unit per_mM_per_second

Name per mM per second

Definition $\mathrm{mmol}^{-1} \cdot \mathrm{l} \cdot \mathrm{s}^{-1}$

2.6 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

2.7 Unit area

Notes Square metre is the predefined SBML unit for area since SBML Level 2 Version 1.

Definition m^2

2.8 Unit length

Notes Metre is the predefined SBML unit for length since SBML Level 2 Version 1.

Definition m

2.9 Unit time

Notes Second is the predefined SBML unit for time.

Definition s

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
extracellular			3	65	l	☑	
cytosol			3	1	litre	☑	extracellular

3.1 Compartment extracellular

This is a three dimensional compartment with a constant size of 65 litre.

3.2 Compartment `cytosol`

This is a three dimensional compartment with a constant size of one litre, which is surrounded by `extracellular`.

4 Species

This model contains 26 species. Section 7 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
cpep	Phosphoenol pyruvate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
cglcex	Extracellular Glucose	extracellular	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
cg6p	Glucose-6-Phosphate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
cpyr	Pyruvate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
cf6p	Fructose-6-Phosphate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
cg1p	Glucose-1-Phosphate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
cpg	6-Phosphogluconate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
cfdp	Fructose-1,6-bisphosphate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
csed7p	sedoheptulose-7-phosphate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
cgap	Glyceraldehyde-3-Phosphate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ce4p	Erythrose-4-phosphate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
cxyl5p	Xylulose-5-phosphate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
crib5p	Ribose-5-phosphate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
cdhap	Dihydroxyacetonephosphate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
cpgp	1,3-diphosphosphoglycerate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
cpg3	3-Phosphoglycerate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
cpg2	2-Phosphoglycerate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
cribu5p	Ribulose-5-phosphate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
accoa		cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
malcoa		cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
fer		cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
fer_ext		extracellular	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
fercoa		cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ferdicoa		cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
cur		cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
cur_ext		extracellular	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains eight global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
catp			4.270	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
cadp			0.595	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
camp			0.955	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
cnadp			0.195	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
cnadph			0.062	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
cnad			1.470	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
cnadh			0.100	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Dil			0.000	s^{-1}	☑

6 Reactions

This model contains 64 reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 5: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	vPTS	Phosphotransferase system	$\mathrm{cglcex} + \mathrm{cpep} \xrightarrow{\mathrm{cglcex,\ cpep,\ cpyr,\ cg6p}} \mathrm{cg6p} + \mathrm{cpyr}$	
2	vPGI	Glucose-6-phosphate isomerase	$\mathrm{cg6p} \xrightleftharpoons{\mathrm{cpg,\ cg6p,\ cf6p,\ cpg}} \mathrm{cf6p}$	
3	vPGM	Phosphoglucomutase	$\mathrm{cg6p} \xrightleftharpoons{\mathrm{cg6p,\ cg1p}} \mathrm{cg1p}$	
4	vG6PDH	Glucose-6-phosphate dehydrogenase	$\mathrm{cg6p} \xrightarrow{\mathrm{cg6p}} \mathrm{cpg}$	
5	vPFK	Phosphofructokinase	$\mathrm{cf6p} \xrightarrow{\mathrm{cpep,\ cf6p,\ cpep}} \mathrm{cfdp}$	
6	vTA	Transaldolase	$\mathrm{cgap} + \mathrm{csed7p} \xrightleftharpoons{\mathrm{cgap,\ csed7p,\ ce4p,\ cf6p}} \mathrm{cf6p} + \mathrm{ce4p}$	
7	vTKA	Transketolase a	$\mathrm{crib5p} + \mathrm{cxyl5p} \xrightleftharpoons{\mathrm{crib5p,\ cxyl5p,\ csed7p,\ cgap}} \mathrm{cgap} + \mathrm{csed7p}$	
8	vTKB	Transketolase b	$\mathrm{ce4p} + \mathrm{cxyl5p} \xrightleftharpoons{\mathrm{cxyl5p,\ ce4p,\ cf6p,\ cgap}} \mathrm{cgap} + \mathrm{cf6p}$	
9	vMURSyNTH	Mureine synthesis	$2\,\mathrm{cf6p} \longrightarrow \emptyset$	
10	vALDO	Aldolase	$\mathrm{cfdp} \xrightleftharpoons{\mathrm{cfdp,\ cgap,\ cdhap}} \mathrm{cdhap} + \mathrm{cgap}$	
11	vGAPDH	Glyceraldehyde-3-phosphate dehydrogenase	$\mathrm{cgap} \xrightleftharpoons{\mathrm{cgap,\ cpgp}} \mathrm{cpgp}$	
12	vTIS	Triosephosphate isomerase	$\mathrm{cdhap} \xrightleftharpoons{\mathrm{cdhap,\ cgap}} \mathrm{cgap}$	
13	vTRPSYNTH	Tryptophan synthesis	$\emptyset \longrightarrow \mathrm{cpyr} + \mathrm{cgap}$	
14	vG3PDH	Glycerol-3-phosphate dehydrogenase	$\mathrm{cdhap} \xrightarrow{\mathrm{cdhap}} \emptyset$	

№	Id	Name	Reaction Equation	SBO
15	vPGK	Phosphoglycerate kinase	$\text{cpgp} \overset{\text{cpgp, cpg3}}{\rightleftharpoons} \text{cpg3}$	
16	vsersynth	Serine synthesis	$\text{cpg3} \overset{\text{cpg3}}{\longrightarrow} \emptyset$	
17	vrpGluMu	Phosphoglycerate mutase	$\text{cpg3} \overset{\text{cpg3, cpg2}}{\rightleftharpoons} \text{cpg2}$	
18	vENO	Enolase	$\text{cpg2} \overset{\text{cpg2, cpep}}{\rightleftharpoons} \text{cpep}$	
19	vPK	Pyruvate kinase	$\text{cpep} \overset{\text{cfdp, cpep, cfdp}}{\longrightarrow} \text{cpyr}$	
20	vpepCxylase	PEP carboxylase	$\text{cpep} \overset{\text{cfdp, cpep, cfdp}}{\longrightarrow} \emptyset$	
21	vSynth1	Synthesis 1	$\text{cpep} \overset{\text{cpep}}{\longrightarrow} \emptyset$	
22	vSynth2	Synthesis 2	$\text{cpyr} \overset{\text{cpyr}}{\longrightarrow} \emptyset$	
23	vDAHPS	DAHP synthesis	$\text{ce4p} + \text{cpep} \overset{\text{ce4p, cpep}}{\longrightarrow} \emptyset$	
24	vPDH	Pyruvate dehydrogenase	$\text{cpyr} \overset{\text{cpyr, accoa}}{\longrightarrow} \text{accoa}$	
25	vMethSynth	Methionine synthesis	$\emptyset \longrightarrow \text{cpyr}$	
26	vPGDH	6-Phosphogluconate dehydrogenase	$\text{cpg} \overset{\text{cpg}}{\longrightarrow} \text{cribu5p}$	
27	vR5PI	Ribose-phosphate isomerase	$\text{cribu5p} \overset{\text{cribu5p, crib5p}}{\rightleftharpoons} \text{crib5p}$	
28	vRu5P	Ribulose-phosphate epimerase	$\text{cribu5p} \overset{\text{cribu5p, cxyl5p}}{\rightleftharpoons} \text{cxyl5p}$	
29	vPPK	Ribose phosphate pyrophosphokinase	$\text{crib5p} \overset{\text{crib5p}}{\longrightarrow} \emptyset$	
30	vG1PAT	Glucose-1-phosphate adenyltransferase	$\text{cg1p} \overset{\text{cfdp, cg1p, cfdp}}{\longrightarrow} \emptyset$	
31	vG6P	G6P degradation	$\text{cg6p} \overset{\text{cg6p}}{\rightleftharpoons} \emptyset$	
32	vf6P	F6P degradation	$\text{cf6p} \overset{\text{cf6p}}{\rightleftharpoons} \emptyset$	
33	vfdP	FDP degradation	$\text{cfdp} \overset{\text{cfdp}}{\rightleftharpoons} \emptyset$	
34	vGAP	GAP degradation	$\text{cgap} \overset{\text{cgap}}{\rightleftharpoons} \emptyset$	

№	Id	Name	Reaction Equation	SBO
35	vDHAP	DHAP degradation	$\text{cdhap} \overset{\text{cdhap}}{\rightleftharpoons} \emptyset$	
36	vPGP	PGP degradation	$\text{cpgp} \overset{\text{cpgp}}{\rightleftharpoons} \emptyset$	
37	vPG3	PG3 degradation	$\text{cpg3} \overset{\text{cpg3}}{\rightleftharpoons} \emptyset$	
38	vpg2	PG2 degradation	$\text{cpg2} \overset{\text{cpg2}}{\rightleftharpoons} \emptyset$	
39	vPEP	PEP degradation	$\text{cpep} \overset{\text{cpep}}{\rightleftharpoons} \emptyset$	
40	vRibu5p	Ribu5P dilution	$\text{cribu5p} \overset{\text{cribu5p}}{\rightleftharpoons} \emptyset$	
41	vRIB5P	Rib5P dilution	$\text{crib5p} \overset{\text{crib5p}}{\rightleftharpoons} \emptyset$	
42	vXYL5P	XYL5P dilution	$\text{cxyl5p} \overset{\text{cxyl5p}}{\rightleftharpoons} \emptyset$	
43	vSED7P	SED7P dilution	$\text{csed7p} \overset{\text{csed7p}}{\rightleftharpoons} \emptyset$	
44	vpyr	Pyruvate dilution	$\text{cpyr} \overset{\text{cpyr}}{\rightleftharpoons} \emptyset$	
45	vPG	PG dilution	$\text{cpg} \overset{\text{cpg}}{\rightleftharpoons} \emptyset$	
46	vE4P	E4P dilution	$\text{ce4p} \overset{\text{ce4p}}{\rightleftharpoons} \emptyset$	
47	vGLP	GLP dilution	$\text{cg1p} \overset{\text{cg1p}}{\rightleftharpoons} \emptyset$	
48	vEXTER	Extracellular glucose kinetics	$\emptyset \overset{\text{cglcex}}{\longrightarrow} \text{cglcex}$	
49	ACCOAC		$\text{accoa} \overset{\text{accoa, malcoa}}{\longrightarrow} \text{malcoa}$	
50	Synth3	Synthesis 3	$\text{accoa} \overset{\text{accoa}}{\longrightarrow} \emptyset$	
51	Synth4	Synthesis 4	$\text{malcoa} \overset{\text{malcoa}}{\longrightarrow} \emptyset$	
52	R4CL		$\text{fer} \overset{\text{fer}}{\longrightarrow} \text{fercoa}$	
53	DCS		$\text{fercoa} + \text{malcoa} \overset{\text{fercoa, malcoa}}{\longrightarrow} \text{ferdicoa}$	
54	CURS		$\text{fercoa} + \text{ferdicoa} \overset{\text{fercoa, ferdicoa}}{\longrightarrow} \text{cur}$	

№	Id	Name	Reaction Equation	SBO
55	FER_t		$\text{fer\_ext} \xrightleftharpoons{\text{fer\_ext, fer}} \text{fer}$	
56	CUR_t		$\text{cur} \xrightleftharpoons{\text{cur, cur\_ext}} \text{cur\_ext}$	
57	EX_FER		$\emptyset \xrightarrow{\text{fer\_ext}} \text{fer\_ext}$	
58	EX_CUR		$\text{cur\_ext} \xrightarrow{\text{cur\_ext}} \emptyset$	
59	vACCOA	ACCOA dilution	$\text{accoa} \xrightleftharpoons{\text{accoa}} \emptyset$	
60	vMALCOA	MALCOA dilution	$\text{malcoa} \xrightleftharpoons{\text{malcoa}} \emptyset$	
61	vFER	FER dilution	$\text{fer} \xrightleftharpoons{\text{fer}} \emptyset$	
62	vFERCOA	FERCOA dilution	$\text{fercoa} \xrightleftharpoons{\text{fercoa}} \emptyset$	
63	vFERDICOA	FERDICOA dilution	$\text{ferdicoa} \xrightleftharpoons{\text{ferdicoa}} \emptyset$	
64	vCUR	CUR dilution	$\text{cur} \xrightleftharpoons{\text{cur}} \emptyset$	

6.1 Reaction vPTS

This is an irreversible reaction of two reactants forming two products influenced by four modifiers.

Name Phosphotransferase system

Reaction equation

$$\text{cglcex} + \text{cpep} \xrightarrow{\text{cglcex, cpep, cpyr, cg6p}} \text{cg6p} + \text{cpyr} \tag{1}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
cglcex	Extracellular Glucose	
cpep	Phosphoenol pyruvate	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
cglcex	Extracellular Glucose	
cpep	Phosphoenol pyruvate	
cpyr	Pyruvate	
cg6p	Glucose-6-Phosphate	

Products

Table 8: Properties of each product.

Id	Name	SBO
cg6p	Glucose-6-Phosphate	
cpyr	Pyruvate	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{\text{vol}\,(\text{extracellular}) \cdot \text{rmaxPTS} \cdot [\text{cglcex}] \cdot \frac{[\text{cpep}]}{[\text{cpyr}]}}{\left(\text{KPTSa1} + \text{KPTSa2} \cdot \frac{[\text{cpep}]}{[\text{cpyr}]} + \text{KPTSa3} \cdot [\text{cglcex}] + [\text{cglcex}] \cdot \frac{[\text{cpep}]}{[\text{cpyr}]}\right) \cdot \left(1 + \frac{[\text{cg6p}]^{\text{nPTSg6p}}}{\text{KPTSg6p}}\right)} \tag{2}$$

Table 9: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxPTS			7829.78	$\text{mmol} \cdot \text{l}^{-1} \cdot \text{s}^{-1}$	☑
KPTSa1			3082.30	$\text{mmol} \cdot \text{l}^{-1}$	☑
KPTSa2			0.01	$\text{mmol} \cdot \text{l}^{-1}$	☑
KPTSa3			245.30	dimensionless	☑
nPTSg6p			3.66	dimensionless	☑
KPTSg6p			2.15	$\text{mmol} \cdot \text{l}^{-1}$	☑

6.2 Reaction vPGI

This is a reversible reaction of one reactant forming one product influenced by four modifiers.

Name Glucose-6-phosphate isomerase

Reaction equation

$$\text{cg6p} \xrightleftharpoons{\text{cpg, cg6p, cf6p, cpg}} \text{cf6p} \tag{3}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
cg6p	Glucose-6-Phosphate	

Modifiers

Table 11: Properties of each modifier.

Id	Name	SBO
cpg	6-Phosphogluconate	
cg6p	Glucose-6-Phosphate	
cf6p	Fructose-6-Phosphate	
cpg	6-Phosphogluconate	

Product

Table 12: Properties of each product.

Id	Name	SBO
cf6p	Fructose-6-Phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{rmaxPGI} \cdot \left([\mathrm{cg6p}] - \frac{[\mathrm{cf6p}]}{\mathrm{KPGIeq}}\right)}{\mathrm{KPGIg6p} \cdot \left(1 + \frac{[\mathrm{cf6p}]}{\mathrm{KPGIf6p} \cdot \left(1 + \frac{[\mathrm{cpg}]}{\mathrm{KPGIf6ppginh}}\right)} + \frac{[\mathrm{cpg}]}{\mathrm{KPGIg6ppginh}}\right) + [\mathrm{cg6p}]} \tag{4}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxPGI			650.988	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot \mathrm{s}^{-1}$	☑
KPGIeq			0.173	dimensionless	☑
KPGIg6p			2.900	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KPGIf6p			0.266	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KPGIf6ppginh			0.200	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KPGIg6ppginh			0.200	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

6.3 Reaction vPGM

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name Phosphoglucomutase

Reaction equation

$$\mathrm{cg6p} \underset{\mathrm{cg6p,\ cg1p}}{\rightleftharpoons} \mathrm{cg1p} \tag{5}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
cg6p	Glucose-6-Phosphate	

Modifiers

Table 15: Properties of each modifier.

Id	Name	SBO
cg6p	Glucose-6-Phosphate	
cg1p	Glucose-1-Phosphate	

Product

Table 16: Properties of each product.

Id	Name	SBO
cg1p	Glucose-1-Phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \frac{\mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{rmaxPGM} \cdot \left([\mathrm{cg6p}] - \frac{[\mathrm{cg1p}]}{\mathrm{KPGMeq}}\right)}{\mathrm{KPGMg6p} \cdot \left(1 + \frac{[\mathrm{cg1p}]}{\mathrm{KPGMg1p}}\right) + [\mathrm{cg6p}]} \tag{6}$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxPGM			0.840	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot \mathrm{s}^{-1}$	☑
KPGMeq			0.196	dimensionless	☑
KPGMg6p			1.038	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KPGMg1p			0.014	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

6.4 Reaction vG6PDH

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

Name Glucose-6-phosphate dehydrogenase

Reaction equation

$$\mathrm{cg6p} \xrightarrow{\mathrm{cg6p}} \mathrm{cpg} \tag{7}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
cg6p	Glucose-6-Phosphate	

Modifier

Table 19: Properties of each modifier.

Id	Name	SBO
cg6p	Glucose-6-Phosphate	

Product

Table 20: Properties of each product.

Id	Name	SBO
cpg	6-Phosphogluconate	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \frac{\mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{rmaxG6PDH} \cdot [\mathrm{cg6p}] \cdot \mathrm{cnadp}}{([\mathrm{cg6p}] + \mathrm{KG6PDHg6p}) \cdot \left(1 + \frac{\mathrm{cnadph}}{\mathrm{KG6PDHnadphg6pinh}}\right) \cdot \left(\mathrm{KG6PDHnadp} \cdot \left(1 + \frac{\mathrm{cnadph}}{\mathrm{KG6PDHnadphnadpinh}}\right) + \mathrm{cnadp}\right)} \tag{8}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxG6PDH			1.380	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot \mathrm{s}^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
KG6PDHg6p			14.400	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KG6PDHnadphg6pinh			6.430	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KG6PDHnadp			0.025	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KG6PDHnadphnadpinh			0.010	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

6.5 Reaction vPFK

This is an irreversible reaction of one reactant forming one product influenced by three modifiers.

Name Phosphofructokinase

Reaction equation

$$\mathrm{cf6p} \xrightarrow{\mathrm{cpep,\ cf6p,\ cpep}} \mathrm{cfdp} \tag{9}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
cf6p	Fructose-6-Phosphate	

Modifiers

Table 23: Properties of each modifier.

Id	Name	SBO
cpep	Phosphoenol pyruvate	
cf6p	Fructose-6-Phosphate	
cpep	Phosphoenol pyruvate	

Product

Table 24: Properties of each product.

Id	Name	SBO
cfdp	Fructose-1,6-bisphosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \frac{\mathrm{vol}\left(\mathrm{cytosol}\right) \cdot \mathrm{rmaxPFK} \cdot \mathrm{catp} \cdot [\mathrm{cf6p}]}{\left(\mathrm{catp} + \mathrm{KPFKatps} \cdot \left(1 + \frac{\mathrm{cadp}}{\mathrm{KPFKadpc}}\right)\right) \cdot \left([\mathrm{cf6p}] + \frac{\mathrm{KPFKf6ps} \cdot \left(1 + \frac{[\mathrm{cpep}]}{\mathrm{KPFKpep}} + \frac{\mathrm{cadp}}{\mathrm{KPFKadpb}} + \frac{\mathrm{camp}}{\mathrm{KPFKampb}}\right)}{1 + \frac{\mathrm{cadp}}{\mathrm{KPFKadpa}} + \frac{\mathrm{camp}}{\mathrm{KPFKampa}}}\right) \cdot \left(1 + \frac{\cdots}{\left(1 + \frac{[\mathrm{cf6p}] \cdot \left(1 + \cdots\right.}{\mathrm{KPFKf6ps} \cdot \left(1 + \cdots\right.}\right.}\right.} \tag{10}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxPFK			1840.585	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot \mathrm{s}^{-1}$	☑
KPFKatps			0.123	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KPFKadpc			4.140	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KPFKf6ps			0.325	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KPFKpep			3.260	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KPFKadpb			3.890	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KPFKampb			3.200	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KPFKadpa			128.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KPFKampa			19.100	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
LPFK			5629067.000	dimensionless	☑
nPFK			11.100	dimensionless	☑

6.6 Reaction vTA

This is a reversible reaction of two reactants forming two products influenced by four modifiers.

Name Transaldolase

Reaction equation

$$\mathrm{cgap} + \mathrm{csed7p} \xrightleftharpoons{\mathrm{cgap,\ csed7p,\ ce4p,\ cf6p}} \mathrm{cf6p} + \mathrm{ce4p} \tag{11}$$

Reactants

Table 26: Properties of each reactant.

Id	Name	SBO
cgap	Glyceraldehyde-3-Phosphate	

Id	Name	SBO
csed7p	sedoheptulose-7-phosphate	

Modifiers

Table 27: Properties of each modifier.

Id	Name	SBO
cgap	Glyceraldehyde-3-Phosphate	
csed7p	sedoheptulose-7-phosphate	
ce4p	Erythrose-4-phosphate	
cf6p	Fructose-6-Phosphate	

Products

Table 28: Properties of each product.

Id	Name	SBO
cf6p	Fructose-6-Phosphate	
ce4p	Erythrose-4-phosphate	

Kinetic Law

Derived unit $0.0010\,\mathrm{mol}\cdot\mathrm{s}^{-1}$

$$v_6 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{rmaxTA} \cdot \left([\mathrm{cgap}] \cdot [\mathrm{csed7p}] - \frac{[\mathrm{ce4p}] \cdot [\mathrm{cf6p}]}{\mathrm{KTAeq}} \right) \tag{12}$$

Table 29: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxTA			10.872	$\mathrm{mmol}^{-1}\cdot 1\cdot \mathrm{s}^{-1}$	☑
KTAeq			1.050	dimensionless	☑

6.7 Reaction vTKA

This is a reversible reaction of two reactants forming two products influenced by four modifiers.

Name Transketolase a

Reaction equation

$$\text{crib5p} + \text{cxyl5p} \xrightleftharpoons{\text{crib5p, cxyl5p, csed7p, cgap}} \text{cgap} + \text{csed7p} \tag{13}$$

Reactants

Table 30: Properties of each reactant.

Id	Name	SBO
`crib5p`	Ribose-5-phosphate	
`cxyl5p`	Xylulose-5-phosphate	

Modifiers

Table 31: Properties of each modifier.

Id	Name	SBO
`crib5p`	Ribose-5-phosphate	
`cxyl5p`	Xylulose-5-phosphate	
`csed7p`	sedoheptulose-7-phosphate	
`cgap`	Glyceraldehyde-3-Phosphate	

Products

Table 32: Properties of each product.

Id	Name	SBO
`cgap`	Glyceraldehyde-3-Phosphate	
`csed7p`	sedoheptulose-7-phosphate	

Kinetic Law

Derived unit $0.0010\,\text{mol}\cdot\text{s}^{-1}$

$$v_7 = \text{vol}\,(\text{cytosol}) \cdot \text{rmaxTKa} \cdot \left([\text{crib5p}] \cdot [\text{cxyl5p}] - \frac{[\text{csed7p}] \cdot [\text{cgap}]}{\text{KTKaeq}} \right) \tag{14}$$

Table 33: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxTKa			9.473	$\mathrm{mmol}^{-1} \cdot 1 \cdot \mathrm{s}^{-1}$	☑
KTKaeq			1.200	dimensionless	☑

6.8 Reaction vTKB

This is a reversible reaction of two reactants forming two products influenced by four modifiers.

Name Transketolase b

Reaction equation

$$\mathrm{ce4p} + \mathrm{cxyl5p} \xrightleftharpoons{\mathrm{cxyl5p,\ ce4p,\ cf6p,\ cgap}} \mathrm{cgap} + \mathrm{cf6p} \tag{15}$$

Reactants

Table 34: Properties of each reactant.

Id	Name	SBO
ce4p	Erythrose-4-phosphate	
cxyl5p	Xylulose-5-phosphate	

Modifiers

Table 35: Properties of each modifier.

Id	Name	SBO
cxyl5p	Xylulose-5-phosphate	
ce4p	Erythrose-4-phosphate	
cf6p	Fructose-6-Phosphate	
cgap	Glyceraldehyde-3-Phosphate	

Products

Table 36: Properties of each product.

Id	Name	SBO
cgap	Glyceraldehyde-3-Phosphate	
cf6p	Fructose-6-Phosphate	

Kinetic Law

Derived unit $0.0010\,\mathrm{mol}\cdot\mathrm{s}^{-1}$

$$v_8 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{rmaxTKb} \cdot \left([\mathrm{cxyl5p}] \cdot [\mathrm{ce4p}] - \frac{[\mathrm{cf6p}] \cdot [\mathrm{cgap}]}{\mathrm{KTKbeq}} \right) \tag{16}$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`rmaxTKb`			86.559	$\mathrm{mmol}^{-1}\cdot 1\cdot \mathrm{s}^{-1}$	☑
`KTKbeq`			10.000	dimensionless	☑

6.9 Reaction `vMURSyNTH`

This is an irreversible reaction of one reactant forming no product.

Name Mureine synthesis

Reaction equation

$$2\,\mathrm{cf6p} \longrightarrow \emptyset \tag{17}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
`cf6p`	Fructose-6-Phosphate	

Kinetic Law

Derived unit $\mathrm{mmol}\cdot\mathrm{s}^{-1}$

$$v_9 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{rmaxMurSynth} \tag{18}$$

Table 39: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`rmaxMurSynth`			0.0	$\mathrm{mmol}\cdot 1^{-1}\cdot \mathrm{s}^{-1}$	☑

6.10 Reaction vALDO

This is a reversible reaction of one reactant forming two products influenced by three modifiers.

Name Aldolase

Reaction equation

$$\text{cfdp} \xrightleftharpoons{\text{cfdp, cgap, cdhap}} \text{cdhap} + \text{cgap} \tag{19}$$

Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
cfdp	Fructose-1,6-bisphosphate	

Modifiers

Table 41: Properties of each modifier.

Id	Name	SBO
cfdp	Fructose-1,6-bisphosphate	
cgap	Glyceraldehyde-3-Phosphate	
cdhap	Dihydroxyacetonephosphate	

Products

Table 42: Properties of each product.

Id	Name	SBO
cdhap	Dihydroxyacetonephosphate	
cgap	Glyceraldehyde-3-Phosphate	

Kinetic Law

Derived unit $0.0010\ \text{mol} \cdot \text{s}^{-1}$

$$v_{10} = \frac{\text{vol}\,(\text{cytosol}) \cdot \text{rmaxALDO} \cdot \left([\text{cfdp}] - \frac{[\text{cgap}] \cdot [\text{cdhap}]}{\text{kALDOeq}}\right)}{\text{kALDOfdp} + [\text{cfdp}] + \frac{\text{kALDOgap} \cdot [\text{cdhap}]}{\text{kALDOeq} \cdot \text{VALDOblf}} + \frac{\text{kALDOdhap} \cdot [\text{cgap}]}{\text{kALDOeq} \cdot \text{VALDOblf}} + \frac{[\text{cfdp}] \cdot [\text{cgap}]}{\text{kALDOgapinh}} + \frac{[\text{cgap}] \cdot [\text{cdhap}]}{\text{VALDOblf} \cdot \text{kALDOeq}}} \tag{20}$$

Table 43: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxALDO			17.415	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot \mathrm{s}^{-1}$	☑
kALDOeq			0.144	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
kALDOfdp			1.750	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
kALDOgap			0.088	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
VALDOblf			2.000	dimensionless	☑
kALDOdhap			0.088	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
kALDOgapinh			0.600	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

6.11 Reaction vGAPDH

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name Glyceraldehyde-3-phosphate dehydrogenase

Reaction equation

$$\mathrm{cgap} \xrightleftharpoons{\mathrm{cgap},\ \mathrm{cpgp}} \mathrm{cpgp} \tag{21}$$

Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
cgap	Glyceraldehyde-3-Phosphate	

Modifiers

Table 45: Properties of each modifier.

Id	Name	SBO
cgap	Glyceraldehyde-3-Phosphate	
cpgp	1,3-diphosphosphoglycerate	

Product

Table 46: Properties of each product.

Id	Name	SBO
cpgp	1,3-diphosphosphoglycerate	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \frac{\text{vol}\,(\text{cytosol}) \cdot \text{rmaxGAPDH} \cdot \left([\text{cgap}] \cdot \text{cnad} - \frac{[\text{cpgp}] \cdot \text{cnadh}}{\text{KGAPDHeq}}\right)}{\left(\text{KGAPDHgap} \cdot \left(1 + \frac{[\text{cpgp}]}{\text{KGAPDHpgp}}\right) + [\text{cgap}]\right) \cdot \left(\text{KGAPDHnad} \cdot \left(1 + \frac{\text{cnadh}}{\text{KGAPDHnadh}}\right) + \text{cnad}\right)} \tag{22}$$

Table 47: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxGAPDH			921.594	$\text{mmol} \cdot \text{l}^{-1} \cdot \text{s}^{-1}$	☑
KGAPDHeq			0.630	dimensionless	☑
KGAPDHgap			0.683	$\text{mmol} \cdot \text{l}^{-1}$	☑
KGAPDHpgp			$1.04 \cdot 10^{-5}$	$\text{mmol} \cdot \text{l}^{-1}$	☑
KGAPDHnad			0.252	$\text{mmol} \cdot \text{l}^{-1}$	☑
KGAPDHnadh			1.090	$\text{mmol} \cdot \text{l}^{-1}$	☑

6.12 Reaction vTIS

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name Triosephosphate isomerase

Reaction equation

$$\text{cdhap} \underset{\text{cdhap, cgap}}{\rightleftharpoons} \text{cgap} \tag{23}$$

Reactant

Table 48: Properties of each reactant.

Id	Name	SBO
cdhap	Dihydroxyacetonephosphate	

Modifiers

Table 49: Properties of each modifier.

Id	Name	SBO
cdhap	Dihydroxyacetonephosphate	
cgap	Glyceraldehyde-3-Phosphate	

Product

Table 50: Properties of each product.

Id	Name	SBO
cgap	Glyceraldehyde-3-Phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \frac{\mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{rmaxTIS} \cdot \left([\mathrm{cdhap}] - \frac{[\mathrm{cgap}]}{\mathrm{kTISeq}}\right)}{\mathrm{kTISdhap} \cdot \left(1 + \frac{[\mathrm{cgap}]}{\mathrm{kTISgap}}\right) + [\mathrm{cdhap}]} \tag{24}$$

Table 51: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxTIS			68.675	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot \mathrm{s}^{-1}$	☑
kTISeq			1.390	dimensionless	☑
kTISdhap			2.800	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
kTISgap			0.300	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

6.13 Reaction vTRPSYNTH

This is an irreversible reaction of no reactant forming two products.

Name Tryptophan synthesis

Reaction equation

$$\emptyset \longrightarrow \mathrm{cpyr} + \mathrm{cgap} \tag{25}$$

Products

Table 52: Properties of each product.

Id	Name	SBO
cpyr	Pyruvate	
cgap	Glyceraldehyde-3-Phosphate	

Kinetic Law

Derived unit $\text{mmol} \cdot \text{s}^{-1}$

$$v_{13} = \text{vol}(\text{cytosol}) \cdot \text{rmaxTrpSynth} \tag{26}$$

Table 53: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxTrpSynth			0.001	$\text{mmol} \cdot \text{l}^{-1} \cdot \text{s}^{-1}$	☑

6.14 Reaction vG3PDH

This is an irreversible reaction of one reactant forming no product influenced by one modifier.

Name Glycerol-3-phosphate dehydrogenase

Reaction equation

$$\text{cdhap} \xrightarrow{\text{cdhap}} \emptyset \tag{27}$$

Reactant

Table 54: Properties of each reactant.

Id	Name	SBO
cdhap	Dihydroxyacetonephosphate	

Modifier

Table 55: Properties of each modifier.

Id	Name	SBO
cdhap	Dihydroxyacetonephosphate	

Kinetic Law

Derived unit $0.0010\ \mathrm{mol} \cdot \mathrm{s}^{-1}$

$$v_{14} = \frac{\mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{rmaxG3PDH} \cdot [\mathrm{cdhap}]}{\mathrm{KG3PDHdhap} + [\mathrm{cdhap}]} \tag{28}$$

Table 56: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxG3PDH			0.012	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot \mathrm{s}^{-1}$	☑
KG3PDHdhap			1.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

6.15 Reaction vPGK

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name Phosphoglycerate kinase

Reaction equation

$$\mathrm{cpgp} \overset{\mathrm{cpgp,\ cpg3}}{\rightleftharpoons} \mathrm{cpg3} \tag{29}$$

Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
cpgp	1,3-diphosphosphoglycerate	

Modifiers

Table 58: Properties of each modifier.

Id	Name	SBO
cpgp	1,3-diphosphosphoglycerate	

Id	Name	SBO
cpg3	3-Phosphoglycerate	

Product

Table 59: Properties of each product.

Id	Name	SBO
cpg3	3-Phosphoglycerate	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \frac{\text{vol}\,(\text{cytosol}) \cdot \text{rmaxPGK} \cdot \left(\text{cadp} \cdot [\text{cpgp}] - \frac{\text{catp} \cdot [\text{cpg3}]}{\text{KPGKeq}}\right)}{\left(\text{KPGKadp} \cdot \left(1 + \frac{\text{catp}}{\text{KPGKatp}}\right) + \text{cadp}\right) \cdot \left(\text{KPGKpgp} \cdot \left(1 + \frac{[\text{cpg3}]}{\text{KPGKpg3}}\right) + [\text{cpgp}]\right)} \tag{30}$$

Table 60: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxPGK			3021.774	$\text{mmol} \cdot \text{l}^{-1} \cdot \text{s}^{-1}$	☑
KPGKeq			1934.400	dimensionless	☑
KPGKadp			0.185	$\text{mmol} \cdot \text{l}^{-1}$	☑
KPGKatp			0.653	$\text{mmol} \cdot \text{l}^{-1}$	☑
KPGKpgp			0.047	$\text{mmol} \cdot \text{l}^{-1}$	☑
KPGKpg3			0.473	$\text{mmol} \cdot \text{l}^{-1}$	☑

6.16 Reaction vsersynth

This is an irreversible reaction of one reactant forming no product influenced by one modifier.

Name Serine synthesis

Reaction equation

$$\text{cpg3} \xrightarrow{\text{cpg3}} \emptyset \tag{31}$$

Reactant

Table 61: Properties of each reactant.

Id	Name	SBO
cpg3	3-Phosphoglycerate	

Modifier

Table 62: Properties of each modifier.

Id	Name	SBO
cpg3	3-Phosphoglycerate	

Kinetic Law

Derived unit $0.0010\,\mathrm{mol}\cdot\mathrm{s}^{-1}$

$$v_{16} = \frac{\mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{rmaxSerSynth} \cdot [\mathrm{cpg3}]}{\mathrm{KSerSynthpg3} + [\mathrm{cpg3}]} \tag{32}$$

Table 63: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxSerSynth			0.026	$\mathrm{mmol}\cdot\mathrm{l}^{-1}\cdot\mathrm{s}^{-1}$	☑
KSerSynthpg3			1.000	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑

6.17 Reaction vrpGluMu

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name Phosphoglycerate mutase

Reaction equation

$$\mathrm{cpg3} \overset{\mathrm{cpg3,\ cpg2}}{\rightleftharpoons} \mathrm{cpg2} \tag{33}$$

Reactant

Table 64: Properties of each reactant.

Id	Name	SBO
cpg3	3-Phosphoglycerate	

Id	Name	SBO

Modifiers

Table 65: Properties of each modifier.

Id	Name	SBO
cpg3	3-Phosphoglycerate	
cpg2	2-Phosphoglycerate	

Product

Table 66: Properties of each product.

Id	Name	SBO
cpg2	2-Phosphoglycerate	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \frac{\mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{rmaxPGluMu} \cdot \left([\mathrm{cpg3}] - \frac{[\mathrm{cpg2}]}{\mathrm{KPGluMueq}}\right)}{\mathrm{KPGluMupg3} \cdot \left(1 + \frac{[\mathrm{cpg2}]}{\mathrm{KPGluMupg2}}\right) + [\mathrm{cpg3}]} \tag{34}$$

Table 67: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxPGluMu			89.050	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot \mathrm{s}^{-1}$	☑
KPGluMueq			0.188	dimensionless	☑
KPGluMupg3			0.200	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KPGluMupg2			0.369	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

6.18 Reaction vENO

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name Enolase

Reaction equation

$$\text{cpg2} \underset{}{\overset{\text{cpg2, cpep}}{\rightleftharpoons}} \text{cpep} \tag{35}$$

Reactant

Table 68: Properties of each reactant.

Id	Name	SBO
cpg2	2-Phosphoglycerate	

Modifiers

Table 69: Properties of each modifier.

Id	Name	SBO
cpg2	2-Phosphoglycerate	
cpep	Phosphoenol pyruvate	

Product

Table 70: Properties of each product.

Id	Name	SBO
cpep	Phosphoenol pyruvate	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \frac{\text{vol}\,(\text{cytosol}) \cdot \text{rmaxENO} \cdot \left([\text{cpg2}] - \frac{[\text{cpep}]}{\text{KENOeq}}\right)}{\text{KENOpg2} \cdot \left(1 + \frac{[\text{cpep}]}{\text{KENOpep}}\right) + [\text{cpg2}]} \tag{36}$$

Table 71: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxENO			330.448	$\text{mmol} \cdot \text{l}^{-1} \cdot \text{s}^{-1}$	☑
KENOeq			6.730	$\text{mmol} \cdot \text{l}^{-1}$	☑
KENOpg2			0.100	$\text{mmol} \cdot \text{l}^{-1}$	☑
KENOpep			0.135	$\text{mmol} \cdot \text{l}^{-1}$	☑

6.19 Reaction vPK

This is an irreversible reaction of one reactant forming one product influenced by three modifiers.

Name Pyruvate kinase

Reaction equation

$$\text{cpep} \xrightarrow{\text{cfdp, cpep, cfdp}} \text{cpyr} \tag{37}$$

Reactant

Table 72: Properties of each reactant.

Id	Name	SBO
cpep	Phosphoenol pyruvate	

Modifiers

Table 73: Properties of each modifier.

Id	Name	SBO
cfdp	Fructose-1,6-bisphosphate	
cpep	Phosphoenol pyruvate	
cfdp	Fructose-1,6-bisphosphate	

Product

Table 74: Properties of each product.

Id	Name	SBO
cpyr	Pyruvate	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \frac{\text{vol}\,(\text{cytosol}) \cdot \text{rmaxPK} \cdot [\text{cpep}] \cdot \left(\frac{[\text{cpep}]}{\text{KPKpep}} + 1\right)^{\text{nPK}-1} \cdot \text{cadp}}{\text{KPKpep} \cdot \left(\text{LPK} \cdot \left(\frac{1+\frac{\text{catp}}{\text{KPKatp}}}{\frac{[\text{cfdp}]}{\text{KPKfdp}} + \frac{\text{camp}}{\text{KPKamp}} + 1}\right)^{\text{nPK}} + \left(\frac{[\text{cpep}]}{\text{KPKpep}} + 1\right)^{\text{nPK}}\right) \cdot (\text{cadp} + \text{KPKadp})} \tag{38}$$

Table 75: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxPK			0.061	$\mathrm{mmol \cdot l^{-1} \cdot s^{-1}}$	☑
KPKpep			0.310	$\mathrm{mmol \cdot l^{-1}}$	☑
nPK			4.000	dimensionless	☑
LPK			1000.000	dimensionless	☑
KPKatp			22.500	$\mathrm{mmol \cdot l^{-1}}$	☑
KPKfdp			0.190	$\mathrm{mmol \cdot l^{-1}}$	☑
KPKamp			0.200	$\mathrm{mmol \cdot l^{-1}}$	☑
KPKadp			0.260	$\mathrm{mmol \cdot l^{-1}}$	☑

6.20 Reaction vpepCxylase

This is an irreversible reaction of one reactant forming no product influenced by three modifiers.

Name PEP carboxylase

Reaction equation

$$\mathrm{cpep} \xrightarrow{\mathrm{cfdp,\ cpep,\ cfdp}} \emptyset \tag{39}$$

Reactant

Table 76: Properties of each reactant.

Id	Name	SBO
cpep	Phosphoenol pyruvate	

Modifiers

Table 77: Properties of each modifier.

Id	Name	SBO
cfdp	Fructose-1,6-bisphosphate	
cpep	Phosphoenol pyruvate	
cfdp	Fructose-1,6-bisphosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \frac{\mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{rmaxpepCxylase} \cdot [\mathrm{cpep}] \cdot \left(1 + \left(\frac{[\mathrm{cfdp}]}{\mathrm{KpepCxylasefdp}}\right)^{\mathrm{npepCxylasefdp}}\right)}{\mathrm{KpepCxylasepep} + [\mathrm{cpep}]} \tag{40}$$

Table 78: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxpepCxylase			0.107	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot \mathrm{s}^{-1}$	☑
KpepCxylasefdp			0.700	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
npepCxylasefdp			4.210	dimensionless	☑
KpepCxylasepep			4.070	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

6.21 Reaction vSynth1

This is an irreversible reaction of one reactant forming no product influenced by one modifier.

Name Synthesis 1

Reaction equation

$$\mathrm{cpep} \xrightarrow{\mathrm{cpep}} \emptyset \tag{41}$$

Reactant

Table 79: Properties of each reactant.

Id	Name	SBO
cpep	Phosphoenol pyruvate	

Modifier

Table 80: Properties of each modifier.

Id	Name	SBO
cpep	Phosphoenol pyruvate	

Kinetic Law

Derived unit $0.0010\ \mathrm{mol} \cdot \mathrm{s}^{-1}$

$$v_{21} = \frac{\mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{rmaxSynth1} \cdot [\mathrm{cpep}]}{\mathrm{KSynth1pep} + [\mathrm{cpep}]} \tag{42}$$

Table 81: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxSynth1			0.020	$\mathrm{mmol \cdot l^{-1} \cdot s^{-1}}$	☑
KSynth1pep			1.000	$\mathrm{mmol \cdot l^{-1}}$	☑

6.22 Reaction vSynth2

This is an irreversible reaction of one reactant forming no product influenced by one modifier.

Name Synthesis 2

Reaction equation

$$\mathrm{cpyr} \xrightarrow{\mathrm{cpyr}} \emptyset \tag{43}$$

Reactant

Table 82: Properties of each reactant.

Id	Name	SBO
cpyr	Pyruvate	

Modifier

Table 83: Properties of each modifier.

Id	Name	SBO
cpyr	Pyruvate	

Kinetic Law

Derived unit $0.0010\ \mathrm{mol \cdot s^{-1}}$

$$v_{22} = \frac{\mathrm{vol\,(cytosol)} \cdot \mathrm{rmaxSynth2} \cdot [\mathrm{cpyr}]}{\mathrm{KSynth2pyr} + [\mathrm{cpyr}]} \tag{44}$$

Table 84: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxSynth2			0.074	$\mathrm{mmol \cdot l^{-1} \cdot s^{-1}}$	☑
KSynth2pyr			1.000	$\mathrm{mmol \cdot l^{-1}}$	☑

6.23 Reaction vDAHPS

This is an irreversible reaction of two reactants forming no product influenced by two modifiers.

Name DAHP synthesis

Reaction equation

$$\mathrm{ce4p} + \mathrm{cpep} \xrightarrow{\mathrm{ce4p},\ \mathrm{cpep}} \emptyset \tag{45}$$

Reactants

Table 85: Properties of each reactant.

Id	Name	SBO
ce4p	Erythrose-4-phosphate	
cpep	Phosphoenol pyruvate	

Modifiers

Table 86: Properties of each modifier.

Id	Name	SBO
ce4p	Erythrose-4-phosphate	
cpep	Phosphoenol pyruvate	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \frac{\mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{rmaxDAHPS} \cdot [\mathrm{ce4p}]^{\mathrm{nDAHPSe4p}} \cdot [\mathrm{cpep}]^{\mathrm{nDAHPSpep}}}{(\mathrm{KDAHPSe4p} + [\mathrm{ce4p}]^{\mathrm{nDAHPSe4p}}) \cdot (\mathrm{KDAHPSpep} + [\mathrm{cpep}]^{\mathrm{nDAHPSpep}})} \tag{46}$$

Table 87: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxDAHPS			0.108	$\mathrm{mmol \cdot l^{-1} \cdot s^{-1}}$	☑
nDAHPSe4p			2.600	dimensionless	☑
nDAHPSpep			2.200	dimensionless	☑
KDAHPSe4p			0.035	$\mathrm{mmol \cdot l^{-1}}$	☑
KDAHPSpep			0.005	$\mathrm{mmol \cdot l^{-1}}$	☑

6.24 Reaction vPDH

This is an irreversible reaction of one reactant forming one product influenced by two modifiers.

Name Pyruvate dehydrogenase

Reaction equation

$$\text{cpyr} \xrightarrow{\text{cpyr, accoa}} \text{accoa} \tag{47}$$

Reactant

Table 88: Properties of each reactant.

Id	Name	SBO
cpyr	Pyruvate	

Modifiers

Table 89: Properties of each modifier.

Id	Name	SBO
cpyr	Pyruvate	
accoa		

Product

Table 90: Properties of each product.

Id	Name	SBO
accoa		

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \frac{\text{vol}\,(\text{cytosol}) \cdot \text{rmaxPDH} \cdot [\text{cpyr}]^{\text{nPDH}}}{\text{KPDHpyr} \cdot \left(1 + \frac{[\text{accoa}]}{\text{Ki\_PDH\_accoa}}\right) + [\text{cpyr}]^{\text{nPDH}}} \tag{48}$$

Table 91: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxPDH			270.277	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot \mathrm{s}^{-1}$	☑
nPDH			3.680	dimensionless	☑
KPDHpyr			1159.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Ki_PDH_accoa			0.022	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

6.25 Reaction vMethSynth

This is an irreversible reaction of no reactant forming one product.

Name Methionine synthesis

Reaction equation

$$\emptyset \longrightarrow \mathrm{cpyr} \tag{49}$$

Product

Table 92: Properties of each product.

Id	Name	SBO
cpyr	Pyruvate	

Kinetic Law

Derived unit $\mathrm{mmol} \cdot \mathrm{s}^{-1}$

$$v_{25} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{rmaxMetSynth} \tag{50}$$

Table 93: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxMetSynth			0.002	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot \mathrm{s}^{-1}$	☑

6.26 Reaction vPGDH

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

Name 6-Phosphogluconate dehydrogenase

Reaction equation

$$\text{cpg} \xrightarrow{\text{cpg}} \text{cribu5p} \tag{51}$$

Reactant

Table 94: Properties of each reactant.

Id	Name	SBO
cpg	6-Phosphogluconate	

Modifier

Table 95: Properties of each modifier.

Id	Name	SBO
cpg	6-Phosphogluconate	

Product

Table 96: Properties of each product.

Id	Name	SBO
cribu5p	Ribulose-5-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = \frac{\text{vol}\,(\text{cytosol}) \cdot \text{rmaxPGDH} \cdot [\text{cpg}] \cdot \text{cnadp}}{([\text{cpg}] + \text{KPGDHpg}) \cdot \left(\text{cnadp} + \text{KPGDHnadp} \cdot \left(1 + \frac{\text{cnadph}}{\text{KPGDHnadphinh}}\right) \cdot \left(1 + \frac{\text{catp}}{\text{KPGDHatpinh}}\right)\right)} \tag{52}$$

Table 97: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxPGDH			16.232	$\text{mmol} \cdot \text{l}^{-1} \cdot \text{s}^{-1}$	☑
KPGDHpg			37.500	$\text{mmol} \cdot \text{l}^{-1}$	☑
KPGDHnadp			0.051	$\text{mmol} \cdot \text{l}^{-1}$	☑
KPGDHnadphinh			0.014	$\text{mmol} \cdot \text{l}^{-1}$	☑
KPGDHatpinh			208.000	$\text{mmol} \cdot \text{l}^{-1}$	☑

6.27 Reaction vR5PI

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name Ribose-phosphate isomerase

Reaction equation

$$\text{cribu5p} \xrightleftharpoons{\text{cribu5p, crib5p}} \text{crib5p} \tag{53}$$

Reactant

Table 98: Properties of each reactant.

Id	Name	SBO
cribu5p	Ribulose-5-phosphate	

Modifiers

Table 99: Properties of each modifier.

Id	Name	SBO
cribu5p	Ribulose-5-phosphate	
crib5p	Ribose-5-phosphate	

Product

Table 100: Properties of each product.

Id	Name	SBO
crib5p	Ribose-5-phosphate	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{27} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{rmaxR5PI} \cdot \left([\mathrm{cribu5p}] - \frac{[\mathrm{crib5p}]}{\mathrm{KR5PIeq}} \right) \tag{54}$$

Table 101: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxR5PI			4.838	s^{-1}	☑
KR5PIeq			4.000	dimensionless	☑

6.28 Reaction vRu5P

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name Ribulose-phosphate epimerase

Reaction equation

$$\text{cribu5p} \underset{}{\overset{\text{cribu5p, cxyl5p}}{\rightleftharpoons}} \text{cxyl5p} \tag{55}$$

Reactant

Table 102: Properties of each reactant.

Id	Name	SBO
cribu5p	Ribulose-5-phosphate	

Modifiers

Table 103: Properties of each modifier.

Id	Name	SBO
cribu5p	Ribulose-5-phosphate	
cxyl5p	Xylulose-5-phosphate	

Product

Table 104: Properties of each product.

Id	Name	SBO
cxyl5p	Xylulose-5-phosphate	

Kinetic Law

Derived unit $s^{-1} \cdot mmol$

$$v_{28} = \text{vol}\,(\text{cytosol}) \cdot \text{rmaxRu5P} \cdot \left([\text{cribu5p}] - \frac{[\text{cxyl5p}]}{\text{KRu5Peq}} \right) \tag{56}$$

Table 105: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxRu5P			6.739	s^{-1}	☑
KRu5Peq			1.400	dimensionless	☑

6.29 Reaction vPPK

This is an irreversible reaction of one reactant forming no product influenced by one modifier.

Name Ribose phosphate pyrophosphokinase

Reaction equation

$$\text{crib5p} \xrightarrow{\text{crib5p}} \emptyset \tag{57}$$

Reactant

Table 106: Properties of each reactant.

Id	Name	SBO
crib5p	Ribose-5-phosphate	

Modifier

Table 107: Properties of each modifier.

Id	Name	SBO
crib5p	Ribose-5-phosphate	

Kinetic Law

Derived unit $0.0010\ \text{mol} \cdot \text{s}^{-1}$

$$v_{29} = \frac{\text{vol}\,(\text{cytosol}) \cdot \text{rmaxRPPK} \cdot [\text{crib5p}]}{\text{KRPPKrib5p} + [\text{crib5p}]} \tag{58}$$

Table 108: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxRPPK			0.013	$\mathrm{mmol \cdot l^{-1} \cdot s^{-1}}$	☑
KRPPKrib5p			0.100	$\mathrm{mmol \cdot l^{-1}}$	☑

6.30 Reaction vG1PAT

This is an irreversible reaction of one reactant forming no product influenced by three modifiers.

Name Glucose-1-phosphate adenyltransferase

Reaction equation

$$\mathrm{cg1p} \xrightarrow{\mathrm{cfdp,\ cg1p,\ cfdp}} \emptyset \tag{59}$$

Reactant

Table 109: Properties of each reactant.

Id	Name	SBO
cg1p	Glucose-1-Phosphate	

Modifiers

Table 110: Properties of each modifier.

Id	Name	SBO
cfdp	Fructose-1,6-bisphosphate	
cg1p	Glucose-1-Phosphate	
cfdp	Fructose-1,6-bisphosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{30} = \frac{\mathrm{vol\,(cytosol)} \cdot \mathrm{rmaxG1PAT} \cdot [\mathrm{cg1p}] \cdot \mathrm{catp} \cdot \left(1 + \left(\frac{[\mathrm{cfdp}]}{\mathrm{KG1PATfdp}}\right)^{\mathrm{nG1PATfdp}}\right)}{(\mathrm{KG1PATatp} + \mathrm{catp}) \cdot (\mathrm{KG1PATg1p} + [\mathrm{cg1p}])} \tag{60}$$

Table 111: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxG1PAT			0.008	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot \mathrm{s}^{-1}$	☑
KG1PATfdp			0.119	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
nG1PATfdp			1.200	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KG1PATatp			4.420	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KG1PATg1p			3.200	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

6.31 Reaction vG6P

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name G6P degradation

Reaction equation

$$\mathrm{cg6p} \overset{\mathrm{cg6p}}{\rightleftharpoons} \emptyset \tag{61}$$

Reactant

Table 112: Properties of each reactant.

Id	Name	SBO
cg6p	Glucose-6-Phosphate	

Modifier

Table 113: Properties of each modifier.

Id	Name	SBO
cg6p	Glucose-6-Phosphate	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{31} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{cg6p}] \tag{62}$$

6.32 Reaction vf6P

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name F6P degradation

Reaction equation

$$\text{cf6p} \overset{\text{cf6p}}{\rightleftharpoons} \emptyset \tag{63}$$

Reactant

Table 114: Properties of each reactant.

Id	Name	SBO
`cf6p`	Fructose-6-Phosphate	

Modifier

Table 115: Properties of each modifier.

Id	Name	SBO
`cf6p`	Fructose-6-Phosphate	

Kinetic Law

Derived unit $\text{s}^{-1} \cdot \text{mmol}$

$$v_{32} = \text{vol}\,(\text{cytosol}) \cdot \text{Dil} \cdot [\text{cf6p}] \tag{64}$$

6.33 Reaction `vfdP`

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name FDP degradation

Reaction equation

$$\text{cfdp} \overset{\text{cfdp}}{\rightleftharpoons} \emptyset \tag{65}$$

Reactant

Table 116: Properties of each reactant.

Id	Name	SBO
`cfdp`	Fructose-1,6-bisphosphate	

Modifier

Table 117: Properties of each modifier.

Id	Name	SBO
cfdp	Fructose-1,6-bisphosphate	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{33} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{cfdp}] \tag{66}$$

6.34 Reaction vGAP

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name GAP degradation

Reaction equation

$$\mathrm{cgap} \overset{\mathrm{cgap}}{\rightleftharpoons} \emptyset \tag{67}$$

Reactant

Table 118: Properties of each reactant.

Id	Name	SBO
cgap	Glyceraldehyde-3-Phosphate	

Modifier

Table 119: Properties of each modifier.

Id	Name	SBO
cgap	Glyceraldehyde-3-Phosphate	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{34} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{cgap}] \tag{68}$$

6.35 Reaction vDHAP

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name DHAP degradation

Reaction equation

$$\text{cdhap} \underset{}{\overset{\text{cdhap}}{\rightleftharpoons}} \emptyset \tag{69}$$

Reactant

Table 120: Properties of each reactant.

Id	Name	SBO
cdhap	Dihydroxyacetonephosphate	

Modifier

Table 121: Properties of each modifier.

Id	Name	SBO
cdhap	Dihydroxyacetonephosphate	

Kinetic Law

Derived unit $\text{s}^{-1} \cdot \text{mmol}$

$$v_{35} = \text{vol}\,(\text{cytosol}) \cdot \text{Dil} \cdot [\text{cdhap}] \tag{70}$$

6.36 Reaction vPGP

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name PGP degradation

Reaction equation

$$\text{cpgp} \underset{}{\overset{\text{cpgp}}{\rightleftharpoons}} \emptyset \tag{71}$$

Reactant

Table 122: Properties of each reactant.

Id	Name	SBO
cpgp	1,3-diphosphophoglycerate	

Modifier

Table 123: Properties of each modifier.

Id	Name	SBO
cpgp	1,3-diphosphophoglycerate	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{36} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{cpgp}] \tag{72}$$

6.37 Reaction vPG3

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name PG3 degradation

Reaction equation

$$\mathrm{cpg3} \overset{\mathrm{cpg3}}{\rightleftharpoons} \emptyset \tag{73}$$

Reactant

Table 124: Properties of each reactant.

Id	Name	SBO
cpg3	3-Phosphoglycerate	

Modifier

Table 125: Properties of each modifier.

Id	Name	SBO
cpg3	3-Phosphoglycerate	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{37} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{cpg3}] \tag{74}$$

6.38 Reaction vpg2

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name PG2 degradation

Reaction equation

$$\mathrm{cpg2} \xrightleftharpoons{\mathrm{cpg2}} \emptyset \tag{75}$$

Reactant

Table 126: Properties of each reactant.

Id	Name	SBO
cpg2	2-Phosphoglycerate	

Modifier

Table 127: Properties of each modifier.

Id	Name	SBO
cpg2	2-Phosphoglycerate	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{38} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{cpg2}] \tag{76}$$

6.39 Reaction vPEP

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name PEP degradation

Reaction equation

$$\text{cpep} \underset{}{\overset{\text{cpep}}{\rightleftharpoons}} \emptyset \tag{77}$$

Reactant

Table 128: Properties of each reactant.

Id	Name	SBO
cpep	Phosphoenol pyruvate	

Modifier

Table 129: Properties of each modifier.

Id	Name	SBO
cpep	Phosphoenol pyruvate	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{39} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{cpep}] \tag{78}$$

6.40 Reaction vRibu5p

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name Ribu5P dilution

Reaction equation

$$\text{cribu5p} \underset{}{\overset{\text{cribu5p}}{\rightleftharpoons}} \emptyset \tag{79}$$

Reactant

Table 130: Properties of each reactant.

Id	Name	SBO
cribu5p	Ribulose-5-phosphate	

Modifier

Table 131: Properties of each modifier.

Id	Name	SBO
cribu5p	Ribulose-5-phosphate	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{40} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{cribu5p}] \tag{80}$$

6.41 Reaction vRIB5P

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name Rib5P dilution

Reaction equation

$$\mathrm{crib5p} \overset{\mathrm{crib5p}}{\rightleftharpoons} \emptyset \tag{81}$$

Reactant

Table 132: Properties of each reactant.

Id	Name	SBO
crib5p	Ribose-5-phosphate	

Modifier

Table 133: Properties of each modifier.

Id	Name	SBO
crib5p	Ribose-5-phosphate	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{41} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{crib5p}] \tag{82}$$

6.42 Reaction vXYL5P

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name XYL5P dilution

Reaction equation

$$\text{cxyl5p} \xrightleftharpoons{\text{cxyl5p}} \emptyset \tag{83}$$

Reactant

Table 134: Properties of each reactant.

Id	Name	SBO
cxyl5p	Xylulose-5-phosphate	

Modifier

Table 135: Properties of each modifier.

Id	Name	SBO
cxyl5p	Xylulose-5-phosphate	

Kinetic Law

Derived unit $\text{s}^{-1} \cdot \text{mmol}$

$$v_{42} = \text{vol}\,(\text{cytosol}) \cdot \text{Dil} \cdot [\text{cxyl5p}] \tag{84}$$

6.43 Reaction vSED7P

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name SED7P dilution

Reaction equation

$$\text{csed7p} \xrightleftharpoons{\text{csed7p}} \emptyset \tag{85}$$

Reactant

Table 136: Properties of each reactant.

Id	Name	SBO
csed7p	sedoheptulose-7-phosphate	

Modifier

Table 137: Properties of each modifier.

Id	Name	SBO
csed7p	sedoheptulose-7-phosphate	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{43} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{csed7p}] \tag{86}$$

6.44 Reaction vpyr

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name Pyruvate dilution

Reaction equation

$$\mathrm{cpyr} \overset{\mathrm{cpyr}}{\rightleftharpoons} \emptyset \tag{87}$$

Reactant

Table 138: Properties of each reactant.

Id	Name	SBO
cpyr	Pyruvate	

Modifier

Table 139: Properties of each modifier.

Id	Name	SBO
cpyr	Pyruvate	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{44} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{cpyr}] \tag{88}$$

6.45 Reaction vPG

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name PG dilution

Reaction equation

$$\mathrm{cpg} \overset{\mathrm{cpg}}{\rightleftharpoons} \emptyset \tag{89}$$

Reactant

Table 140: Properties of each reactant.

Id	Name	SBO
cpg	6-Phosphogluconate	

Modifier

Table 141: Properties of each modifier.

Id	Name	SBO
cpg	6-Phosphogluconate	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{45} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{cpg}] \tag{90}$$

6.46 Reaction vE4P

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name E4P dilution

Reaction equation

$$\text{ce4p} \xrightleftharpoons{\text{ce4p}} \emptyset \tag{91}$$

Reactant

Table 142: Properties of each reactant.

Id	Name	SBO
ce4p	Erythrose-4-phosphate	

Modifier

Table 143: Properties of each modifier.

Id	Name	SBO
ce4p	Erythrose-4-phosphate	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{46} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{ce4p}] \tag{92}$$

6.47 Reaction vGLP

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name GLP dilution

Reaction equation

$$\text{cg1p} \xrightleftharpoons{\text{cg1p}} \emptyset \tag{93}$$

Reactant

Table 144: Properties of each reactant.

Id	Name	SBO
cg1p	Glucose-1-Phosphate	

Modifier

Table 145: Properties of each modifier.

Id	Name	SBO
cg1p	Glucose-1-Phosphate	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{47} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{cg1p}] \tag{94}$$

6.48 Reaction vEXTER

This is an irreversible reaction of no reactant forming one product influenced by one modifier.

Name Extracellular glucose kinetics

Reaction equation

$$\emptyset \xrightarrow{\mathrm{cglcex}} \mathrm{cglcex} \tag{95}$$

Modifier

Table 146: Properties of each modifier.

Id	Name	SBO
cglcex	Extracellular Glucose	

Product

Table 147: Properties of each product.

Id	Name	SBO
cglcex	Extracellular Glucose	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{48} = \mathrm{vol}\,(\mathrm{extracellular}) \cdot \mathrm{Dil} \cdot (\mathrm{cfeed\_glc} - [\mathrm{cglcex}]) \tag{96}$$

Table 148: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
cfeed_glc			110.96	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

6.49 Reaction ACCOAC

This is an irreversible reaction of one reactant forming one product influenced by two modifiers.

Reaction equation

$$\mathrm{accoa} \xrightarrow{\mathrm{accoa,\ malcoa}} \mathrm{malcoa} \tag{97}$$

Reactant

Table 149: Properties of each reactant.

Id	Name	SBO
accoa		

Modifiers

Table 150: Properties of each modifier.

Id	Name	SBO
accoa		
malcoa		

Product

Table 151: Properties of each product.

Id	Name	SBO
malcoa		

Kinetic Law

Derived unit contains undeclared units

$$v_{49} = \frac{\mathrm{vol\,(cytosol)} \cdot \mathrm{rmaxACCOAC} \cdot [\mathrm{accoa}]}{\mathrm{K\_ACCOAC\_accoa} \cdot \left(1 + \frac{[\mathrm{malcoa}]}{\mathrm{Ki\_ACCOAC\_malcoa}}\right) + [\mathrm{accoa}]} \tag{98}$$

Table 152: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxACCOAC			0.046	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot \mathrm{s}^{-1}$	☑
K_ACCOAC-_accoa			$3 \cdot 10^{-4}$	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Ki_ACCOAC-_malcoa			0.100	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

6.50 Reaction Synth3

This is an irreversible reaction of one reactant forming no product influenced by one modifier.

Name Synthesis 3

Reaction equation

$$\mathrm{accoa} \xrightarrow{\mathrm{accoa}} \emptyset \tag{99}$$

Reactant

Table 153: Properties of each reactant.

Id	Name	SBO
accoa		

Modifier

Table 154: Properties of each modifier.

Id	Name	SBO
accoa		

Kinetic Law

Derived unit $0.0010\ \mathrm{mol} \cdot \mathrm{s}^{-1}$

$$v_{50} = \frac{\mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{rmaxSynth3} \cdot [\mathrm{accoa}]}{\mathrm{KSynth3accoa} + [\mathrm{accoa}]} \tag{100}$$

Table 155: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxSynth3			0.284	$\mathrm{mmol \cdot l^{-1} \cdot s^{-1}}$	☑
KSynth3accoa			1.000	$\mathrm{mmol \cdot l^{-1}}$	☑

6.51 Reaction Synth4

This is an irreversible reaction of one reactant forming no product influenced by one modifier.

Name Synthesis 4

Reaction equation

$$\mathrm{malcoa} \xrightarrow{\mathrm{malcoa}} \emptyset \tag{101}$$

Reactant

Table 156: Properties of each reactant.

Id	Name	SBO
malcoa		

Modifier

Table 157: Properties of each modifier.

Id	Name	SBO
malcoa		

Kinetic Law

Derived unit $0.0010\ \mathrm{mol \cdot s^{-1}}$

$$v_{51} = \frac{\mathrm{vol\,(cytosol)} \cdot \mathrm{rmaxSynth4} \cdot [\mathrm{malcoa}]}{\mathrm{KSynth4malcoa} + [\mathrm{malcoa}]} \tag{102}$$

Table 158: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxSynth4			0.092	$\mathrm{mmol \cdot l^{-1} \cdot s^{-1}}$	☑
KSynth4malcoa			1.000	$\mathrm{mmol \cdot l^{-1}}$	☑

6.52 Reaction R4CL

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

Reaction equation

$$\text{fer} \xrightarrow{\text{fer}} \text{fercoa} \tag{103}$$

Reactant

Table 159: Properties of each reactant.

Id	Name	SBO
fer		

Modifier

Table 160: Properties of each modifier.

Id	Name	SBO
fer		

Product

Table 161: Properties of each product.

Id	Name	SBO
fercoa		

Kinetic Law

Derived unit contains undeclared units

$$v_{52} = \frac{\text{E\_4CL} \cdot \text{kcat\_4CL} \cdot [\text{fer}]}{\text{Km\_4CL} + [\text{fer}]} \tag{104}$$

Table 162: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
E_4CL			100.000		☑
kcat_4CL			9.572		☑

Id	Name	SBO	Value	Unit	Constant
Km_4CL			0.026		☑

6.53 Reaction DCS

This is an irreversible reaction of two reactants forming one product influenced by two modifiers.

Reaction equation

$$\text{fercoa} + \text{malcoa} \xrightarrow{\text{fercoa, malcoa}} \text{ferdicoa} \tag{105}$$

Reactants

Table 163: Properties of each reactant.

Id	Name	SBO
fercoa		
malcoa		

Modifiers

Table 164: Properties of each modifier.

Id	Name	SBO
fercoa		
malcoa		

Product

Table 165: Properties of each product.

Id	Name	SBO
ferdicoa		

Kinetic Law

Derived unit contains undeclared units

$$v_{53} = \text{E\_DCS} \cdot \text{kcat\_DCS} \cdot \frac{[\text{fercoa}]^{\text{n\_DCS\_fercoa}}}{\text{Km\_DCS\_fercoa}^{\text{n\_DCS\_fercoa}} + [\text{fercoa}]^{\text{n\_DCS\_fercoa}}} \cdot \frac{[\text{malcoa}]}{\text{Km\_DCS\_malcoa} + [\text{malcoa}]} \tag{106}$$

Table 166: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
E_DCS			100.000		☑
kcat_DCS			0.013		☑
Km_DCS-_fercoa			0.046		☑
Km_DCS-_malcoa			0.008		☑
n_DCS_fercoa			1.800		☑

6.54 Reaction CURS

This is an irreversible reaction of two reactants forming one product influenced by two modifiers.

Reaction equation

$$\text{fercoa} + \text{ferdicoa} \xrightarrow{\text{fercoa, ferdicoa}} \text{cur} \tag{107}$$

Reactants

Table 167: Properties of each reactant.

Id	Name	SBO
fercoa		
ferdicoa		

Modifiers

Table 168: Properties of each modifier.

Id	Name	SBO
fercoa		
ferdicoa		

Product

Table 169: Properties of each product.

Id	Name	SBO
cur		

Kinetic Law

Derived unit contains undeclared units

$$v_{54} = \text{E\_CURS} \cdot \text{kcat\_CURS} \cdot \frac{[\text{fercoa}]}{\text{Km\_CURS\_fercoa} + [\text{fercoa}]} \cdot \frac{[\text{ferdicoa}]}{\text{Km\_CURS\_ferdicoa} + [\text{ferdicoa}]} \tag{108}$$

Table 170: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
E_CURS			100.000		☑
kcat_CURS			0.022		☑
Km_CURS-_fercoa			0.018		☑
Km_CURS-_ferdicoa			0.018		☑

6.55 Reaction FER_t

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Reaction equation

$$\text{fer\_ext} \underset{\text{fer\_ext, fer}}{\rightleftharpoons} \text{fer} \tag{109}$$

Reactant

Table 171: Properties of each reactant.

Id	Name	SBO
fer_ext		

Modifiers

Table 172: Properties of each modifier.

Id	Name	SBO
fer_ext		
fer		

Product

Table 173: Properties of each product.

Id	Name	SBO
fer		

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{55} = \mathrm{vol}\,(\mathrm{extracellular}) \cdot \mathrm{k\_FER\_t} \cdot \left([\mathrm{fer\_ext}] - \frac{[\mathrm{fer}]}{\mathrm{Keq\_FER\_t}} \right) \tag{110}$$

Table 174: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_FER_t			1000.0	s^{-1}	☑
Keq_FER_t			1.0	dimensionless	☑

6.56 Reaction CUR_t

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Reaction equation

$$\mathrm{cur} \underset{\leftarrow}{\overset{\mathrm{cur,\ cur\_ext}}{\rightleftharpoons}} \mathrm{cur\_ext} \tag{111}$$

Reactant

Table 175: Properties of each reactant.

Id	Name	SBO
cur		

Modifiers

Table 176: Properties of each modifier.

Id	Name	SBO
cur		
cur_ext		

Product

Table 177: Properties of each product.

Id	Name	SBO
cur_ext		

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{56} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{k\_CUR\_t} \cdot \left([\mathrm{cur}] - \frac{[\mathrm{cur\_ext}]}{\mathrm{Keq\_CUR\_t}} \right) \tag{112}$$

Table 178: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_CUR_t			1000.0	s^{-1}	☑
Keq_CUR_t			1.0	dimensionless	☑

6.57 Reaction EX_FER

This is an irreversible reaction of no reactant forming one product influenced by one modifier.

Reaction equation

$$\emptyset \xrightarrow{\mathrm{fer\_ext}} \mathrm{fer\_ext} \tag{113}$$

Modifier

Table 179: Properties of each modifier.

Id	Name	SBO
fer_ext		

Product

Table 180: Properties of each product.

Id	Name	SBO
fer_ext		

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{57} = \mathrm{vol}\,(\mathrm{extracellular}) \cdot \mathrm{Dil} \cdot (\mathrm{cfeed\_fer} - [\mathrm{fer\_ext}]) \tag{114}$$

Table 181: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
cfeed_fer			500.0	$\mathrm{mmol} \cdot 1^{-1}$	☑

6.58 Reaction EX_CUR

This is an irreversible reaction of one reactant forming no product influenced by one modifier.

Reaction equation

$$\mathrm{cur\_ext} \xrightarrow{\mathrm{cur\_ext}} \emptyset \tag{115}$$

Reactant

Table 182: Properties of each reactant.

Id	Name	SBO
cur_ext		

Modifier

Table 183: Properties of each modifier.

Id	Name	SBO
cur_ext		

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{58} = \mathrm{vol}\,(\mathrm{extracellular}) \cdot \mathrm{Dil} \cdot [\mathrm{cur\_ext}] \tag{116}$$

6.59 Reaction vACCOA

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name ACCOA dilution

Reaction equation

$$\mathrm{accoa} \overset{\mathrm{accoa}}{\rightleftharpoons} \emptyset \tag{117}$$

Reactant

Table 184: Properties of each reactant.

Id	Name	SBO
accoa		

Modifier

Table 185: Properties of each modifier.

Id	Name	SBO
accoa		

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{59} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{accoa}] \tag{118}$$

6.60 Reaction vMALCOA

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name MALCOA dilution

Reaction equation

$$\text{malcoa} \overset{\text{malcoa}}{\rightleftharpoons} \emptyset \tag{119}$$

Reactant

Table 186: Properties of each reactant.

Id	Name	SBO
malcoa		

Modifier

Table 187: Properties of each modifier.

Id	Name	SBO
malcoa		

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{60} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{malcoa}] \tag{120}$$

6.61 Reaction vFER

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name FER dilution

Reaction equation

$$\text{fer} \overset{\text{fer}}{\rightleftharpoons} \emptyset \tag{121}$$

Reactant

Table 188: Properties of each reactant.

Id	Name	SBO
fer		

Modifier

Table 189: Properties of each modifier.

Id	Name	SBO
fer		

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{61} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{fer}] \tag{122}$$

6.62 Reaction vFERCOA

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name FERCOA dilution

Reaction equation

$$\mathrm{fercoa} \underset{}{\overset{\mathrm{fercoa}}{\rightleftharpoons}} \emptyset \tag{123}$$

Reactant

Table 190: Properties of each reactant.

Id	Name	SBO
fercoa		

Modifier

Table 191: Properties of each modifier.

Id	Name	SBO
fercoa		

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{62} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{fercoa}] \tag{124}$$

6.63 Reaction vFERDICOA

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name FERDICOA dilution

Reaction equation

$$\mathrm{ferdicoa} \xrightleftharpoons{\mathrm{ferdicoa}} \emptyset \tag{125}$$

Reactant

Table 192: Properties of each reactant.

Id	Name	SBO
ferdicoa		

Modifier

Table 193: Properties of each modifier.

Id	Name	SBO
ferdicoa		

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{63} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{ferdicoa}] \tag{126}$$

6.64 Reaction vCUR

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name CUR dilution

Reaction equation

$$\text{cur} \overset{\text{cur}}{\rightleftharpoons} \emptyset \tag{127}$$

Reactant

Table 194: Properties of each reactant.

Id	Name	SBO
cur		

Modifier

Table 195: Properties of each modifier.

Id	Name	SBO
cur		

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{64} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Dil} \cdot [\mathrm{cur}] \tag{128}$$

7 Derived Rate Equations

When interpreted as an ordinary differential equation framework, this model implies the following set of equations for the rates of change of each species.

Identifiers for kinetic laws highlighted in gray cannot be verified to evaluate to units of SBML `substance` per `time`. As a result, some SBML interpreters may not be able to verify the consistency of the units on quantities in the model. Please check if

- parameters without an unit definition are involved or
- volume correction is necessary because the `hasOnlySubstanceUnits` flag may be set to `false` and `spacialDimensions`> 0 for certain species.

7.1 Species `cpep`

Name Phosphoenol pyruvate

Initial concentration $2.67\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in 16 reactions (as a reactant in vPTS, vPK, vpepCxylase, vSynth1, vDAHPS, vPEP and as a product in vENO and as a modifier in vPTS, vPFK, vPFK, vENO, vPK, vpepCxylase, vSynth1, vDAHPS, vPEP).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cpep} = v_{18} - v_1 - v_{19} - v_{20} - v_{21} - v_{23} - v_{39} \tag{129}$$

7.2 Species cglcex

Name Extracellular Glucose

Initial concentration $55.5\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in vPTS and as a product in vEXTER and as a modifier in vPTS, vEXTER).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cglcex} = v_{48} - v_1 \tag{130}$$

7.3 Species cg6p

Name Glucose-6-Phosphate

Initial concentration $3.48\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in ten reactions (as a reactant in vPGI, vPGM, vG6PDH, vG6P and as a product in vPTS and as a modifier in vPTS, vPGI, vPGM, vG6PDH, vG6P).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cg6p} = v_1 - v_2 - v_3 - v_4 - v_{31} \tag{131}$$

7.4 Species cpyr

Name Pyruvate

Initial concentration $2.67\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eleven reactions (as a reactant in vSynth2, vPDH, vpyr and as a product in vPTS, vTRPSYNTH, vPK, vMethSynth and as a modifier in vPTS, vSynth2, vPDH, vpyr).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cpyr} = v_1 + v_{13} + v_{19} + v_{25} - v_{22} - v_{24} - v_{44} \tag{132}$$

7.5 Species cf6p

Name Fructose-6-Phosphate

Initial concentration $0.6\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eleven reactions (as a reactant in vPFK, vMURSyNTH, vf6P and as a product in vPGI, vTA, vTKB and as a modifier in vPGI, vPFK, vTA, vTKB, vf6P).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cf6p} = v_2 + v_6 + v_8 - v_5 - 2v_9 - v_{32} \tag{133}$$

7.6 Species cg1p

Name Glucose-1-Phosphate

Initial concentration $0.653\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in vG1PAT, vGLP and as a product in vPGM and as a modifier in vPGM, vG1PAT, vGLP).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cg1p} = v_3 - v_{30} - v_{47} \tag{134}$$

7.7 Species cpg

Name 6-Phosphogluconate

Initial concentration $0.808\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in seven reactions (as a reactant in vPGDH, vPG and as a product in vG6PDH and as a modifier in vPGI, vPGI, vPGDH, vPG).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cpg} = v_4 - v_{26} - v_{45} \tag{135}$$

7.8 Species cfdp

Name Fructose-1,6-bisphosphate

Initial concentration $0.272\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eleven reactions (as a reactant in vALDO, vfdP and as a product in vPFK and as a modifier in vALDO, vPK, vPK, vpepCxylase, vpepCxylase, vG1PAT, vG1PAT, vfdP).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cfdp} = v_5 - v_{10} - v_{33} \tag{136}$$

7.9 Species csed7p

Name sedoheptulose-7-phosphate

Initial concentration $0.276\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in vTA, vSED7P and as a product in vTKA and as a modifier in vTA, vTKA, vSED7P).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{csed7p} = v_7 - v_6 - v_{43} \tag{137}$$

7.10 Species cgap

Name Glyceraldehyde-3-Phosphate

Initial concentration $0.218\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in 15 reactions (as a reactant in vTA, vGAPDH, vGAP and as a product in vTKA, vTKB, vALDO, vTIS, vTRPSYNTH and as a modifier in vTA, vTKA, vTKB, vALDO, vGAPDH, vTIS, vGAP).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cgap} = v_7 + v_8 + v_{10} + v_{12} + v_{13} - v_6 - v_{11} - v_{34} \tag{138}$$

7.11 Species ce4p

Name Erythrose-4-phosphate

Initial concentration $0.098\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in vTKB, vDAHPS, vE4P and as a product in vTA and as a modifier in vTA, vTKB, vDAHPS, vE4P).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ce4p} = v_6 - v_8 - v_{23} - v_{46} \tag{139}$$

7.12 Species cxyl5p

Name Xylulose-5-phosphate

Initial concentration $0.138\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in vTKA, vTKB, vXYL5P and as a product in vRu5P and as a modifier in vTKA, vTKB, vRu5P, vXYL5P).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cxyl5p} = v_{28} - v_7 - v_8 - v_{42} \tag{140}$$

7.13 Species crib5p

Name Ribose-5-phosphate

Initial concentration $0.398\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in vTKA, vPPK, vRIB5P and as a product in vR5PI and as a modifier in vTKA, vR5PI, vPPK, vRIB5P).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{crib5p} = v_{27} - v_{7} - v_{29} - v_{41} \tag{141}$$

7.14 Species cdhap

Name Dihydroxyacetonephosphate

Initial concentration $0.167\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in vTIS, vG3PDH, vDHAP and as a product in vALDO and as a modifier in vALDO, vTIS, vG3PDH, vDHAP).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cdhap} = v_{10} - v_{12} - v_{14} - v_{35} \tag{142}$$

7.15 Species cpgp

Name 1,3-diphosphosphoglycerate

Initial concentration $0.0080\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in vPGK, vPGP and as a product in vGAPDH and as a modifier in vGAPDH, vPGK, vPGP).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cpgp} = v_{11} - v_{15} - v_{36} \tag{143}$$

7.16 Species cpg3

Name 3-Phosphoglycerate

Initial concentration $2.13\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in vsersynth, vrpGluMu, vPG3 and as a product in vPGK and as a modifier in vPGK, vsersynth, vrpGluMu, vPG3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cpg3} = v_{15} - v_{16} - v_{17} - v_{37} \tag{144}$$

7.17 Species cpg2

Name 2-Phosphoglycerate

Initial concentration $0.399\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in vENO, vpg2 and as a product in vrpGluMu and as a modifier in vrpGluMu, vENO, vpg2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cpg2} = v_{17} - v_{18} - v_{38} \tag{145}$$

7.18 Species cribu5p

Name Ribulose-5-phosphate

Initial concentration $0.111\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in seven reactions (as a reactant in vR5PI, vRu5P, vRibu5p and as a product in vPGDH and as a modifier in vR5PI, vRu5P, vRibu5p).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cribu5p} = v_{26} - v_{27} - v_{28} - v_{40} \tag{146}$$

7.19 Species accoa

Initial concentration $1\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in ACCOAC, Synth3, vACCOA and as a product in vPDH and as a modifier in vPDH, ACCOAC, Synth3, vACCOA).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{accoa} = v_{24} - v_{49} - v_{50} - v_{59} \tag{147}$$

7.20 Species malcoa

Initial concentration $1\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in Synth4, DCS, vMALCOA and as a product in ACCOAC and as a modifier in ACCOAC, Synth4, DCS, vMALCOA).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{malcoa} = v_{49} - v_{51} - v_{53} - v_{60} \tag{148}$$

7.21 Species fer

Initial concentration $0\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in R4CL, vFER and as a product in FER_t and as a modifier in R4CL, FER_t, vFER).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{fer} = v_{55} - v_{52} - v_{61} \tag{149}$$

7.22 Species fer_ext

Initial concentration $271.5\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in FER_t and as a product in EX_FER and as a modifier in FER_t, EX_FER).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{fer\_ext} = v_{57} - v_{55} \tag{150}$$

7.23 Species fercoa

Initial concentration $0\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in seven reactions (as a reactant in DCS, CURS, vFERCOA and as a product in R4CL and as a modifier in DCS, CURS, vFERCOA).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{fercoa} = v_{52} - v_{53} - v_{54} - v_{62} \tag{151}$$

7.24 Species ferdicoa

Initial concentration $0\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in CURS, vFERDICOA and as a product in DCS and as a modifier in CURS, vFERDICOA).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ferdicoa} = v_{53} - v_{54} - v_{63} \tag{152}$$

7.25 Species cur

Initial concentration $0\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in CUR_t, vCUR and as a product in CURS and as a modifier in CUR_t, vCUR).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cur} = v_{54} - v_{56} - v_{64} \tag{153}$$

7.26 Species cur_ext

Initial concentration $0\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in EX_CUR and as a product in CUR_t and as a modifier in CUR_t, EX_CUR).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cur\_ext} = v_{56} - v_{58} \tag{154}$$

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