SBML Model Report

Model name: "Chassagnole2002_Carbon_Metabolism"



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Jacky L Snoep¹ and Harish Dharuri² at January 18th 2006 at 10:51 p.m. and last time modified at April eighth 2016 at 3:26 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	18
events	0	constraints	0
reactions	48	function definitions	0
global parameters	7	unit definitions	5
rules	7	initial assignments	0

Model Notes

The model reproduces Figures 4,5 and 6 of the publication. The analytical functions for cometabolites Catp, Camp, Cnadph, and Cnadp slightly differ from the equations given in the paper. These

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changes were made in consultation with Dr. Christophe Chassagnole and are essential for reproducing the figures. The dependency of the rate of change of extracellular glucose concentration on the ratio of biomass concentration to specific weight of biomass (Cx*rPTS/Rhox) is taken into account by appropriately adjusting the stoichiometries of the species involved in the phosphotransferase system (rPTS). The rmax values for the various reactions are obtained from experiments and are not provided in the paper. However, these were personally communicated to the JWS repository. The model has been successfully tested on MathSBML.

SBML level 2 code generated for the JWS Online project by Jacky Snoep using PySCeS Run this model online at http://jjj.biochem.sun.ac.za

To cite JWS Online please refer to: Olivier, B.G. and Snoep, J.L. (2004) Web-based modelling using JWS Online, Bioinformatics, 20:2143-2144

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To cite BioModels Database, please use: Li C, Donizelli M, Rodriguez N, Dharuri H, Endler L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novre N, Laibe C (2010) BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models. BMC Syst Biol., 4:92.

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 $mmol \cdot l^{-1}$

2.3 Unit second_inverse

Name second inverse

Definition s^{-1}

2.4 Unit mM_per_second

Name mM per second

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

2.5 Unit per_mM_per_second

Name per mM per second

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

2.6 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition 1

2.7 Unit area

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

Definition m²

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	Size	Unit	Constant	Outside
			Dimensions				
extracellular			3	1	litre		

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
cytosol			3	1	litre	Ø	extracellular

3.1 Compartment extracellular

This is a three dimensional compartment with a constant size of one 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 18 species. Section 8 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 Condi- tion
cpep	Phosphoenol pyruvate	cytosol	$\operatorname{mmol} \cdot 1^{-1}$		
cglcex	Extracellular Glucose	extracellular	$\text{mmol} \cdot l^{-1}$		\Box
cg6p	Glucose-6-Phosphate	cytosol	$mmol \cdot l^{-1}$		
cpyr	Pyruvate	cytosol	$mmol \cdot l^{-1}$		
cf6p	Fructose-6-Phosphate	cytosol	$mmol \cdot l^{-1}$		
cg1p	Glucose-1-Phosphate	cytosol	$mmol \cdot l^{-1}$		
cpg	6-Phosphogluconate	cytosol	$\text{mmol} \cdot 1^{-1}$		
cfdp	Fructose-1,6-bisphosphate	cytosol	$\text{mmol} \cdot 1^{-1}$		
csed7p	sedoheptulose-7-phosphate	cytosol	$\text{mmol} \cdot 1^{-1}$		
cgap	Glyceraldehyde-3-Phosphate	cytosol	$\text{mmol} \cdot 1^{-1}$		\Box
ce4p	Erythrose-4-phosphate	cytosol	$mmol \cdot l^{-1}$		
cxy15p	Xylulose-5-phosphate	cytosol	$mmol \cdot l^{-1}$		
crib5p	Ribose-5-phosphate	cytosol	$mmol \cdot l^{-1}$		
cdhap	Dihydroxyacetonephosphate	cytosol	$\text{mmol} \cdot 1^{-1}$		
cpgp	1,3-diphosphosphoglycerate	cytosol	$\text{mmol} \cdot 1^{-1}$		
cpg3	3-Phosphoglycerate	cytosol	$\text{mmol} \cdot 1^{-1}$		\Box
cpg2	2-Phosphoglycerate	cytosol	$\text{mmol} \cdot 1^{-1}$		\Box
cribu5p	Ribulose-5-phosphate	cytosol	$\text{mmol} \cdot l^{-1}$		

5 Parameters

This model contains seven global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
catp			4.270	$\operatorname{mmol} \cdot l^{-1}$	
cadp			0.595	$\operatorname{mmol} \cdot 1^{-1}$	\Box
camp			0.955	$\text{mmol} \cdot 1^{-1}$	
cnadp			0.195	$\operatorname{mmol} \cdot 1^{-1}$	
cnadph			0.062	$\operatorname{mmol} \cdot 1^{-1}$	\Box
cnad			1.470	$\operatorname{mmol} \cdot 1^{-1}$	
cnadh			0.100	$mmol \cdot l^{-1}$	

6 Rules

This is an overview of seven rules.

6.1 Rule catp

Rule catp is an assignment rule for parameter catp:

$$catp = 4.27 - 4.163 \cdot \frac{t}{0.657 + 1.43 \cdot t + 0.0364 \cdot t^2}$$
 (1)

6.2 Rule cadp

Rule cadp is an assignment rule for parameter cadp:

$$cadp = 0.582 + 1.73 \cdot 2.731^{-0.15 \cdot t} \cdot (0.12 \cdot t + 2.14 \cdot 10^{-4} \cdot t3)$$
 (2)

6.3 Rule camp

Rule camp is an assignment rule for parameter camp:

camp =
$$0.123 + 7.25 \cdot \frac{t}{7.25 + 1.47 \cdot t + 0.17 \cdot t^2} + \frac{1.073}{1.29 + 8.05 \cdot t}$$
 (3)

6.4 Rule cnadph

Rule cnadph is an assignment rule for parameter cnadph:

$$\begin{aligned} \text{cnadph} &= 0.062 + 0.332 \cdot 2.718^{-0.464 \cdot t} \cdot \left(0.0166 \cdot t^{1.58} + 1.66 \cdot 10^{-4} \cdot t^{4.73} \right. \\ &\quad + 0.1312 \cdot 10^{-9} \cdot t^{7.89} + 0.1362 \cdot 10^{-12} \cdot t^{11} + 0.1233 \cdot 10^{-15} \cdot t_{14.2} \end{aligned} \tag{4}$$

6.5 Rule cnadp

Rule cnadp is an assignment rule for parameter cnadp:

$$cnadp = 0.159 - 0.00554 \cdot \frac{t}{2.8 - 0.271 \cdot t + 0.01 \cdot t^2} + \frac{0.182}{4.82 + 0.526 \cdot t}$$
 (5)

6.6 Rule cnadh

Rule cnadh is an assignment rule for parameter cnadh:

$$cnadh = 0.0934 + 0.00111 \cdot 2.371^{-0.123 \cdot t} \cdot \left(0.844 \cdot t + 0.104 \cdot t^{3}\right) \tag{6}$$

6.7 Rule cnad

Rule cnad is an assignment rule for parameter cnad:

$$cnad = 1.314 + 1.314 \cdot 2.73^{-0.0435 \cdot t - 0.342} - (t + 7.871) \cdot \frac{2.73^{-0.0218 \cdot t - 0.171}}{8.481 + t}$$
 (7)

7 Reactions

This model contains 48 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

Nº	Id	Name	Reaction Equation	SBO
1	vPTS	Phosphotransferase system	$cglcex + 65 cpep \Longrightarrow 65 cg6p + 65 cpyr$	
2	vPGI	Glucose-6-phosphate isomerase	$cg6p \stackrel{cpg}{\rightleftharpoons} cf6p$	
3	vPGM	Phosphoglucomutase	cg6p ← cg1p	
4	vG6PDH	Glucose-6-phosphate dehydrogenase	cg6p ← cpg	
5	vPFK	Phosphofructokinase	cf6p cpep cfdp	
6	vTA	Transaldolase	$cgap + csed7p \Longrightarrow cf6p + ce4p$	
7	vTKA	Transketolase a	$crib5p + cxyl5p \Longrightarrow cgap + csed7p$	
8	vTKB	Transketolase b	$ce4p + cxyl5p \Longrightarrow cgap + cf6p$	
9	vMURSyNTH	Mureine synthesis	$2 \operatorname{cf6p} \Longrightarrow \emptyset$	
10	vALDO	Aldolase	$cfdp \Longrightarrow cdhap + cgap$	
11	vGAPDH	Glyceraldehyde-3-phosphate dehydrogenase	cgap ← cpgp	
12	vTIS	Triosephosphate isomerase	cdhap ← cgap	
13	vTRPSYNTH	Tryptophan synthesis	$\emptyset \Longrightarrow cpyr + cgap$	
14	vG3PDH	Glycerol-3-phosphate dehydrogenase	cdhap ← ∅	
15	vPGK	Phosphoglycerate kinase	cpgp ← cpg3	
16	vsersynth	Serine synthesis	cpg3 ==== ∅	
17	vrpGluMu	Phosphoglycerate mutase	$cpg3 \Longrightarrow cpg2$	
18	vENO	Enolase	cpg2 ← cpep	
19	vPK	Pyruvate kinase	$\operatorname{cpep} \stackrel{\operatorname{cfdp}}{===} \operatorname{cpyr}$	
20	vpepCxylase	PEP carboxylase	$\operatorname{cpep} \stackrel{\operatorname{cfdp}}{\longleftarrow} \emptyset$	
21	vSynth1	Synthesis 1	$cpep \Longrightarrow \emptyset$	

N₀	Id	Name	Reaction Equation	SBO
22	vSynth2	Synthesis 2	cpyr ← Ø	
23	vDAHPS	DAHP synthesis	$ce4p + cpep \Longrightarrow \emptyset$	
24	vPDH	Pyruvate dehydrogenase	$\operatorname{cpyr} \rightleftharpoons \emptyset$	
25	vMethSynth	Methionine synthesis	$\emptyset \Longrightarrow \text{cpyr}$	
26	vPGDH	6-Phosphogluconate dehydrogenase	cpg ← cribu5p	
27	vR5PI	Ribose-phosphate isomerase	cribu5p ← crib5p	
28	vRu5P	Ribulose-phosphate epimerase	cribu5p ← cxyl5p	
29	vPPK	Ribose phosphate pyrophosphokinase	crib5p ← ∅	
30	vG1PAT	Glucose-1-phosphate adenyltransferase	$cg1p \stackrel{cfdp}{\longleftarrow} \emptyset$	
31	vG6P	G6P degradation	$cg6p \rightleftharpoons \emptyset$	
32	vf6P	F6P degradation	$cf6p \rightleftharpoons \emptyset$	
33	vfdP	FDP degradation	$\operatorname{cfdp} \rightleftharpoons \emptyset$	
34	vGAP	GAP degradation	$\operatorname{cgap} \Longrightarrow \emptyset$	
35	vDHAP	DHAP degradation	cdhap ==== ∅	
36	vPGP	PGP degradation	$\operatorname{cpgp} \Longrightarrow \emptyset$	
37	vPG3	PG3 degradation	cpg3 ==== ∅	
38	vpg2	PG2 degradation	$cpg2 \Longrightarrow \emptyset$	
39	vPEP	PEP degradation	$\operatorname{cpep} \Longrightarrow \emptyset$	
40	vRibu5p	Ribu5P dilution	cribu $5p \Longrightarrow \emptyset$	
41	vRIB5P	Rib5P dilution	crib5p ← ∅	
42	vXYL5P	XYL5P dilution	$cxyl5p \Longrightarrow \emptyset$	
43	vSED7P	SED7P dilution	$\operatorname{csed7p} \rightleftharpoons \emptyset$	
44	vpyr	Pyruvate dilution	$\operatorname{cpyr} \rightleftharpoons \emptyset$	
45	vPG	PG dilution	$cpg \Longrightarrow \emptyset$	
46	vE4P	E4P dilution	ce4p ← ∅	
47	vGLP	GLP dilution	$cg1p \rightleftharpoons \emptyset$	
48	vEXTER	Extracellular glucose kinetics	$\emptyset \Longrightarrow \operatorname{cglcex}$	

7.1 Reaction vPTS

This is a reversible reaction of two reactants forming two products.

Name Phosphotransferase system

Reaction equation

$$cglcex + 65 cpep \Longrightarrow 65 cg6p + 65 cpyr$$
 (8)

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
cglcex cpep	Extracellular Glucose Phosphoenol pyruvate	

Products

Table 7: Properties of each product.

Id	Name	SBO
٠.	Glucose-6-Phosphate Pyruvate	

Kinetic Law

$$\nu_{1} = \frac{\text{vol}\left(\text{extracellular}\right) \cdot \text{rmaxPTS} \cdot \left[\text{cglcex}\right] \cdot \frac{\left[\text{cpep}\right]}{\left[\text{cpyr}\right]}}{\left(\text{KPTSa1} + \text{KPTSa2} \cdot \frac{\left[\text{cpep}\right]}{\left[\text{cpyr}\right]} + \text{KPTSa3} \cdot \left[\text{cglcex}\right] + \left[\text{cglcex}\right] \cdot \frac{\left[\text{cpep}\right]}{\left[\text{cpyr}\right]}\right) \cdot \left(1 + \frac{\left[\text{cg6p}\right]^{nPTSg6p}}{\text{KPTSg6p}}\right)}$$
(9)

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxPTS			7829.78	$mmol \cdot l^{-1} \cdot s^{-1}$	\square
KPTSa1			3082.30	$mmol \cdot l^{-1}$	
KPTSa2			0.01	$\operatorname{mmol} \cdot 1^{-1}$	
KPTSa3			245.30	dimensionless	

Id	Name	SBO	Value	Unit	Constant
nPTSg6p KPTSg6p				$\begin{array}{c} \text{dimensionless} \\ \text{mmol} \cdot l^{-1} \end{array}$	✓

7.2 Reaction vPGI

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

Name Glucose-6-phosphate isomerase

Reaction equation

$$cg6p \rightleftharpoons cf6p$$
 (10)

Reactant

Table 9: Properties of each reactant.

	, , F	
Id	Name	SBO
cg6p	Glucose-6-Phosphate	

Modifier

Table 10: Properties of each modifier.

Id	Name	SBO
cpg	6-Phosphogluconate	

Product

Table 11: Properties of each product.

Id	Name	SBO
cf6p	Fructose-6-Phosphate	

Kinetic Law

$$v_{2} = \frac{\text{vol}\left(\text{cytosol}\right) \cdot \text{rmaxPGI} \cdot \left(\left[\text{cg6p}\right] - \frac{\left[\text{cf6p}\right]}{\text{KPGIeq}}\right)}{\text{KPGIg6p} \cdot \left(1 + \frac{\left[\text{cf6p}\right]}{\text{KPGIf6p} \cdot \left(1 + \frac{\left[\text{cpg}\right]}{\text{KPGIf6ppginh}}\right)} + \frac{\left[\text{cpg}\right]}{\text{KPGIg6ppginh}}\right) + \left[\text{cg6p}\right]}$$
(11)

Table 12: Properties of each parameter.

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

7.3 Reaction vPGM

This is a reversible reaction of one reactant forming one product.

Name Phosphoglucomutase

Reaction equation

$$cg6p \rightleftharpoons cg1p$$
 (12)

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
cg6p	Glucose-6-Phosphate	

Product

Table 14: Properties of each product.

Id	Name	SBO
cg1p	Glucose-1-Phosphate	

Derived unit contains undeclared units

$$v_{3} = \frac{\text{vol}(\text{cytosol}) \cdot \text{rmaxPGM} \cdot \left([\text{cg6p}] - \frac{[\text{cg1p}]}{\text{KPGMeq}} \right)}{\text{KPGMg6p} \cdot \left(1 + \frac{[\text{cg1p}]}{\text{KPGMg1p}} \right) + [\text{cg6p}]}$$
(13)

Table 15: Properties of each parameter.

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

7.4 Reaction vG6PDH

This is a reversible reaction of one reactant forming one product.

Name Glucose-6-phosphate dehydrogenase

Reaction equation

$$cg6p \rightleftharpoons cpg$$
 (14)

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
cg6p	Glucose-6-Phosphate	

Product

Table 17: Properties of each product.

Id	Name	SBO
cpg	6-Phosphogluconate	

Derived unit contains undeclared units

$$v_{4} = \frac{\text{vol}\left(\text{cytosol}\right) \cdot \text{rmaxG6PDH} \cdot \left[\text{cg6p}\right] \cdot \text{cnadp}}{\left(\left[\text{cg6p}\right] + \text{KG6PDHg6p}\right) \cdot \left(1 + \frac{\text{cnadph}}{\text{KG6PDHnadphg6pinh}}\right) \cdot \left(\text{KG6PDHnadp} \cdot \left(1 + \frac{\text{cnadph}}{\text{KG6PDHnadphnadpinh}}\right) + \text{cnadp}\right)}$$

Table 18: Properties of each parameter.

		1	1		
Id	Name	SBO	Value	Unit	Constant
rmaxG6PDH			1.380	$mmol \cdot l^{-1} \cdot s^{-1}$	
KG6PDHg6p			14.400	$mmol \cdot l^{-1}$	
KG6PDHnadphg6	pinh		6.430	$mmol \cdot l^{-1}$	
KG6PDHnadp			0.025	$mmol \cdot l^{-1}$	
KG6PDHnadphna	dpinh		0.010	$mmol \cdot l^{-1}$	

7.5 Reaction vPFK

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

Name Phosphofructokinase

Reaction equation

$$cf6p \stackrel{cpep}{\rightleftharpoons} cfdp \tag{16}$$

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
cf6p	Fructose-6-Phosphate	

Modifier

Table 20: Properties of each modifier.

Id	Name	SBO
cpep	Phosphoenol pyruvate	

Table 21: Properties of each product.

Id	Name	SBO
cfdp	Fructose-1,6-bisphosphate	

Kinetic Law

Derived unit contains undeclared units

$$=\frac{\text{vol}\left(\text{cytosol}\right)\cdot\text{rmaxPFK}\cdot\text{catp}\cdot\left[\text{cf6p}\right]}{\left(\text{catp}+\text{KPFKatps}\cdot\left(1+\frac{\text{cadp}}{\text{KPFKadpc}}\right)\right)\cdot\left(\left[\text{cf6p}\right]+\frac{\text{KPFKf6ps}\cdot\left(1+\frac{\left[\text{cpep}\right]}{\text{KPFKadpa}}+\frac{\text{cadp}}{\text{KPFKadpb}}+\frac{\text{camp}}{\text{KPFKampb}}\right)}{1+\frac{\text{cadp}}{\text{KPFKadpa}}+\frac{\text{camp}}{\text{KPFKampa}}}\right)\cdot\left(1+\frac{\left(1+\frac{\left[\text{cf6p}\right]\cdot\left[\text{cf6p}\right]\cdot\left(1+\frac{\left[\text{cf6p}\right]\cdot\left(1+\frac{\left[\text{cf6p}\right]\cdot\left(1+\frac{\left[\text{cf6p}\right]\cdot\left(1+\frac{\left[\text{cf6p}\right]\cdot\left(1+\frac{\left[\text{cf6p}\right]\cdot\left(1+\frac{\left[\text{cf6p}\right]\cdot\left(1+\frac{\left[\text{cf6p}\right]\cdot\left(1+\frac{\left[\text{cf6p}\right]\cdot\left(1+\frac{\left[\text{cf6p}\right]\cdot\left[\text{cf$$

Table 22: Properties of each parameter.

		1	1		
Id	Name	SBO	Value	Unit	Constant
rmaxPFK			1840.585	$mmol \cdot l^{-1} \cdot s^{-1}$	$\overline{\hspace{1cm}}$
KPFKatps			0.123	$\text{mmol} \cdot 1^{-1}$	
KPFKadpc			4.140	$\text{mmol} \cdot 1^{-1}$	
KPFKf6ps			0.325	$\operatorname{mmol} \cdot 1^{-1}$	$\overline{\mathbf{Z}}$
KPFKpep			3.260	$\operatorname{mmol} \cdot 1^{-1}$	
KPFKadpb			3.890	$\operatorname{mmol} \cdot 1^{-1}$	$\overline{\mathbf{Z}}$
KPFKampb			3.200	$\operatorname{mmol} \cdot 1^{-1}$	
KPFKadpa			128.000	$\operatorname{mmol} \cdot 1^{-1}$	$\overline{\mathbf{Z}}$
KPFKampa			19.100	$\operatorname{mmol} \cdot 1^{-1}$	$\overline{\mathbf{Z}}$
LPFK		5	629067.000	dimensionless	$\overline{\mathbf{Z}}$
nPFK			11.100	dimensionless	

7.6 Reaction vTA

This is a reversible reaction of two reactants forming two products.

Name Transaldolase

Reaction equation

$$cgap + csed7p \Longrightarrow cf6p + ce4p \tag{18}$$

Reactants

Table 23: Properties of each reactant.

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

Products

Table 24: Properties of each product.

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

Kinetic Law

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

$$v_6 = \text{vol}(\text{cytosol}) \cdot \text{rmaxTA} \cdot \left([\text{cgap}] \cdot [\text{csed7p}] - \frac{[\text{ce4p}] \cdot [\text{cf6p}]}{\text{KTAeq}} \right)$$
 (19)

Table 25: Properties of each parameter.

		1	I		
Id	Name	SBO	Value	Unit	Constant
rmaxTA			10.872	$\text{mmol}^{-1} \cdot 1 \cdot \text{s}^{-1}$	
KTAeq			1.050	dimensionless	$\overline{\mathbf{Z}}$

7.7 Reaction vTKA

This is a reversible reaction of two reactants forming two products.

Name Transketolase a

Reaction equation

$$crib5p + cxyl5p \rightleftharpoons cgap + csed7p$$
 (20)

Table 26: Properties of each reactant.

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

Table 27: Properties of each product.

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

Kinetic Law

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

$$v_7 = \text{vol} (\text{cytosol}) \cdot \text{rmaxTKa} \cdot \left([\text{crib5p}] \cdot [\text{cxyl5p}] - \frac{[\text{csed7p}] \cdot [\text{cgap}]}{\text{KTKaeq}} \right)$$
 (21)

Table 28: Properties of each parameter.

			I	
Id	Name	SBO Va	lue Unit	Constant
rmaxTKa KTKaeq			$\frac{1}{1}$ mmol ⁻¹ ·1·s ⁻¹ dimensionless	

7.8 Reaction vTKB

This is a reversible reaction of two reactants forming two products.

Name Transketolase b

Reaction equation

$$ce4p + cxyl5p \rightleftharpoons cgap + cf6p$$
 (22)

Table 29: Properties of each reactant.

Id	Name	SBO
ce4p cxy15p	Erythrose-4-phosphate Xylulose-5-phosphate	

Table 30: Properties of each product.

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

Kinetic Law

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

$$v_8 = vol (cytosol) \cdot rmaxTKb \cdot \left([cxyl5p] \cdot [ce4p] - \frac{[cf6p] \cdot [cgap]}{KTKbeq} \right)$$
 (23)

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxTKb KTKbeq				$mmol^{-1} \cdot l \cdot s^{-1}$ dimensionless	Z

7.9 Reaction vMURSyNTH

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

Name Mureine synthesis

Reaction equation

$$2\operatorname{cf6p} \Longrightarrow \emptyset \tag{24}$$

Table 32: Properties of each reactant.

Id	Name	SBO
cf6p	Fructose-6-Phosphate	

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

$$v_9 = \text{vol}(\text{cytosol}) \cdot \text{rmaxMurSynth}$$
 (25)

Table 33: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxMurS	ynth		$4.3711 \cdot 10^{-4}$	$mmol \cdot l^{-1} \cdot s^{-1}$	

7.10 Reaction vALDO

This is a reversible reaction of one reactant forming two products.

Name Aldolase

Reaction equation

$$cfdp \Longrightarrow cdhap + cgap$$
 (26)

Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
cfdp	Fructose-1,6-bisphosphate	

Products

Table 35: Properties of each product.

Id	Name	SBO
cdhap cgap	Dihydroxyacetonephosphate Glyceraldehyde-3-Phosphate	

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

$$\begin{aligned} & v_{10} \\ &= \frac{\text{vol}\left(\text{cytosol}\right) \cdot \text{rmaxALDO} \cdot \left(\left[\text{cfdp}\right] - \frac{\left[\text{cgap}\right] \cdot \left[\text{cdhap}\right]}{\text{kALDOeq}}\right)}{\text{kALDOfdp} + \left[\text{cfdp}\right] + \frac{\text{kALDOgap} \cdot \left[\text{cdhap}\right]}{\text{kALDOeq} \cdot \text{VALDOblf}} + \frac{\text{kALDOdhap} \cdot \left[\text{cgap}\right]}{\text{kALDOeq} \cdot \text{VALDOblf}} + \frac{\left[\text{cfdp}\right] \cdot \left[\text{cgap}\right]}{\text{kALDOeq} \cdot \text{VALDOblf}} + \frac{\left[\text{cgap}\right] \cdot \left[\text{cdhap}\right]}{\text{kALDOeq} \cdot \text{VALDOblf}} + \frac{\left[\text{cfdp}\right] \cdot \left[\text{cgap}\right]}{\text{kALDOeq} \cdot \text{VALDOblf}} + \frac{\left[\text{cfdp}\right] \cdot \left[\text{cgap}\right]}{\text{kALDOeq} \cdot \text{VALDOblf}} + \frac{\left[\text{cfdp}\right] \cdot \left[\text{cgap}\right]}{\text{kALDOeq}} + \frac{\left[\text{cfdp}\right] \cdot \left[\text{cgap}\right]}{\text{valdoblf} \cdot \text{kALDOeq}} + \frac{\left[\text{cfdp}\right] \cdot \left[\text{cfdp}\right]}{\text{valdoblf} \cdot \text{kALDOeq}} + \frac{\left[\text{cfdp}\right] \cdot \left[\text{cgap}\right]}{\text{valdoblf} \cdot \text{kALDOeq}} + \frac{\left[\text{cfdp}\right] \cdot \left[\text{cgap}\right]}{\text{valdoblf} \cdot \text{kALDOeq}} + \frac{\left[\text{cfdp}\right] \cdot \left[\text{cfdp}\right]}{\text{valdoblf} \cdot \text{valdoblf}} + \frac{\left[\text{cfdp}\right] \cdot \left[\text{cfdp}\right]}{\text{valdoblf} \cdot \text{valdoblf}} + \frac{\left[\text{cfdp}\right] \cdot \left[\text{cfdp}\right]}{\text{valdoblf}} + \frac{\left[\text{cfdp}\right]}{\text{valdoblf}} + \frac{\left$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxALDO			17.415	$mmol \cdot l^{-1} \cdot s^{-1}$	
kALD0eq			0.144	$\operatorname{mmol} \cdot l^{-1}$	
kALDOfdp			1.750	$\operatorname{mmol} \cdot l^{-1}$	
kALDOgap			0.088	$mmol \cdot l^{-1}$	$ \overline{\mathbf{Z}} $
VALDOblf			2.000	dimensionless	$ \overline{\mathbf{Z}} $
kALDOdhap			0.088	$mmol \cdot l^{-1}$	$ \overline{\mathscr{L}} $
kALD0gapinh			0.600	$\operatorname{mmol} \cdot l^{-1}$	$\overline{\mathbf{Z}}$

7.11 Reaction vGAPDH

This is a reversible reaction of one reactant forming one product.

Name Glyceraldehyde-3-phosphate dehydrogenase

Reaction equation

$$cgap \rightleftharpoons cpgp$$
 (28)

Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
cgap	Glyceraldehyde-3-Phosphate	

Product

Table 38: Properties of each product.

Id Name		SBO
cpgp	1,3-diphosphosphoglycerate	

Derived unit contains undeclared units

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

Table 39: Properties of each parameter.

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

7.12 Reaction vTIS

This is a reversible reaction of one reactant forming one product.

Name Triosephosphate isomerase

Reaction equation

$$cdhap \rightleftharpoons cgap \tag{30}$$

Reactant

Table 40: Properties of each reactant.

	1	
Id	Name	SBO
cdhap	Dihydroxyacetonephosphate	

Product

Table 41: Properties of each product.

Id	Name	SBO
cgap	Glyceraldehyde-3-Phosphate	

Derived unit contains undeclared units

$$v_{12} = \frac{\text{vol}(\text{cytosol}) \cdot \text{rmaxTIS} \cdot \left([\text{cdhap}] - \frac{[\text{cgap}]}{\text{kTISeq}} \right)}{\text{kTISdhap} \cdot \left(1 + \frac{[\text{cgap}]}{\text{kTISgap}} \right) + [\text{cdhap}]}$$
(31)

Table 42: Properties of each parameter.

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

7.13 Reaction vTRPSYNTH

This is a reversible reaction of no reactant forming two products.

Name Tryptophan synthesis

Reaction equation

$$\emptyset \rightleftharpoons cpyr + cgap \tag{32}$$

Products

Table 43: Properties of each product.

Id	Name	SBO
10	Pyruvate Glyceraldehyde-3-Phosphate	

Kinetic Law

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

$$v_{13} = \text{vol}(\text{cytosol}) \cdot \text{rmaxTrpSynth}$$
 (33)

Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxTrpS	ynth		0.001	$mmol \cdot l^{-1} \cdot s^{-1}$	\overline{Z}

7.14 Reaction vG3PDH

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

Name Glycerol-3-phosphate dehydrogenase

Reaction equation

$$cdhap \rightleftharpoons \emptyset \tag{34}$$

Reactant

Table 45: Properties of each reactant.

Id Name		SBO
cdhap	Dihydroxyacetonephosphate	

Kinetic Law

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

$$v_{14} = \frac{\text{vol}\left(\text{cytosol}\right) \cdot \text{rmaxG3PDH} \cdot \left[\text{cdhap}\right]}{\text{KG3PDHdhap} + \left[\text{cdhap}\right]} \tag{35}$$

Table 46: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxG3PDH KG3PDHdhap				$\begin{array}{c} \text{mmol} \cdot l^{-1} \cdot s^{-1} \\ \text{mmol} \cdot l^{-1} \end{array}$	✓

7.15 Reaction vPGK

This is a reversible reaction of one reactant forming one product.

Name Phosphoglycerate kinase

Reaction equation

$$cpgp \rightleftharpoons cpg3 \tag{36}$$

Reactant

Table 47: Properties of each reactant.

Id	Name	SBO
cpgp	1,3-diphosphosphoglycerate	

Product

Table 48: Properties of each product.

Id	Name	SBO
cpg3	3-Phosphoglycerate	

Kinetic Law

$$v_{15} = \frac{\text{vol}\left(\text{cytosol}\right) \cdot \text{rmaxPGK} \cdot \left(\text{cadp} \cdot [\text{cpgp}] - \frac{\text{catp} \cdot [\text{cpg3}]}{\text{KPGKeq}}\right)}{\left(\text{KPGKadp} \cdot \left(1 + \frac{\text{catp}}{\text{KPGKatp}}\right) + \text{cadp}\right) \cdot \left(\text{KPGKpgp} \cdot \left(1 + \frac{[\text{cpg3}]}{\text{KPGKpg3}}\right) + [\text{cpgp}]\right)}$$
(37)

Table 49: Properties of each parameter.

		1		
Name	SBO	Value	Unit	Constant
		3021.774	$mmol \cdot l^{-1} \cdot s^{-1}$	
		1934.400	dimensionless	
		0.185	$\operatorname{mmol} \cdot 1^{-1}$	
		0.653	$\operatorname{mmol} \cdot 1^{-1}$	
		0.047	$\text{mmol} \cdot 1^{-1}$	
		0.473	$mmol \cdot l^{-1}$	\square
	Name	Name SBO	3021.774 1934.400 0.185 0.653 0.047	$\begin{array}{cccc} 3021.774 & \text{mmol} \cdot l^{-1} \cdot s^{-1} \\ 1934.400 & \text{dimensionless} \\ 0.185 & \text{mmol} \cdot l^{-1} \\ 0.653 & \text{mmol} \cdot l^{-1} \\ 0.047 & \text{mmol} \cdot l^{-1} \end{array}$

7.16 Reaction vsersynth

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

Name Serine synthesis

Reaction equation

$$cpg3 \rightleftharpoons \emptyset \tag{38}$$

Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
cpg3	3-Phosphoglycerate	

Kinetic Law

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

$$v_{16} = \frac{\text{vol}(\text{cytosol}) \cdot \text{rmaxSerSynth} \cdot [\text{cpg3}]}{\text{KSerSynthpg3} + [\text{cpg3}]}$$
(39)

Table 51: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxSerSynth KSerSynthpg3				$\begin{array}{c} \operatorname{mmol} \cdot l^{-1} \cdot s^{-1} \\ \operatorname{mmol} \cdot l^{-1} \end{array}$	2

7.17 Reaction vrpGluMu

This is a reversible reaction of one reactant forming one product.

Name Phosphoglycerate mutase

Reaction equation

$$cpg3 \Longrightarrow cpg2 \tag{40}$$

Table 52: Properties of each reactant.

There exists of the streether.					
Id	Name	SBO			
cpg3	3-Phosphoglycerate				

Table 53: Properties of each product.

	F	
Id	Name	SBO
cpg2	2-Phosphoglycerate	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \frac{\text{vol}\left(\text{cytosol}\right) \cdot \text{rmaxPGluMu} \cdot \left(\left[\text{cpg3}\right] - \frac{\left[\text{cpg2}\right]}{\text{KPGluMueq}}\right)}{\text{KPGluMupg3} \cdot \left(1 + \frac{\left[\text{cpg2}\right]}{\text{KPGluMupg2}}\right) + \left[\text{cpg3}\right]}$$
(41)

Table 54: Properties of each parameter.

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

7.18 Reaction vENO

This is a reversible reaction of one reactant forming one product.

Name Enolase

Reaction equation

$$cpg2 \rightleftharpoons cpep$$
 (42)

Table 55: Properties of each reactant.

Id	Name	SBO
cpg2	2-Phosphoglycerate	

Table 56: Properties of each product.

Id	Name	SBO
срер	Phosphoenol pyruvate	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \frac{\text{vol}(\text{cytosol}) \cdot \text{rmaxENO} \cdot \left([\text{cpg2}] - \frac{[\text{cpep}]}{\text{KENOeq}} \right)}{\text{KENOpg2} \cdot \left(1 + \frac{[\text{cpep}]}{\text{KENOpep}} \right) + [\text{cpg2}]}$$
(43)

Table 57: Properties of each parameter.

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

7.19 Reaction vPK

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

Name Pyruvate kinase

Reaction equation

$$cpep \xrightarrow{cfdp} cpyr \tag{44}$$

Table 58: Properties of each reactant.

Id	Name	SBO
срер	Phosphoenol pyruvate	

Modifier

Table 59: Properties of each modifier.

Id	Name	SBO
cfdp	Fructose-1,6-bisphosphate	

Product

Table 60: Properties of each product.

Id	Name	SBO
cpyr	Pyruvate	

Kinetic Law

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

$$\tag{45}$$

Table 61: Properties of each parameter.

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

7.20 Reaction vpepCxylase

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

Name PEP carboxylase

Reaction equation

$$cpep \stackrel{cfdp}{\longleftarrow} \emptyset \tag{46}$$

Reactant

Table 62: Properties of each reactant.

Id	Name	SBO
срер	Phosphoenol pyruvate	

Modifier

Table 63: Properties of each modifier.

Id	Name	SBO
cfdp	Fructose-1,6-bisphosphate	

Kinetic Law

$$v_{20} = \frac{\text{vol}(\text{cytosol}) \cdot \text{rmaxpepCxylase} \cdot [\text{cpep}] \cdot \left(1 + \left(\frac{[\text{cfdp}]}{\text{KpepCxylasefdp}}\right)^{\text{npepCxylasefdp}}\right)}{\text{KpepCxylasepep} + [\text{cpep}]}$$
(47)

Table 64: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxpepCx	kylase		0.107	$mmol \cdot l^{-1} \cdot s^{-1}$	\square
KpepCxyla	asefdp		0.700	$\text{mmol} \cdot 1^{-1}$	\square
npepCxyla	asefdp		4.210	dimensionless	\square
KpepCxyla	asepep		4.070	$mmol \cdot l^{-1}$	\square

7.21 Reaction vSynth1

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

Name Synthesis 1

Reaction equation

$$\operatorname{cpep} \Longrightarrow \emptyset \tag{48}$$

Reactant

Table 65: Properties of each reactant.

Id	Name	SBO
cpep	Phosphoenol pyruvate	

Kinetic Law

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

$$v_{21} = \frac{\text{vol}(\text{cytosol}) \cdot \text{rmaxSynth1} \cdot [\text{cpep}]}{\text{KSynth1pep} + [\text{cpep}]}$$
(49)

Table 66: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxSynth1 KSynth1pep				$\begin{array}{c} \text{mmol} \cdot \mathbf{l}^{-1} \cdot \mathbf{s}^{-1} \\ \text{mmol} \cdot \mathbf{l}^{-1} \end{array}$	1

7.22 Reaction vSynth2

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

Name Synthesis 2

Reaction equation

$$\operatorname{cpyr} \Longrightarrow \emptyset \tag{50}$$

Table 67: Properties of each reactant.

Id	Name	SBO
cpyr	Pyruvate	

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

$$v_{22} = \frac{\text{vol}\left(\text{cytosol}\right) \cdot \text{rmaxSynth2} \cdot [\text{cpyr}]}{\text{KSynth2pyr} + [\text{cpyr}]} \tag{51}$$

Table 68: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxSynth2 KSynth2pyr			0.074 1.000	$\begin{array}{c} mmol \cdot \mathbf{l}^{-1} \cdot \mathbf{s}^{-1} \\ mmol \cdot \mathbf{l}^{-1} \end{array}$	1

7.23 Reaction vDAHPS

This is a reversible reaction of two reactants forming no product.

Name DAHP synthesis

Reaction equation

$$ce4p + cpep \Longrightarrow \emptyset \tag{52}$$

Reactants

Table 69: Properties of each reactant.

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

Kinetic Law

$$\nu_{23} = \frac{\text{vol}\left(\text{cytosol}\right) \cdot \text{rmaxDAHPS} \cdot [\text{ce4p}]^{\text{nDAHPSe4p}} \cdot [\text{cpep}]^{\text{nDAHPSpep}}}{(\text{KDAHPSe4p} + [\text{ce4p}]^{\text{nDAHPSe4p}}) \cdot (\text{KDAHPSpep} + [\text{cpep}]^{\text{nDAHPSpep}})} \tag{53}$$

Table 70: Properties of each parameter.

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

7.24 Reaction vPDH

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

Name Pyruvate dehydrogenase

Reaction equation

$$cpyr \Longrightarrow \emptyset \tag{54}$$

Reactant

Table 71: Properties of each reactant.

Id	Name	SBO
cpyr	Pyruvate	

Kinetic Law

$$v_{24} = \frac{\text{vol}(\text{cytosol}) \cdot \text{rmaxPDH} \cdot [\text{cpyr}]^{\text{nPDH}}}{\text{KPDHpyr} + [\text{cpyr}]^{\text{nPDH}}}$$
(55)

Table 72: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxPDH			6.060	$mmol \cdot l^{-1} \cdot s^{-1}$	$ \mathbf{Z} $
\mathtt{nPDH}			3.680	dimensionless	
KPDHpyr			1159.000	$\operatorname{mmol} \cdot 1^{-1}$	

7.25 Reaction vMethSynth

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

Name Methionine synthesis

Reaction equation

$$\emptyset \rightleftharpoons \text{cpyr}$$
 (56)

Product

Table 73: Properties of each product.

Id	Name	SBO
cpyr	Pyruvate	

Kinetic Law

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

$$v_{25} = \text{vol}(\text{cytosol}) \cdot \text{rmaxMetSynth}$$
 (57)

Table 74: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxMetSyn	ıth		0.002	$mmol \cdot l^{-1} \cdot s^{-1}$	

7.26 Reaction vPGDH

This is a reversible reaction of one reactant forming one product.

Name 6-Phosphogluconate dehydrogenase

Reaction equation

$$cpg \Longrightarrow cribu5p \tag{58}$$

Table 75: Properties of each reactant.				
Id	Name	SBO		
cpg	6-Phosphogluconate			

Table 76: Properties of each product

Id	Name	SBO
cribu5p	Ribulose-5-phosphate	

Kinetic Law

Derived unit contains undeclared units

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

Table 77: Properties of each parameter.

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

7.27 Reaction vR5PI

This is a reversible reaction of one reactant forming one product.

Name Ribose-phosphate isomerase

Reaction equation

$$cribu5p \rightleftharpoons crib5p$$
 (60)

Table 78: Properties of each reactant.

Id	Name	SBO
cribu5p	Ribulose-5-phosphate	

Table 79: Properties of each product.

Id	Name	SBO
crib5p	Ribose-5-phosphate	

Kinetic Law

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

$$v_{27} = \text{vol}(\text{cytosol}) \cdot \text{rmaxR5PI} \cdot \left([\text{cribu5p}] - \frac{[\text{crib5p}]}{\text{KR5PIeq}} \right)$$
 (61)

Table 80: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxR5PI KR5PIeq			4.838 4.000	s ⁻¹ dimensionless	<u>✓</u>

7.28 Reaction vRu5P

This is a reversible reaction of one reactant forming one product.

Name Ribulose-phosphate epimerase

Reaction equation

$$cribu5p \Longrightarrow cxyl5p$$
 (62)

Table 81: Properties of each reactant.

Id	Name	SBO
cribu5p	Ribulose-5-phosphate	

Table 82: Properties of each product.

Id	Name	SBO
cxyl5p	Xylulose-5-phosphate	

Kinetic Law

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

$$v_{28} = \text{vol}(\text{cytosol}) \cdot \text{rmaxRu5P} \cdot \left([\text{cribu5p}] - \frac{[\text{cxyl5p}]}{\text{KRu5Peq}} \right)$$
 (63)

Table 83: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxRu5P			6.739	s^{-1}	\overline{Z}
KRu5Peq			1.400	dimensionless	\square

7.29 Reaction vPPK

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

Name Ribose phosphate pyrophosphokinase

Reaction equation

$$crib5p \Longrightarrow \emptyset$$
 (64)

Reactant

Table 84: Properties of each reactant.

Id	Name	SBO
crib5p	Ribose-5-phosphate	

Kinetic Law

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

$$v_{29} = \frac{\text{vol}(\text{cytosol}) \cdot \text{rmaxRPPK} \cdot [\text{crib5p}]}{\text{KRPPKrib5p} + [\text{crib5p}]}$$
(65)

Table 85: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
rmaxRPPK KRPPKrib5p			0.013 0.100	$\begin{array}{c} mmol \cdot \mathbf{l}^{-1} \cdot \mathbf{s}^{-1} \\ mmol \cdot \mathbf{l}^{-1} \end{array}$	✓

7.30 Reaction vG1PAT

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

Name Glucose-1-phosphate adenyltransferase

Reaction equation

$$cg1p \stackrel{cfdp}{\rightleftharpoons} \emptyset \tag{66}$$

Reactant

Table 86: Properties of each reactant.

Id	Name	SBO
cg1p	Glucose-1-Phosphate	

Modifier

Table 87: Properties of each modifier.

Id	Name	SBO
cfdp	Fructose-1,6-bisphosphate	

Kinetic Law

Derived unit contains undeclared units

$$\nu_{30} = \frac{\text{vol}\left(\text{cytosol}\right) \cdot \text{rmaxG1PAT} \cdot \left[\text{cg1p}\right] \cdot \text{catp} \cdot \left(1 + \left(\frac{\left[\text{cfdp}\right]}{\text{KG1PATfdp}}\right)^{\text{nG1PATfdp}}\right)}{\left(\text{KG1PATatp} + \text{catp}\right) \cdot \left(\text{KG1PATg1p} + \left[\text{cg1p}\right]\right)} \tag{67}$$

Table 88: Properties of each parameter.

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

7.31 Reaction vG6P

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

Name G6P degradation

Reaction equation

$$cg6p \rightleftharpoons \emptyset$$
 (68)

Reactant

Table 89: Properties of each reactant.

Table 67. I Toperties of Cach reactain.					
Id	Name	SBO			
cg6p	Glucose-6-Phosphate				

Kinetic Law

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

$$v_{31} = \text{vol}(\text{cytosol}) \cdot \text{mu} \cdot [\text{cg6p}] \tag{69}$$

Table 90: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			$2.78 \cdot 10^{-5}$	s^{-1}	

7.32 Reaction vf6P

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

Name F6P degradation

$$cf6p \rightleftharpoons \emptyset \tag{70}$$

Reactant

Table 91: Properties of each reactant.

Id	Name	SBO
cf6p	Fructose-6-Phosphate	

Kinetic Law

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

$$v_{32} = \text{vol}(\text{cytosol}) \cdot \text{mu} \cdot [\text{cf6p}] \tag{71}$$

Table 92: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			$2.78 \cdot 10^{-5}$	s^{-1}	

7.33 Reaction vfdP

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

Name FDP degradation

Reaction equation

$$cfdp \rightleftharpoons \emptyset \tag{72}$$

Reactant

Table 93: Properties of each reactant.

Id	Name	SBO
cfdp	Fructose-1,6-bisphosphate	

Kinetic Law

$$v_{33} = \text{vol}(\text{cytosol}) \cdot \text{mu} \cdot [\text{cfdp}]$$
 (73)

Table 94: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			$2.78 \cdot 10^{-5}$	s^{-1}	\overline{Z}

7.34 Reaction vGAP

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

Name GAP degradation

Reaction equation

$$\operatorname{cgap} \rightleftharpoons \emptyset \tag{74}$$

Reactant

Table 95: Properties of each reactant.

Id	Name	SBO
cgap	Glyceraldehyde-3-Phosphate	

Kinetic Law

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

$$v_{34} = \text{vol}(\text{cytosol}) \cdot \text{mu} \cdot [\text{cgap}]$$
 (75)

Table 96: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			$2.78 \cdot 10^{-5}$	s^{-1}	Ø

7.35 Reaction vDHAP

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

Name DHAP degradation

$$cdhap \rightleftharpoons \emptyset \tag{76}$$

Reactant

Table 97: Properties of each reactant.

Id	Name	SBO
cdhap	Dihydroxyacetonephosphate	

Kinetic Law

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

$$v_{35} = \text{vol}(\text{cytosol}) \cdot \text{mu} \cdot [\text{cdhap}] \tag{77}$$

Table 98: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			$2.78 \cdot 10^{-5}$	s^{-1}	

7.36 Reaction vPGP

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

Name PGP degradation

Reaction equation

$$\operatorname{cpgp} \Longrightarrow \emptyset \tag{78}$$

Reactant

Table 99: Properties of each reactant.

Id	Name	SBO
cpgp	1,3-diphosphosphoglycerate	

Kinetic Law

$$v_{36} = \text{vol}(\text{cytosol}) \cdot \text{mu} \cdot [\text{cpgp}]$$
 (79)

Table 100: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			$2.78 \cdot 10^{-5}$	s^{-1}	\overline{Z}

7.37 Reaction vPG3

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

Name PG3 degradation

Reaction equation

$$cpg3 \rightleftharpoons \emptyset \tag{80}$$

Reactant

Table 101: Properties of each reactant.

Id	Name	SBO
cpg3	3-Phosphoglycerate	

Kinetic Law

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

$$v_{37} = \text{vol}(\text{cytosol}) \cdot \text{mu} \cdot [\text{cpg3}]$$
 (81)

Table 102: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			$2.78 \cdot 10^{-5}$	s^{-1}	Ø

7.38 Reaction vpg2

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

Name PG2 degradation

$$cpg2 \rightleftharpoons \emptyset \tag{82}$$

Reactant

Table 103: Properties of each reactant.

Id	Name	SBO
cpg2	2-Phosphoglycerate	

Kinetic Law

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

$$v_{38} = \text{vol}(\text{cytosol}) \cdot \text{mu} \cdot [\text{cpg2}]$$
 (83)

Table 104: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			$2.78 \cdot 10^{-5}$	s^{-1}	

7.39 Reaction vPEP

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

Name PEP degradation

Reaction equation

$$\operatorname{cpep} \Longrightarrow \emptyset \tag{84}$$

Reactant

Table 105: Properties of each reactant.

Id	Name	SBO
срер	Phosphoenol pyruvate	

Kinetic Law

$$v_{39} = \text{vol}(\text{cytosol}) \cdot \text{mu} \cdot [\text{cpep}]$$
 (85)

Table 106: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			$2.78 \cdot 10^{-5}$	s^{-1}	\overline{Z}

7.40 Reaction vRibu5p

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

Name Ribu5P dilution

Reaction equation

$$cribu5p \Longrightarrow \emptyset \tag{86}$$

Reactant

Table 107: Properties of each reactant.

	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	
Id	Name	SBO
cribu5p	Ribulose-5-phosphate	

Kinetic Law

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

$$v_{40} = \text{vol}(\text{cytosol}) \cdot \text{mu} \cdot [\text{cribu5p}]$$
 (87)

Table 108: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			$2.78 \cdot 10^{-5}$	s^{-1}	Ø

7.41 Reaction vRIB5P

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

Name Rib5P dilution

$$crib5p \Longrightarrow \emptyset \tag{88}$$

Reactant

Table 109: Properties of each reactant.

Id	Name	SBO
crib5p	Ribose-5-phosphate	

Kinetic Law

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

$$v_{41} = \text{vol}(\text{cytosol}) \cdot \text{mu} \cdot [\text{crib5p}]$$
 (89)

Table 110: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			$2.78 \cdot 10^{-5}$	s^{-1}	

7.42 Reaction vXYL5P

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

Name XYL5P dilution

Reaction equation

$$cxyl5p \Longrightarrow \emptyset \tag{90}$$

Reactant

Table 111: Properties of each reactant.

Id	Name	SBO
cxyl5p	Xylulose-5-phosphate	

Kinetic Law

$$v_{42} = \text{vol}(\text{cytosol}) \cdot \text{mu} \cdot [\text{cxyl5p}]$$
 (91)

Table 112: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			$2.78 \cdot 10^{-5}$	s^{-1}	\overline{Z}

7.43 Reaction vSED7P

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

Name SED7P dilution

Reaction equation

$$\csc d7p \Longrightarrow \emptyset \tag{92}$$

Reactant

Table 113: Properties of each reactant.

Id	Name	SBO
csed7p	sedoheptulose-7-phosphate	

Kinetic Law

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

$$v_{43} = \text{vol}(\text{cytosol}) \cdot \text{mu} \cdot [\text{csed7p}]$$
 (93)

Table 114: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			$2.78 \cdot 10^{-5}$	s^{-1}	Ø

7.44 Reaction vpyr

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

Name Pyruvate dilution

$$cpyr \rightleftharpoons \emptyset \tag{94}$$

Reactant

Table 115: Properties of each reactant.

Id	Name	SBO
cpyr	Pyruvate	

Kinetic Law

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

$$v_{44} = \text{vol}(\text{cytosol}) \cdot \text{mu} \cdot [\text{cpyr}] \tag{95}$$

Table 116: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			$2.78 \cdot 10^{-5}$	s^{-1}	Ø

7.45 Reaction vPG

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

Name PG dilution

Reaction equation

$$cpg \Longrightarrow \emptyset \tag{96}$$

Reactant

Table 117: Properties of each reactant.

Id	Name	SBO
cpg	6-Phosphogluconate	

Kinetic Law

$$v_{45} = \text{vol}(\text{cytosol}) \cdot \text{mu} \cdot [\text{cpg}]$$
 (97)

Table 118: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			$2.78 \cdot 10^{-5}$	s^{-1}	\overline{Z}

7.46 Reaction vE4P

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

Name E4P dilution

Reaction equation

$$ce4p \rightleftharpoons \emptyset \tag{98}$$

Reactant

Table 119: Properties of each reactant.

Id	Name	SBO
ce4p	Erythrose-4-phosphate	

Kinetic Law

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

$$v_{46} = \text{vol}(\text{cytosol}) \cdot \text{mu} \cdot [\text{ce4p}] \tag{99}$$

Table 120: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			$2.78 \cdot 10^{-5}$	s^{-1}	

7.47 Reaction vGLP

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

Name GLP dilution

$$cg1p \rightleftharpoons \emptyset \tag{100}$$

Reactant

Table 121: Properties of each reactant.

Tuese 121: 11 openies of each reactant.					
Id	Name	SBO			
cg1p	Glucose-1-Phosphate				

Kinetic Law

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

$$v_{47} = \text{vol}(\text{cytosol}) \cdot \text{mu} \cdot [\text{cg1p}] \tag{101}$$

Table 122: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			$2.78 \cdot 10^{-5}$	s^{-1}	

7.48 Reaction **VEXTER**

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

Name Extracellular glucose kinetics

Reaction equation

$$\emptyset \rightleftharpoons \text{cglcex}$$
 (102)

Product

Table 123: Properties of each product.

Id	Name	SBO
cglcex	Extracellular Glucose	

Kinetic Law

$$v_{48} = \text{vol}(\text{extracellular}) \cdot \text{Dil} \cdot (\text{cfeed} - [\text{cglcex}])$$
 (103)

Table 124: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Dil cfeed			$2.78 \cdot 10^{-5} \\ 110.960$	s^{-1} mmol·1 ⁻¹	Ø

8 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.

8.1 Species cpep

Name Phosphoenol pyruvate

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

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

$$\frac{d}{dt}cpep = v_{18} - 65 v_1 - v_{19} - v_{20} - v_{21} - v_{23} - v_{39}$$
(104)

8.2 Species cglcex

Name Extracellular Glucose

Initial concentration $2 \text{ mmol} \cdot 1^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cglcex} = v_{48} - v_1 \tag{105}$$

8.3 Species cg6p

Name Glucose-6-Phosphate

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cg6p} = 65\ v_1 - v_2 - v_3 - v_4 - v_{31} \tag{106}$$

8.4 Species cpyr

Name Pyruvate

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cpyr} = 65 v_1 + v_{13} + v_{19} + v_{25} - v_{22} - v_{24} - v_{44}$$
 (107)

8.5 Species cf6p

Name Fructose-6-Phosphate

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cf6p} = v_2 + v_6 + v_8 - v_5 - 2v_9 - v_{32} \tag{108}$$

8.6 Species cg1p

Name Glucose-1-Phosphate

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

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

$$\frac{d}{dt}cg1p = v_3 - v_{30} - v_{47} \tag{109}$$

8.7 Species cpg

Name 6-Phosphogluconate

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

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

$$\frac{d}{dt}cpg = v_4 - v_{26} - v_{45} \tag{110}$$

8.8 Species cfdp

Name Fructose-1,6-bisphosphate

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

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

$$\frac{d}{dt}cfdp = v_5 - v_{10} - v_{33} \tag{111}$$

8.9 Species csed7p

Name sedoheptulose-7-phosphate

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

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

$$\frac{d}{dt}\csc 7p = v_7 - v_6 - v_{43} \tag{112}$$

8.10 Species cgap

Name Glyceraldehyde-3-Phosphate

Initial concentration 0.218 mmol·l⁻¹

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cgap} = v_7 + v_8 + v_{10} + v_{12} + v_{13} - v_6 - v_{11} - v_{34}$$
 (113)

8.11 Species ce4p

Name Erythrose-4-phosphate

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ce4p} = v_6 - v_8 - v_{23} - v_{46} \tag{114}$$

8.12 Species cxy15p

Name Xylulose-5-phosphate

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

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

$$\frac{d}{dt} \exp(5p) = v_{28} - v_7 - v_8 - v_{42}$$
 (115)

8.13 Species crib5p

Name Ribose-5-phosphate

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{crib5p} = v_{27} - v_7 - v_{29} - v_{41} \tag{116}$$

8.14 Species cdhap

Name Dihydroxyacetonephosphate

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cdhap} = v_{10} - v_{12} - v_{14} - v_{35} \tag{117}$$

8.15 Species cpgp

Name 1,3-diphosphosphoglycerate

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

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

$$\frac{d}{dt}cpgp = v_{11} - v_{15} - v_{36} \tag{118}$$

8.16 Species cpg3

Name 3-Phosphoglycerate

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cpg3} = v_{15} - v_{16} - v_{17} - v_{37} \tag{119}$$

8.17 Species cpg2

Name 2-Phosphoglycerate

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

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

$$\frac{d}{dt}cpg2 = v_{17} - v_{18} - v_{38} \tag{120}$$

8.18 Species cribu5p

Name Ribulose-5-phosphate

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

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

$$\frac{d}{dt}\text{cribu5p} = v_{26} - v_{27} - v_{28} - v_{40} \tag{121}$$

 $\mathfrak{BML2}^{AT}$ EX was developed by Andreas Dräger^a, Hannes Planatscher^a, Dieudonné M Wouamba^a, Adrian Schröder^a, Michael Hucka^b, Lukas Endler^c, Martin Golebiewski^d and Andreas Zell^a. Please see http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX for more information.

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