SBML Model Report

Model name: “Jiang2007 - GSIS system, Pancreatic Beta Cells”

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah[1] and Kieran Smallbone[2] at November 29th 2011 at 12:14 a. m. and last time modified at April eighth 2016 at 4:06 p. m. Table 1 provides 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	4
species types	0	species	59
events	0	constraints	0
reactions	45	function definitions	0
global parameters	1	unit definitions	0
rules	0	initial assignments	0

Model Notes

Jiang2007 - GSIS system, Pancreatic Beta CellsDescription of a core kinetic model of the glucose-stimulated insulin secretion system (GSIS) in pancreatic beta cells.

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This model is described in the article:A kinetic core model of the glucose-stimulated insulin secretion network of pancreatic beta cells.Jiang N, Cox RD, Hancock JM.Mamm Genome 2007 Jul; 18(6-7):508-20.

Abstract:

The construction and characterization of a core kinetic model of the glucose-stimulated insulin secretion system (GSIS) in pancreatic beta cells is described. The model consists of 44 enzymatic reactions, 59 metabolic state variables, and 272 parameters. It integrates five subsystems: glycolysis, the TCA cycle, the respiratory chain, NADH shuttles, and the pyruvate cycle. It also takes into account compartmentalization of the reactions in the cytoplasm and mitochondrial matrix. The model shows expected behavior in its outputs, including the response of ATP production to starting glucose concentration and the induction of oscillations of metabolite concentrations in the glycolytic pathway and in ATP and ADP concentrations. Identification of choke points and parameter sensitivity analysis indicate that the glycolytic pathway, and to a lesser extent the TCA cycle, are critical to the proper behavior of the system, while parameters in other components such as the respiratory chain are less critical. Notably, however, sensitivity analysis identifies the first reactions of nonglycolytic pathways as being important for the behavior of the system. The model is robust to deletion of malic enzyme activity, which is absent in mouse pancreatic beta cells. The model represents a step toward the construction of a model with species-specific parameters that can be used to understand mouse models of diabetes and the relationship of these mouse models to the human disease state.

The model reproduces Figure 2 of the paper, and is built using files 'ModelNNT11.xml' and 'changed.m' available from http://www.har.mrc.ac.uk/research/bioinformatics/research_areas/systems_biology.html .

A couple of small errors in the model (in the original SBML file 'ModelNNT11.xml') have been corrected. The errors are:

- v44 now produces Pyr rather than PYR
- the kinetic law of v27 is now dependent on cytoplasmic (rather than mitochondrial) acetyl CoA and OXA

This model is hosted on BioModels Database and identified by: BIOMD0000000239 .

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 five unit definitions which are all predefined by SBML and not mentioned in the model.

2.1 Unit substance

Notes Mole is the predefined SBML unit for substance.

Definition mol

2.2 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

2.3 Unit area

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

Definition m^2

2.4 Unit length

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

Definition m

2.5 Unit time

Notes Second is the predefined SBML unit for time.

Definition s

3 Compartments

This model contains four compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
CYTOPLASM	cytoplasm		3	1	litre	☑	
MT_IMS	mitochondrial intermembrane space		3	1	litre	☑	
MT_IM	mitochondrial inner membrane		3	1	litre	☑	
MATRIX	mitochondrial matrix		3	1	litre	☑	

3.1 Compartment CYTOPLASM

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

Name cytoplasm

3.2 Compartment MT_IMS

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

Name mitochondrial intermembrane space

3.3 Compartment MT_IM

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

Name mitochondrial inner membrane

3.4 Compartment MATRIX

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

Name mitochondrial matrix

4 Species

This model contains 59 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
GLC	glucose	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
F6P	fructose-6-phosphate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
FBP	fructose-1,6-bisphosphate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
GAP	glyceraldehyde 3-phosphate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DPG	1,2-bisphospho-D-glycerate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PEP	phosphoenolpyruvate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PYR_cyt	pyruvate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
AMP	adenine monophosphate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
LAC	lactate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
G3P	glycerol-3-phosphate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DHAP	dihydrohxyacetone-phosphate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
OXA_cyt	oxaloacetate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Asp_cyt	aspartate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Glu_cyt	glutamate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
OG_cyt	oxoglutarate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Mal_cyt	malate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Acetyl_CoA_cyt	acetyl CoA	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CoA_cyt	coenzyme A	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
IsoCitcyt	isocitrate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Cit_cyt	citrate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ATP_cyt	adenine triphosphate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ADP_cyt	adenine diphosphate	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
NAD	NAD	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
NADH_cyt	NADH	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
NADP_cyt	NADP	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
NADPH_cyt	NADPH	CYTOPLASM	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Pyr	pyruvate	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CO2	carbon dioxide	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CoA	coenzyme A	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Acetyl_CoA	acetyl CoA	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Pi	phosphate	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Fum	fumarate	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
SCoA	succinyl-CoA	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Suc	succinate	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
GTP	guanosine triphosphate	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
GDP	guanosine diphosphate	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Ala	slanine	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Asp	aspartate	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Glu	glutamate	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
H2O	water	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ETFred	electron transfer flavoprotein (reduced form)	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ETFox	electron transfer flavoprotein (oxidised form)	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
FADH2	FADH2	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
FAD	FAD	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
OG	oxoglutarate	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Mal	malate	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
OXA	oxaloacetate	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
Cit	citrate	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
IsoCit	isocitrate	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ATP	adenine triphosphate	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ADP	adenine diphosphate	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
NADP_p	NADP+	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
NADPH	NADPH	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
NAD_p	NAD+	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
NADH	NADH	MATRIX	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Q	ubiquinone	MT_IMS	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
QH2	ubiquinol	MT_IMS	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Cytc3p	ferrocytochrome c	MT_IMS	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Cytc2p	ferricytochrome c	MT_IMS	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameter

This model contains one global parameter.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`flow`			0.011		☑

6 Reactions

This model contains 45 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	GLCflow		$\emptyset \rightleftharpoons \mathrm{GLC}$	
2	LACflow		$\mathrm{LAC} \longrightarrow \emptyset$	
3	GAPflow		$\mathrm{GAP} \longrightarrow \emptyset$	
4	v1	glucokinase	$\mathrm{GLC} + \mathrm{ATP\_cyt} \longrightarrow \mathrm{F6P} + \mathrm{ADP\_cyt}$	
5	v2	6-phosphofructokinase	$\mathrm{F6P} + \mathrm{ATP\_cyt} \xrightarrow{\mathrm{AMP}} \mathrm{FBP} + \mathrm{ADP\_cyt}$	
6	v3	fructose-bisphosphate aldolase	$\mathrm{FBP} \rightleftharpoons 2\,\mathrm{GAP}$	
7	v4	glyceraldehyde 3-phosphate dehydrogenase	$\mathrm{GAP} + \mathrm{NAD} \longrightarrow \mathrm{DPG} + \mathrm{NADH\_cyt}$	
8	v5	bisphosphoglycerate phosphotase (1/2)	$\mathrm{DPG} + \mathrm{ADP\_cyt} \rightleftharpoons \mathrm{PEP} + \mathrm{ATP\_cyt}$	
9	v6	pyruvate kinase	$\mathrm{PEP} + \mathrm{ADP\_cyt} \longrightarrow \mathrm{PYR\_cyt} + \mathrm{ATP\_cyt}$	
10	v7	lactate dehydrogenase	$\mathrm{PYR\_cyt} + \mathrm{NADH\_cyt} \rightleftharpoons \mathrm{LAC} + \mathrm{NAD}$	
11	hidden_1		$\mathrm{AMP} + \mathrm{ATP\_cyt} \rightleftharpoons 2\,\mathrm{ADP\_cyt}$	
12	v8	pyruvate carrier	$\mathrm{PYR\_cyt} \rightleftharpoons \mathrm{Pyr}$	
13	v9	pyruvate dehydrogenase complex	$\mathrm{Pyr} + \mathrm{CoA} + \mathrm{NAD\_p} \longrightarrow \mathrm{CO2} + \mathrm{Acetyl\_CoA} + \mathrm{NADH}$	
14	v10	citrate synthase	$\mathrm{OXA} + \mathrm{Acetyl\_CoA} \rightleftharpoons \mathrm{Cit} + \mathrm{CoA}$	
15	v11	aconitase	$\mathrm{Cit} \rightleftharpoons \mathrm{IsoCit}$	
16	v12	isocitrate dehydrogenase (NAD+) (alpha/beta/gamma)	$\mathrm{IsoCit} + \mathrm{NAD\_p} \xrightarrow{\mathrm{ADP}} \mathrm{OG} + \mathrm{NADH}$	
17	v14	oxoglutarate dehydrogenase complex	$\mathrm{OG} + \mathrm{CoA} + \mathrm{NAD\_p} \longrightarrow \mathrm{CO2} + \mathrm{SCoA} + \mathrm{NADH}$	
18	v15	succinyl-CoA synthetase	$\mathrm{GDP} + \mathrm{SCoA} + \mathrm{Pi} \rightleftharpoons \mathrm{Suc} + \mathrm{GTP} + \mathrm{CoA}$	
19	v16	succinate dehydrogenase	$\mathrm{Suc} + \mathrm{Q} \rightleftharpoons \mathrm{Fum} + \mathrm{QH2}$	
20	v17	fumarase	$\mathrm{Fum} \rightleftharpoons \mathrm{Mal}$	

№	Id	Name	Reaction Equation	SBO
21	v18	malate dehydrogenase (mitochondrion)	$\mathrm{Mal} + \mathrm{NAD\_p} \rightleftharpoons \mathrm{NADH} + \mathrm{OXA}$	
22	v20	alanine transaminase	$\mathrm{Ala} + \mathrm{OG} \rightleftharpoons \mathrm{Glu} + \mathrm{Pyr}$	
23	v21	aspartate transaminase	$\mathrm{OXA} + \mathrm{Glu} \rightleftharpoons \mathrm{Asp} + \mathrm{OG}$	
24	v22	aspartate/glutamate carrier	$\mathrm{Glu\_cyt} + \mathrm{Asp} \rightleftharpoons \mathrm{Asp\_cyt} + \mathrm{Glu}$	
25	v24	NADH:ubiquinone oxidoreductase	$\mathrm{NADH} + \mathrm{Q} \rightleftharpoons \mathrm{NAD\_p} + \mathrm{QH2}$	
26	v25	ubiquinol:cytochrome c oxidoreductase	$\mathrm{QH2} + 2\,\mathrm{Cytc3p} \longrightarrow \mathrm{Q} + 2\,\mathrm{Cytc2p}$	
27	v26	cytochrome c oxidase	$\mathrm{Cytc2p} \longrightarrow \mathrm{Cytc3p}$	
28	v27	citrate synthase	$\mathrm{Cit\_cyt} + \mathrm{CoA\_cyt} \rightleftharpoons \mathrm{OXA\_cyt} + \mathrm{Acetyl\_CoA\_cyt}$	
29	v28	ATPase complex	$\mathrm{ADP} + \mathrm{Pi} \rightleftharpoons \mathrm{ATP} + \mathrm{H2O}$	
30	v29	aconitase	$\mathrm{Cit\_cyt} \rightleftharpoons \mathrm{IsoCitcyt}$	
31	v30	oxoglutarate carrier	$\mathrm{Mal\_cyt} + \mathrm{OG} \rightleftharpoons \mathrm{OG\_cyt} + \mathrm{Mal}$	
32	v31	malate dehydrogenase (cytosol)	$\mathrm{NADH\_cyt} + \mathrm{OXA\_cyt} \longrightarrow \mathrm{Mal\_cyt} + \mathrm{NAD}$	
33	v32	aspartate transaminase	$\mathrm{Asp\_cyt} + \mathrm{OG\_cyt} \rightleftharpoons \mathrm{OXA\_cyt} + \mathrm{Glu\_cyt}$	
34	v33	citrate carrier	$\mathrm{Cit\_cyt} + \mathrm{Mal} \rightleftharpoons \mathrm{Mal\_cyt} + \mathrm{Cit}$	
35	v34	ETF:Q oxidoreductase	$\mathrm{ETFred} + \mathrm{Q} \rightleftharpoons \mathrm{ETFox} + \mathrm{QH2}$	
36	v35	glutathione reductase	$\mathrm{FADH2} + \mathrm{ETFox} \rightleftharpoons \mathrm{ETFred} + \mathrm{FAD}$	
37	v36	pyruvate decarboxylase	$\mathrm{ATP} + \mathrm{CO2} + \mathrm{Pyr} \rightleftharpoons \mathrm{Pi} + \mathrm{ADP} + \mathrm{OXA}$	
38	v37	glycerol-3-phosphate dehydrogenase (FAD dependent)	$\mathrm{G3P} + \mathrm{FAD} \longrightarrow \mathrm{FADH2} + \mathrm{DHAP}$	
39	v38	glycerol-3-phosphate dehydrogenase (NAD+ dependent)	$\mathrm{NADH\_cyt} + \mathrm{DHAP} \longrightarrow \mathrm{G3P} + \mathrm{NAD}$	
40	v40	ATP/ADP carrier	$\mathrm{ADP\_cyt} \longrightarrow \mathrm{ADP}$	
41	v41	cytosolic isocitrate dehydrogenase	$\mathrm{IsoCitcyt} + \mathrm{NADP\_cyt} \overset{\mathrm{CO2}}{\rightleftharpoons} \mathrm{OG\_cyt} + \mathrm{NADPH\_cyt}$	
42	v42	citrate carrier	$\mathrm{IsoCitcyt} + \mathrm{Mal} \rightleftharpoons \mathrm{Mal\_cyt} + \mathrm{IsoCit}$	
43	v43	ATP/ADP carrier	$\mathrm{ATP} \longrightarrow \mathrm{ATP\_cyt}$	
44	v39	malate dehydrogenase (oxaloacetate-decarboxylating) (NADP+)	$\mathrm{Mal\_cyt} + \mathrm{NADP\_cyt} \rightleftharpoons \mathrm{NADPH\_cyt} + \mathrm{PYR\_cyt}$	
45	v44	malate dehydrogenase (oxaloacetate-decarboxylating) (NADP+)	$\mathrm{Mal} + \mathrm{NADP\_p} \rightleftharpoons \mathrm{NADPH} + \mathrm{Pyr}$	

№	Id	Name	Reaction Equation	SBO

6.1 Reaction GLCflow

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

Reaction equation

$$\emptyset \rightleftharpoons \mathrm{GLC} \tag{1}$$

Product

Table 6: Properties of each product.

Id	Name	SBO
GLC	glucose	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{CYTOPLASM}) \cdot \left(\mathrm{Glc\_F} \cdot 10^{-3} - [\mathrm{GLC}]\right) \cdot \mathrm{flow} \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Glc_F			64.941		☑

6.2 Reaction LACflow

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

Reaction equation

$$\mathrm{LAC} \longrightarrow \emptyset \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
LAC	lactate	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol}\,(\text{CYTOPLASM}) \cdot [\text{LAC}] \cdot \text{flow} \tag{4}$$

6.3 Reaction GAPflow

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

Reaction equation

$$\text{GAP} \longrightarrow \emptyset \tag{5}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
GAP	glyceraldehyde 3-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}\,(\text{CYTOPLASM}) \cdot [\text{GAP}] \cdot \text{flow} \tag{6}$$

6.4 Reaction v1

This is an irreversible reaction of two reactants forming two products.

Name glucokinase

Reaction equation

$$\text{GLC} + \text{ATP\_cyt} \longrightarrow \text{F6P} + \text{ADP\_cyt} \tag{7}$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
GLC	glucose	
ATP_cyt	adenine triphosphate	

Products

Table 11: Properties of each product.

Id	Name	SBO
F6P	fructose-6-phosphate	
ADP_cyt	adenine diphosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{CYTOPLASM}) \cdot \frac{\mathrm{V1} \cdot [\mathrm{ATP\_cyt}] \cdot [\mathrm{GLC}]}{(\mathrm{K1GLC} + [\mathrm{GLC}]) \cdot (\mathrm{K1ATP} + [\mathrm{ATP\_cyt}])} \tag{8}$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V1			$5 \cdot 10^{-4}$		☑
K1GLC			10^{-4}		☑
K1ATP			$6.3 \cdot 10^{-5}$		☑

6.5 Reaction v2

This is an irreversible reaction of two reactants forming two products influenced by one modifier.

Name 6-phosphofructokinase

Reaction equation

$$\mathrm{F6P} + \mathrm{ATP\_cyt} \xrightarrow{\mathrm{AMP}} \mathrm{FBP} + \mathrm{ADP\_cyt} \tag{9}$$

Reactants

Table 13: Properties of each reactant.

Id	Name	SBO
F6P	fructose-6-phosphate	
ATP_cyt	adenine triphosphate	

Modifier

Table 14: Properties of each modifier.

Id	Name	SBO
AMP	adenine monophosphate	

Products

Table 15: Properties of each product.

Id	Name	SBO
FBP	fructose-1,6-bisphosphate	
ADP_cyt	adenine diphosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{CYTOPLASM}) \cdot \frac{\mathrm{V2} \cdot [\mathrm{ATP\_cyt}] \cdot [\mathrm{F6P}]^2}{\left(\mathrm{K2} \cdot \left(1 + \mathrm{k2} \cdot \left(\frac{[\mathrm{ATP\_cyt}]}{[\mathrm{AMP}]}\right)^2\right) + [\mathrm{F6P}]^2\right) \cdot (\mathrm{K2ATP} + [\mathrm{ATP\_cyt}])} \tag{10}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V2			0.002		☑
K2			$1.6 \cdot 10^{-9}$		☑
k2			0.017		☑
K2ATP			10^{-5}		☑

6.6 Reaction v3

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

Name fructose-bisphosphate aldolase

Reaction equation

$$\mathrm{FBP} \rightleftharpoons 2\,\mathrm{GAP} \tag{11}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
FBP	fructose-1,6-bisphosphate	

Product

Table 18: Properties of each product.

Id	Name	SBO
GAP	glyceraldehyde 3-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{CYTOPLASM}) \cdot \left(\mathrm{k3f} \cdot [\mathrm{FBP}] - \mathrm{k3b} \cdot [\mathrm{GAP}]^2\right) \tag{12}$$

Table 19: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k3f			1.00		☑
k3b			0.05		☑

6.7 Reaction v4

This is an irreversible reaction of two reactants forming two products.

Name glyceraldehyde 3-phosphate dehydrogenase

Reaction equation

$$\mathrm{GAP} + \mathrm{NAD} \longrightarrow \mathrm{DPG} + \mathrm{NADH\_cyt} \tag{13}$$

Reactants

Table 20: Properties of each reactant.

Id	Name	SBO
GAP	glyceraldehyde 3-phosphate	
NAD	NAD	

Products

Table 21: Properties of each product.

Id	Name	SBO
DPG	1,2-bisphospho-D-glycerate	
NADH_cyt	NADH	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{CYTOPLASM}) \cdot \frac{\mathrm{V4} \cdot [\mathrm{NAD}] \cdot [\mathrm{GAP}]}{(\mathrm{K4GAP} + [\mathrm{GAP}]) \cdot (\mathrm{K4NAD} + [\mathrm{NAD}])} \tag{14}$$

Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V4			0.010		☑
K4GAP			0.001		☑
K4NAD			0.001		☑

6.8 Reaction v5

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

Name bisphosphoglycerate phosphotase (1/2)

Reaction equation

$$\mathrm{DPG} + \mathrm{ADP\_cyt} \rightleftharpoons \mathrm{PEP} + \mathrm{ATP\_cyt} \tag{15}$$

Reactants

Table 23: Properties of each reactant.

Id	Name	SBO
DPG	1,2-bisphospho-D-glycerate	
ADP_cyt	adenine diphosphate	

Products

Table 24: Properties of each product.

Id	Name	SBO
PEP	phosphoenolpyruvate	
ATP_cyt	adenine triphosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{CYTOPLASM}) \cdot (\mathrm{k5f} \cdot [\mathrm{DPG}] \cdot [\mathrm{ADP\_cyt}] - \mathrm{k5b} \cdot [\mathrm{PEP}] \cdot [\mathrm{ATP\_cyt}]) \qquad (16)$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k5f			1000.0		☑
k5b			500.0		☑

6.9 Reaction v6

This is an irreversible reaction of two reactants forming two products.

Name pyruvate kinase

Reaction equation

$$\mathrm{PEP} + \mathrm{ADP\_cyt} \longrightarrow \mathrm{PYR\_cyt} + \mathrm{ATP\_cyt} \qquad (17)$$

Reactants

Table 26: Properties of each reactant.

Id	Name	SBO
PEP	phosphoenolpyruvate	
ADP_cyt	adenine diphosphate	

Products

Table 27: Properties of each product.

Id	Name	SBO
PYR_cyt	pyruvate	
ATP_cyt	adenine triphosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{CYTOPLASM}) \cdot \frac{\mathrm{V6} \cdot [\mathrm{ADP\_cyt}] \cdot [\mathrm{PEP}]}{(\mathrm{K6PEP} + [\mathrm{PEP}]) \cdot (\mathrm{K6ADP} + [\mathrm{ADP\_cyt}])} \tag{18}$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V6			0.010		☑
K6PEP			$2 \cdot 10^{-4}$		☑
K6ADP			$3 \cdot 10^{-4}$		☑

6.10 Reaction v7

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

Name lactate dehydrogenase

Reaction equation

$$\mathrm{PYR\_cyt} + \mathrm{NADH\_cyt} \rightleftharpoons \mathrm{LAC} + \mathrm{NAD} \tag{19}$$

Reactants

Table 29: Properties of each reactant.

Id	Name	SBO
PYR_cyt	pyruvate	
NADH_cyt	NADH	

Products

Table 30: Properties of each product.

Id	Name	SBO
LAC	lactate	
NAD	NAD	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\,(\mathrm{CYTOPLASM}) \cdot (\mathrm{k8f} \cdot [\mathrm{NADH\_cyt}] \cdot [\mathrm{PYR\_cyt}] - \mathrm{k8b} \cdot [\mathrm{NAD}] \cdot [\mathrm{LAC}]) \quad (20)$$

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k8f			1000.000		☑
k8b			0.143		☑

6.11 Reaction hidden_1

This is a reversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{AMP} + \mathrm{ATP\_cyt} \rightleftharpoons 2\,\mathrm{ADP\_cyt} \quad (21)$$

Reactants

Table 32: Properties of each reactant.

Id	Name	SBO
AMP	adenine monophosphate	

Id	Name	SBO
ATP_cyt	adenine triphosphate	

Product

Table 33: Properties of each product.

Id	Name	SBO
ADP_cyt	adenine diphosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{CYTOPLASM}) \cdot \left(\mathrm{k9f} \cdot [\mathrm{AMP}] \cdot [\mathrm{ATP\_cyt}] - \mathrm{k9b} \cdot [\mathrm{ADP\_cyt}]^2\right) \tag{22}$$

Table 34: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k9f			10000.0		☑
k9b			10000.0		☑

6.12 Reaction v8

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

Name pyruvate carrier

Reaction equation

$$\mathrm{PYR\_cyt} \rightleftharpoons \mathrm{Pyr} \tag{23}$$

Reactant

Table 35: Properties of each reactant.

Id	Name	SBO
PYR_cyt	pyruvate	

Product

Table 36: Properties of each product.

Id	Name	SBO
Pyr	pyruvate	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\,(\mathrm{MATRIX}) \cdot \frac{\mathrm{V} \cdot [\mathrm{PYR\_cyt}] \cdot \mathrm{v8\_PYC}}{\mathrm{K} + [\mathrm{PYR\_cyt}]} \tag{24}$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V			10^{-8}		☑
K			$1.5 \cdot 10^{-7}$		☑
v8_PYC	PYC		$3.3211 \cdot 10^{-4}$		☑

6.13 Reaction v9

This is an irreversible reaction of three reactants forming three products.

Name pyruvate dehydrogenase complex

Reaction equation

$$\mathrm{Pyr} + \mathrm{CoA} + \mathrm{NAD\_p} \longrightarrow \mathrm{CO2} + \mathrm{Acetyl\_CoA} + \mathrm{NADH} \tag{25}$$

Reactants

Table 38: Properties of each reactant.

Id	Name	SBO
Pyr	pyruvate	
CoA	coenzyme A	
NAD_p	NAD+	

Products

Table 39: Properties of each product.

Id	Name	SBO
CO2	carbon dioxide	
Acetyl_CoA	acetyl CoA	
NADH	NADH	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}\,(\mathrm{MATRIX}) \cdot \frac{\mathrm{K}}{\mathrm{KmC} \cdot [\mathrm{Pyr}] \cdot [\mathrm{CoA}] + \mathrm{KmB} \cdot [\mathrm{Pyr}] \cdot [\mathrm{NAD\_p}] + \mathrm{KmA} \cdot [\mathrm{CoA}] \cdot [\mathrm{NAD\_p}] + [\mathrm{Pyr}] \cdot [\mathrm{CoA}] \cdot [\mathrm{NAD\_p}] + \frac{\frac{\mathrm{KmA} \cdot \mathrm{KmP} \cdot \mathrm{Kib}}{\mathrm{KmR}}}{\mathrm{Kip}}}{\mathrm{Kiq}}} \tag{26}$$

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KmA			$2.5 \cdot 10^{-5}$		☑
KmB			$1.3 \cdot 10^{-5}$		☑
KmC			$5 \cdot 10^{-5}$		☑
KmP			$5.9 \cdot 10^{-7}$		☑
KmR			$6.9 \cdot 10^{-7}$		☑
Kia			$5.5 \cdot 10^{-4}$		☑
Kib			$3 \cdot 10^{-4}$		☑
Kic			$1.8 \cdot 10^{-4}$		☑
Kip			$6 \cdot 10^{-5}$		☑
Kiq			$3.5 \cdot 10^{-5}$		☑
Kir			$3.6 \cdot 10^{-5}$		☑
KcF			856.000		☑
v9_PDC	PDC		$3.8617 \cdot 10^{-7}$		☑

6.14 Reaction v10

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

Name citrate synthase

Reaction equation

$$\mathrm{OXA} + \mathrm{Acetyl\_CoA} \rightleftharpoons \mathrm{Cit} + \mathrm{CoA} \tag{27}$$

Reactants

Table 41: Properties of each reactant.

Id	Name	SBO
OXA	oxaloacetate	
Acetyl_CoA	acetyl CoA	

Products

Table 42: Properties of each product.

Id	Name	SBO
Cit	citrate	
CoA	coenzyme A	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \text{vol}\,(\text{MATRIX}) \cdot \frac{\text{V} \cdot [\text{Acetyl\_CoA}] \cdot [\text{OXA}] \cdot \text{v10\_CS}}{[\text{Acetyl\_CoA}] \cdot [\text{OXA}] + \text{Ka} \cdot [\text{OXA}] + \text{Kb} \cdot [\text{Acetyl\_CoA}] + \text{Kia} \cdot \text{Kib}} \tag{28}$$

Table 43: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V			0.005		☑
Ka			$1.18 \cdot 10^{-5}$		☑
Kb			$4.8 \cdot 10^{-6}$		☑
Kia			10^{-5}		☑
Kib			$4 \cdot 10^{-6}$		☑
v10_CS	CS		$3.8617 \cdot 10^{-7}$		☑

6.15 Reaction v11

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

Name aconitase

Reaction equation

$$\text{Cit} \rightleftharpoons \text{IsoCit} \tag{29}$$

Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
Cit	citrate	

Product

Table 45: Properties of each product.

Id	Name	SBO
IsoCit	isocitrate	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{vol}\,(\text{MATRIX}) \cdot \frac{(\text{KcF} \cdot \text{Kp} \cdot [\text{Cit}] - \text{KcR} \cdot \text{Ks} \cdot [\text{IsoCit}]) \cdot \text{v11\_ACO}}{\text{Ks} \cdot [\text{IsoCit}] + \text{Kp} \cdot [\text{Cit}] + \text{Ks} \cdot \text{Kp}} \tag{30}$$

Table 46: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Ks			$5 \cdot 10^{-4}$		☑
Kp			$1.1 \cdot 10^{-4}$		☑
KcF			20.470		☑
KcR			31.440		☑
v11_ACO	ACO		$3.8617 \cdot 10^{-7}$		☑

6.16 Reaction v12

This is an irreversible reaction of two reactants forming two products influenced by one modifier.

Name isocitrate dehydrogenase (NAD+) (alpha/beta/gamma)

Reaction equation

$$\mathrm{IsoCit} + \mathrm{NAD\_p} \xrightarrow{\mathrm{ADP}} \mathrm{OG} + \mathrm{NADH} \tag{31}$$

Reactants

Table 47: Properties of each reactant.

Id	Name	SBO
IsoCit	isocitrate	
NAD_p	NAD+	

Modifier

Table 48: Properties of each modifier.

Id	Name	SBO
ADP	adenine diphosphate	

Products

Table 49: Properties of each product.

Id	Name	SBO
OG	oxoglutarate	
NADH	NADH	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}\,(\mathrm{MATRIX}) \cdot \frac{\mathrm{KcF} \cdot \mathrm{v12\_IDHa} \cdot (\mathrm{[IsoCit]} \cdot \mathrm{[IsoCit]} + \mathrm{b} \cdot \mathrm{[ADP]} \cdot \mathrm{[IsoCit]})}{\mathrm{[IsoCit]} \cdot \mathrm{[IsoCit]} + \mathrm{c} \cdot \mathrm{[IsoCit]} + \mathrm{d} \cdot \mathrm{[ADP]} + \mathrm{e} \cdot \mathrm{[ADP]} \cdot \mathrm{[IsoCit]} + \mathrm{f}} \tag{32}$$

Table 50: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KcF			105.000		☑
b			29.600		☑

Id	Name	SBO	Value	Unit	Constant
c			$2.3 \cdot 10^{-4}$		☑
d			$7.8 \cdot 10^{-5}$		☑
e			$6.4 \cdot 10^{-4}$		☑
f			$3.6 \cdot 10^{-4}$		☑
v12_IDHa	IDHa		$3.8617 \cdot 10^{-7}$		☑

6.17 Reaction v14

This is an irreversible reaction of three reactants forming three products.

Name oxoglutarate dehydrogenase complex

Reaction equation

$$\mathrm{OG} + \mathrm{CoA} + \mathrm{NAD\_p} \longrightarrow \mathrm{CO2} + \mathrm{SCoA} + \mathrm{NADH} \tag{33}$$

Reactants

Table 51: Properties of each reactant.

Id	Name	SBO
OG	oxoglutarate	
CoA	coenzyme A	
NAD_p	NAD+	

Products

Table 52: Properties of each product.

Id	Name	SBO
CO2	carbon dioxide	
SCoA	succinyl-CoA	
NADH	NADH	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{vol}\,(\mathrm{MATRIX}) \cdot \frac{\mathrm{KcF} \cdot \mathrm{v14\_C}}{\mathrm{KmC} \cdot [\mathrm{OG}] \cdot [\mathrm{CoA}] + \mathrm{KmB} \cdot [\mathrm{OG}] \cdot [\mathrm{NAD\_p}] + \mathrm{KmA} \cdot [\mathrm{CoA}] \cdot [\mathrm{NAD\_p}] + [\mathrm{OG}] \cdot [\mathrm{CoA}] \cdot [\mathrm{NAD\_p}] + \frac{\frac{\mathrm{KmA} \cdot \mathrm{KmP} \cdot \mathrm{Kib}}{\mathrm{KmR}}}{\mathrm{Kip}}}{\mathrm{Kiq}}} \tag{34}$$

Table 53: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KmA			$2.2 \cdot 10^{-4}$		☑
KmB			$2.5 \cdot 10^{-5}$		☑
KmC			$5 \cdot 10^{-5}$		☑
KmP			$3 \cdot 10^{-4}$		☑
KmR			$6 \cdot 10^{-4}$		☑
Kia			$7.2 \cdot 10^{-4}$		☑
Kib			$7.4 \cdot 10^{-4}$		☑
Kic			10^{-4}		☑
Kip			$1.1 \cdot 10^{-6}$		☑
Kiq			$8.1 \cdot 10^{-5}$		☑
Kir			$2.5 \cdot 10^{-5}$		☑
KcF			177.000		☑
v14_OGDC	OGDC		$3.8617 \cdot 10^{-7}$		☑

6.18 Reaction v15

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

Name succinyl-CoA synthetase

Reaction equation

$$\mathrm{GDP} + \mathrm{SCoA} + \mathrm{Pi} \rightleftharpoons \mathrm{Suc} + \mathrm{GTP} + \mathrm{CoA} \tag{35}$$

Reactants

Table 54: Properties of each reactant.

Id	Name	SBO
GDP	guanosine diphosphate	
SCoA	succinyl-CoA	
Pi	phosphate	

Products

Table 55: Properties of each product.

Id	Name	SBO
Suc	succinate	
GTP	guanosine triphosphate	
CoA	coenzyme A	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \mathrm{vol}\,(\mathrm{MATRIX}) \tag{36}$$

.

$$\mathrm{Kia} \cdot \mathrm{KmB} \cdot \pi + \mathrm{KmB} \cdot [\mathrm{GDP}] \cdot \pi + \mathrm{KmA} \cdot [\mathrm{SCoA}] \cdot \pi + \mathrm{KmC} \cdot [\mathrm{GDP}] \cdot [\mathrm{SCoA}] + [\mathrm{GDP}] \cdot [\mathrm{SCoA}] \cdot \pi + \frac{[\mathrm{GDP}] \cdot}{\mathrm{K}}$$

Table 56: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KmA			$5 \cdot 10^{-6}$		☑
KmB			$3.5 \cdot 10^{-5}$		☑
KmC			$4.5 \cdot 10^{-4}$		☑
KmP			$6 \cdot 10^{-4}$		☑
KmQ			$7.5 \cdot 10^{-6}$		☑
KmC2			$4.5 \cdot 10^{-4}$		☑
KmP2			$6 \cdot 10^{-4}$		☑
Keq			8.375		☑
Kia			$4 \cdot 10^{-4}$		☑
Kib			$2 \cdot 10^{-5}$		☑
Kic			$3 \cdot 10^{-5}$		☑
Kip			0.070		☑
Kiq			$5 \cdot 10^{-6}$		☑
Kir			$6.7 \cdot 10^{-6}$		☑
Kc1			100.000		☑
Kc2			100.000		☑
v15_SCS	SCS		$3.8617 \cdot 10^{-7}$		☑

6.19 Reaction v16

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

Name succinate dehydrogenase

Reaction equation

$$\mathrm{Suc} + \mathrm{Q} \rightleftharpoons \mathrm{Fum} + \mathrm{QH2} \tag{37}$$

Reactants

Table 57: Properties of each reactant.

Id	Name	SBO
Suc	succinate	
Q	ubiquinone	

Products

Table 58: Properties of each product.

Id	Name	SBO
Fum	fumarate	
QH2	ubiquinol	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \mathrm{vol}\,(\mathrm{MATRIX}) \tag{38}$$
$$\cdot \frac{\mathrm{KcF} \cdot \mathrm{KcR} \cdot \mathrm{v16\_SDH} \cdot \left([\mathrm{Suc}] \cdot [\mathrm{Q}] - \frac{[\mathrm{Fum}] \cdot [\mathrm{QH2}]}{\mathrm{Keq}} \right)}{\mathrm{KcR} \cdot \mathrm{KmS2} \cdot [\mathrm{Suc}] + \mathrm{KcR} \cdot \mathrm{KmS1} \cdot [\mathrm{Q}] + \frac{\mathrm{KcF} \cdot \mathrm{KmP2} \cdot [\mathrm{Fum}]}{\mathrm{Keq}} + \frac{\mathrm{KcF} \cdot \mathrm{KmP1} \cdot [\mathrm{QH2}]}{\mathrm{Keq}} + \mathrm{KcR} \cdot [\mathrm{Suc}] \cdot [\mathrm{Q}] + \frac{\mathrm{KcF} \cdot \mathrm{KmP2} \cdot [\mathrm{Suc}] \cdot [\mathrm{Fu}}{\mathrm{Keq} \cdot \mathrm{KiS1}}}$$

Table 59: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KmS1			$3 \cdot 10^{-5}$		☑
KmS2			$6.9 \cdot 10^{-5}$		☑
KmP1			$3 \cdot 10^{-7}$		☑
KmP2			$1.5 \cdot 10^{-6}$		☑

Id	Name	SBO	Value	Unit	Constant
KiS1			$4.1 \cdot 10^{-6}$		☑
KiP2			$5.6 \cdot 10^{-6}$		☑
Keq			0.037		☑
KcF			69.300		☑
KcR			1.730		☑
v16_SDH	SDH		$9.9211 \cdot 10^{-5}$		☑

6.20 Reaction v17

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

Name fumarase

Reaction equation

$$\text{Fum} \rightleftharpoons \text{Mal} \tag{39}$$

Reactant

Table 60: Properties of each reactant.

Id	Name	SBO
Fum	fumarate	

Product

Table 61: Properties of each product.

Id	Name	SBO
Mal	malate	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \text{vol}\,(\text{MATRIX}) \cdot \frac{(\text{KcF} \cdot \text{Kp} \cdot [\text{Fum}] - \text{KcR} \cdot \text{Ks} \cdot [\text{Mal}]) \cdot \text{v17\_FM}}{\text{Ks} \cdot [\text{Mal}] + \text{Kp} \cdot [\text{Fum}] + \text{Ks} \cdot \text{Kp}} \tag{40}$$

Table 62: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kp			$2.5 \cdot 10^{-5}$		☑
Ks			$5 \cdot 10^{-6}$		☑
KcF			800.000		☑
KcR			900.000		☑
v17_FM	FM		$3.8617 \cdot 10^{-7}$		☑

6.21 Reaction v18

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

Name malate dehydrogenase (mitochondrion)

Reaction equation

$$\mathrm{Mal} + \mathrm{NAD\_p} \rightleftharpoons \mathrm{NADH} + \mathrm{OXA} \tag{41}$$

Reactants

Table 63: Properties of each reactant.

Id	Name	SBO
Mal	malate	
NAD_p	NAD+	

Products

Table 64: Properties of each product.

Id	Name	SBO
NADH	NADH	
OXA	oxaloacetate	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \mathrm{vol}\,(\mathrm{MATRIX}) \cdot \frac{\left(\frac{\mathrm{KcF}\cdot[\mathrm{Mal}]\cdot[\mathrm{NAD\_p}]}{\mathrm{KiS1}} - \frac{\mathrm{KcR}\cdot[\mathrm{OXA}]\cdot[\mathrm{NADH}]}{\mathrm{KmP1}}\right)}{\mathrm{KmS2}} \cdot \mathrm{v18\_MDH}}{1 + \frac{[\mathrm{Mal}]}{\mathrm{KiS1}} + \frac{\frac{\mathrm{KmS1}\cdot[\mathrm{NAD\_p}]}{\mathrm{KiS1}}}{\mathrm{KmS2}} + \frac{\frac{\mathrm{KmP2}\cdot[\mathrm{OXA}]}{\mathrm{KmP1}}}{\mathrm{KiP2}} + \frac{[\mathrm{NADH}]}{\mathrm{KiP2}} + \frac{\frac{[\mathrm{Mal}]\cdot[\mathrm{NAD\_p}]}{\mathrm{KiS1}}}{\mathrm{KmS2}} + \frac{\frac{\mathrm{KmP2}\cdot[\mathrm{Mal}]\cdot[\mathrm{OXA}]}{\mathrm{KiS1}}}{\mathrm{KmP1}} + \frac{\frac{\mathrm{KmS1}\cdot[\mathrm{NAD\_p}]\cdot[\mathrm{NADH}]}{\mathrm{KiS1}}}{\mathrm{KmS2}} + \frac{[\mathrm{OXA}]\cdot[\mathrm{NADH}]}{\mathrm{KmP1}} \cdot \mathrm{KiP2}} \tag{42}$$

Table 65: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KmS1			$7.2 \cdot 10^{-5}$		☑
KmS2			$1.1 \cdot 10^{-4}$		☑
KmP1			0.002		☑
KmP2			$1.7 \cdot 10^{-4}$		☑
KiS1			$1.1 \cdot 10^{-5}$		☑
KiS2			10^{-4}		☑
KiP1			0.007		☑
KiP2			0.002		☑
KcF			0.390		☑
KcR			0.040		☑
v18_MDH	MDH		$3.8617 \cdot 10^{-7}$		☑

6.22 Reaction v20

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

Name alanine transaminase

Reaction equation

$$\mathrm{Ala} + \mathrm{OG} \rightleftharpoons \mathrm{Glu} + \mathrm{Pyr} \tag{43}$$

Reactants

Table 66: Properties of each reactant.

Id	Name	SBO
Ala	slanine	
OG	oxoglutarate	

Products

Table 67: Properties of each product.

Id	Name	SBO
Glu	glutamate	
Pyr	pyruvate	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \mathrm{vol}\,(\mathrm{MATRIX}) \cdot \frac{\mathrm{KcF} \cdot \mathrm{KcR} \cdot \mathrm{v20\_AlaTA} \cdot \left([\mathrm{Ala}] \cdot [\mathrm{OG}] - \frac{[\mathrm{Glu}] \cdot [\mathrm{Pyr}]}{\mathrm{Keq}}\right)}{\mathrm{KcR} \cdot \mathrm{KmS2} \cdot [\mathrm{Ala}] + \mathrm{KcR} \cdot \mathrm{KmS1} \cdot [\mathrm{OG}] + \frac{\mathrm{KcF} \cdot \mathrm{KmP2} \cdot [\mathrm{Glu}]}{\mathrm{Keq}} + \frac{\mathrm{KcF} \cdot \mathrm{KmP1} \cdot [\mathrm{Pyr}]}{\mathrm{Keq}} + \mathrm{KcR} \cdot [\mathrm{Ala}] \cdot [\mathrm{OG}] + \frac{\mathrm{KcF} \cdot \mathrm{KmP2} \cdot [\mathrm{Ala}] \cdot}{\mathrm{Keq} \cdot \mathrm{KiS1}}} \tag{44}$$

Table 68: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KmS1			0.002		☑
KmS2			$4 \cdot 10^{-4}$		☑
KmP1			0.032		☑
KmP2			$4 \cdot 10^{-4}$		☑
KiS1			0.009		☑
KiP2			0.012		☑
Keq			0.690		☑
KcF			337.000		☑
KcR			0.150		☑
v20_AlaTA	AlaTA		$3.8617 \cdot 10^{-7}$		☑

6.23 Reaction v21

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

Name aspartate transaminase

Reaction equation

$$\mathrm{OXA} + \mathrm{Glu} \rightleftharpoons \mathrm{Asp} + \mathrm{OG} \tag{45}$$

Reactants

Table 69: Properties of each reactant.

Id	Name	SBO
OXA	oxaloacetate	
Glu	glutamate	

Products

Table 70: Properties of each product.

Id	Name	SBO
Asp	aspartate	
OG	oxoglutarate	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \mathrm{vol}\,(\mathrm{MATRIX}) \cdot \frac{\mathrm{KcF} \cdot \mathrm{KcR} \cdot \mathrm{v21\_AspTA} \cdot \left([\mathrm{OXA}] \cdot [\mathrm{Glu}] - \frac{[\mathrm{Asp}] \cdot [\mathrm{OG}]}{\mathrm{Keq}}\right)}{\mathrm{KcR} \cdot \mathrm{KmS2} \cdot [\mathrm{OXA}] + \mathrm{KcR} \cdot \mathrm{KmS1} \cdot [\mathrm{Glu}] + \frac{\mathrm{KcF} \cdot \mathrm{KmP2} \cdot [\mathrm{Asp}]}{\mathrm{Keq}} + \frac{\mathrm{KcF} \cdot \mathrm{KmP1} \cdot [\mathrm{OG}]}{\mathrm{Keq}} + \mathrm{KcR} \cdot [\mathrm{OXA}] \cdot [\mathrm{Glu}] + \frac{\mathrm{KcF} \cdot \mathrm{KmP2} \cdot [}{\mathrm{Keq} \cdot}} \tag{46}$$

Table 71: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KmS1			$9 \cdot 10^{-4}$		☑
KmS2			10^{-4}		☑
KmP1			$4 \cdot 10^{-5}$		☑
KmP2			0.004		☑
KiS1			0.002		☑
KiP2			0.008		☑
Keq			6.200		☑
KcF			300.000		☑
KcR			1000.000		☑
v21_AspTA	AspTA		$3.8617 \cdot 10^{-7}$		☑

6.24 Reaction v22

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

Name aspartate/glutamate carrier

Reaction equation

$$\mathrm{Glu\_cyt} + \mathrm{Asp} \rightleftharpoons \mathrm{Asp\_cyt} + \mathrm{Glu} \tag{47}$$

Reactants

Table 72: Properties of each reactant.

Id	Name	SBO
`Glu_cyt`	glutamate	
`Asp`	aspartate	

Products

Table 73: Properties of each product.

Id	Name	SBO
`Asp_cyt`	aspartate	
`Glu`	glutamate	

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \mathrm{vol}\,(\mathrm{MATRIX}) \cdot \frac{\left(\frac{\frac{[\mathrm{Asp}]\cdot[\mathrm{Glu\_cyt}]}{\mathrm{alpha}}}{\mathrm{KiS1}\cdot\mathrm{KiS2}} \cdot \mathrm{KcF} - \frac{\frac{[\mathrm{Glu}]\cdot[\mathrm{Asp\_cyt}]}{\mathrm{beta}}}{\mathrm{KiP1}\cdot\mathrm{KiP2}} \cdot \mathrm{KcR}\right) \cdot \mathrm{v22\_AGC}}{1 + \frac{[\mathrm{Asp}]}{\mathrm{KiS1}} + \frac{[\mathrm{Glu\_cyt}]}{\mathrm{KiS2}} + \frac{[\mathrm{Glu}]}{\mathrm{KiP1}} + \frac{[\mathrm{Asp\_cyt}]}{\mathrm{KiP2}} + \frac{\frac{[\mathrm{Asp}]\cdot[\mathrm{Glu\_cyt}]}{\mathrm{alpha}}}{\mathrm{KiS1}\cdot\mathrm{KiS2}} + \frac{\frac{[\mathrm{Glu}]\cdot[\mathrm{Asp\_cyt}]}{\mathrm{beta}}}{\mathrm{KiP1}\cdot\mathrm{KiP2}} + \frac{\frac{[\mathrm{Glu\_cyt}]\cdot[\mathrm{Asp\_cyt}]}{\mathrm{gamma}}}{\mathrm{KiS2}\cdot\mathrm{KiP2}} + \frac{\frac{[\mathrm{Asp}]\cdot[\mathrm{Glu}]}{\mathrm{delta}}}{\mathrm{KiS1}\cdot\mathrm{KiP1}}} \tag{48}$$

Table 74: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`KiS1`			$8 \cdot 10^{-5}$		☑
`KiS2`			0.003		☑
`KiP1`			$1.8 \cdot 10^{-4}$		☑
`KiP2`			0.003		☑

Id	Name	SBO	Value	Unit	Constant
KcF			10.000		☑
KcR			10.000		☑
alpha			1.000		☑
beta			1.000		☑
gamma			1.000		☑
delta			1.000		☑
v22_AGC	AGC		$3.3211 \cdot 10^{-4}$		☑

6.25 Reaction v24

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

Name NADH:ubiquinone oxidoreductase

Reaction equation

$$\mathrm{NADH} + \mathrm{Q} \rightleftharpoons \mathrm{NAD\_p} + \mathrm{QH2} \tag{49}$$

Reactants

Table 75: Properties of each reactant.

Id	Name	SBO
NADH	NADH	
Q	ubiquinone	

Products

Table 76: Properties of each product.

Id	Name	SBO
NAD_p	NAD+	
QH2	ubiquinol	

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \mathrm{vol}(\mathrm{MATRIX}) \cdot \frac{\mathrm{KcF} \cdot \mathrm{KcR} \cdot \mathrm{v24\_Complex\_I} \cdot \left([\mathrm{NADH}] \cdot [\mathrm{Q}] - \frac{[\mathrm{NAD\_p}] \cdot [\mathrm{QH2}]}{\mathrm{Keq}}\right.}{\mathrm{KcR} \cdot \mathrm{KmS2} \cdot [\mathrm{NADH}] + \mathrm{KcR} \cdot \mathrm{KmS1} \cdot [\mathrm{Q}] + \frac{\mathrm{KcF} \cdot \mathrm{KmP2} \cdot [\mathrm{NAD\_p}]}{\mathrm{Keq}} + \frac{\mathrm{KcF} \cdot \mathrm{KmP1} \cdot [\mathrm{QH2}]}{\mathrm{Keq}} + \mathrm{KcR} \cdot [\mathrm{NADH}] \cdot [\mathrm{Q}] + \frac{\mathrm{KcF} \cdot \mathrm{Km}}{} \tag{50}$$

Table 77: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KmS1			$9.2 \cdot 10^{-6}$		☑
KmS2			$2.6 \cdot 10^{-4}$		☑
KmP1			$9.9 \cdot 10^{-6}$		☑
KmP2			$5.9 \cdot 10^{-5}$		☑
KiS1			$2.1 \cdot 10^{-8}$		☑
KiP2			$9.8 \cdot 10^{-8}$		☑
Keq			407.900		☑
KcF			498.000		☑
KcR			229.000		☑
v24_Complex_I	Complex_I		$3.3211 \cdot 10^{-4}$		☑

6.26 Reaction v25

This is an irreversible reaction of two reactants forming two products.

Name ubiquinol:cytochrome c oxidoreductase

Reaction equation

$$\mathrm{QH2} + 2\,\mathrm{Cytc3p} \longrightarrow \mathrm{Q} + 2\,\mathrm{Cytc2p} \tag{51}$$

Reactants

Table 78: Properties of each reactant.

Id	Name	SBO
QH2	ubiquinol	
Cytc3p	ferrocytochrome c	

Products

Table 79: Properties of each product.

Id	Name	SBO
Q	ubiquinone	
Cytc2p	ferricytochrome c	

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = \mathrm{vol}(\mathrm{MT\_IMS}) \cdot \frac{\mathrm{KcF} \cdot \mathrm{v25\_Complex\_III} \cdot [\mathrm{QH2}] \cdot [\mathrm{Cytc3p}]}{\left(\mathrm{KmA} \cdot \mathrm{Kq2} \cdot \mathrm{Kb2} + \mathrm{KmA} \cdot \mathrm{Kq2} \cdot [\mathrm{Cytc3p}] + \frac{\mathrm{KcF}}{\mathrm{k8}} \cdot \mathrm{Kq1} \cdot [\mathrm{QH2}] \cdot \mathrm{Kb1} + \frac{\mathrm{KcF}}{\mathrm{k8}} \cdot \mathrm{Kq1} \cdot [\mathrm{QH2}] \cdot [\mathrm{Cytc3p}]\right) \cdot [\mathrm{Cytc2}} \quad (52)$$

Table 80: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KmA			$2.8 \cdot 10^{-5}$		☑
KmB			$3 \cdot 10^{-6}$		☑
Kb1			$5.4 \cdot 10^{-6}$		☑
Kb2			$5.7 \cdot 10^{-6}$		☑
Kq1			$2.8 \cdot 10^{-6}$		☑
Kq2			$1.9 \cdot 10^{-6}$		☑
k8			622.100		☑
KcF			426.800		☑
v25_Complex-_III	Complex_III		$9.963 \cdot 10^{-9}$		☑

6.27 Reaction v26

This is an irreversible reaction of one reactant forming one product.

Name cytochrome c oxidase

Reaction equation

$$\mathrm{Cytc2p} \longrightarrow \mathrm{Cytc3p} \quad (53)$$

Reactant

Table 81: Properties of each reactant.

Id	Name	SBO
Cytc2p	ferricytochrome c	

Product

Table 82: Properties of each product.

Id	Name	SBO
Cytc3p	ferrocytochrome c	

Kinetic Law

Derived unit contains undeclared units

$$v_{27} = \mathrm{vol}\,(\mathrm{MT\_IMS}) \cdot \frac{\mathrm{KcF} \cdot \mathrm{v26\_Complex\_IV} \cdot [\mathrm{Cytc2p}]}{\mathrm{Ks} + [\mathrm{Cytc2p}]} \tag{54}$$

Table 83: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Ks			$1.1 \cdot 10^{-4}$		☑
KcF			$9.35 \cdot 10^{-4}$		☑
v26_Complex_IV	Complex_IV		0.002		☑

6.28 Reaction v27

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

Name citrate synthase

Reaction equation

$$\mathrm{Cit\_cyt} + \mathrm{CoA\_cyt} \rightleftharpoons \mathrm{OXA\_cyt} + \mathrm{Acetyl\_CoA\_cyt} \tag{55}$$

Reactants

Table 84: Properties of each reactant.

Id	Name	SBO
Cit_cyt	citrate	
CoA_cyt	coenzyme A	

Products

Table 85: Properties of each product.

Id	Name	SBO
OXA_cyt	oxaloacetate	
Acetyl_CoA_cyt	acetyl CoA	

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \frac{\mathrm{vol}\,(\mathrm{CYTOPLASM}) \cdot \mathrm{Kid} \cdot \mathrm{Kc} \cdot \frac{\mathrm{V} \cdot [\mathrm{Acetyl\_CoA\_cyt}] \cdot [\mathrm{OXA\_cyt}] \cdot \mathrm{v10\_CS}}{[\mathrm{Acetyl\_CoA\_cyt}] \cdot [\mathrm{OXA\_cyt}] + \mathrm{Ka} \cdot [\mathrm{OXA\_cyt}] + \mathrm{Kb} \cdot [\mathrm{Acetyl\_CoA\_cyt}] + \mathrm{Kia} \cdot \mathrm{Kib}}}{\mathrm{Keq} \cdot \mathrm{Kia} \cdot \mathrm{Kb}} \tag{56}$$

Table 86: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V			0.005		☑
Ka			$5 \cdot 10^{-6}$		☑
Kb			$4.5 \cdot 10^{-6}$		☑
Kc			$3.9 \cdot 10^{-5}$		☑
Kia			$5 \cdot 10^{-6}$		☑
Kib			$4.5 \cdot 10^{-6}$		☑
Kid			0.004		☑
Keq			$1.8 \cdot 10^{7}$		☑
v10_CS	CS		$3.8617 \cdot 10^{-7}$		☑

6.29 Reaction v28

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

Name ATPase complex

Reaction equation

$$\mathrm{ADP} + \mathrm{Pi} \rightleftharpoons \mathrm{ATP} + \mathrm{H2O} \tag{57}$$

Reactants

Table 87: Properties of each reactant.

Id	Name	SBO
ADP	adenine diphosphate	
Pi	phosphate	

Products

Table 88: Properties of each product.

Id	Name	SBO
ATP	adenine triphosphate	
H2O	water	

Kinetic Law

Derived unit contains undeclared units

$$v_{29} = \frac{\text{vol}\,(\text{MATRIX}) \cdot \text{v28\_Complex\_V} \cdot \text{V} \cdot [\text{ADP}]}{\text{Km} + [\text{ADP}] + \frac{[\text{ADP}] \cdot [\text{ADP}]}{\text{Ki}}} \tag{58}$$

Table 89: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V			0.075		☑
Km			0.005		☑
Ki			0.047		☑
v28_Complex_V	Complex_V		0.003		☑

6.30 Reaction v29

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

Name aconitase

Reaction equation

$$\text{Cit\_cyt} \rightleftharpoons \text{IsoCitcyt} \tag{59}$$

Reactant

Table 90: Properties of each reactant.

Id	Name	SBO
Cit_cyt	citrate	

Product

Table 91: Properties of each product.

Id	Name	SBO
IsoCitcyt	isocitrate	

Kinetic Law

Derived unit contains undeclared units

$$v_{30} = \mathrm{vol}\,(\mathrm{CYTOPLASM}) \cdot \frac{(\mathrm{KcF} \cdot \mathrm{Kp} \cdot [\mathrm{Cit\_cyt}] - \mathrm{KcR} \cdot \mathrm{Ks} \cdot [\mathrm{IsoCitcyt}]) \cdot \mathrm{v29\_ACO}}{\mathrm{Ks} \cdot [\mathrm{IsoCitcyt}] + \mathrm{Kp} \cdot [\mathrm{Cit\_cyt}] + \mathrm{Ks} \cdot \mathrm{Kp}} \tag{60}$$

Table 92: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Ks			$5 \cdot 10^{-4}$		☑
Kp			$1.1 \cdot 10^{-4}$		☑
KcF			20.470		☑
KcR			31.440		☑
v29_ACO	ACO		$3.8617 \cdot 10^{-7}$		☑

6.31 Reaction v30

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

Name oxoglutarate carrier

Reaction equation

$$\mathrm{Mal\_cyt} + \mathrm{OG} \rightleftharpoons \mathrm{OG\_cyt} + \mathrm{Mal} \tag{61}$$

Reactants

Table 93: Properties of each reactant.

Id	Name	SBO
Mal_cyt	malate	
OG	oxoglutarate	

Products

Table 94: Properties of each product.

Id	Name	SBO
OG_cyt	oxoglutarate	
Mal	malate	

Kinetic Law

Derived unit contains undeclared units

$$v_{31} = \mathrm{vol}\,(\mathrm{MATRIX}) \cdot \frac{\left(\frac{\frac{[\mathrm{OG}]\cdot[\mathrm{Mal\_cyt}]}{\mathrm{alpha}}}{\mathrm{KiS1}\cdot\mathrm{KiS2}} \cdot \mathrm{KcF} - \frac{\frac{[\mathrm{Mal}]\cdot[\mathrm{OG\_cyt}]}{\mathrm{beta}}}{\mathrm{KiP1}\cdot\mathrm{KiP2}} \cdot \mathrm{KcR}\right) \cdot \mathrm{v30\_OGC}}{1 + \frac{[\mathrm{OG}]}{\mathrm{KiS1}} + \frac{[\mathrm{Mal\_cyt}]}{\mathrm{KiS2}} + \frac{[\mathrm{Mal}]}{\mathrm{KiP1}} + \frac{[\mathrm{OG\_cyt}]}{\mathrm{KiP2}} + \frac{\frac{[\mathrm{OG}]\cdot[\mathrm{Mal\_cyt}]}{\mathrm{alpha}}}{\mathrm{KiS1}\cdot\mathrm{KiS2}} + \frac{\frac{[\mathrm{Mal}]\cdot[\mathrm{OG\_cyt}]}{\mathrm{beta}}}{\mathrm{KiP1}\cdot\mathrm{KiP2}} + \frac{\frac{[\mathrm{Mal\_cyt}]\cdot[\mathrm{OG\_cyt}]}{\mathrm{gamma}}}{\mathrm{KiS2}\cdot\mathrm{KiP2}} + \frac{\frac{[\mathrm{OG}]\cdot[\mathrm{Mal}]}{\mathrm{delta}}}{\mathrm{KiS1}\cdot\mathrm{KiP1}}} \tag{62}$$

Table 95: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KiS1			$3 \cdot 10^{-4}$		☑
KiS2			$7 \cdot 10^{-4}$		☑
KiP1			0.001		☑
KiP2			$1.7 \cdot 10^{-4}$		☑
KcF			3.675		☑
KcR			4.830		☑
alpha			1.000		☑
beta			1.000		☑
gamma			1.000		☑
delta			1.000		☑
v30_OGC	OGC		$3.3211 \cdot 10^{-4}$		☑

6.32 Reaction v31

This is an irreversible reaction of two reactants forming two products.

Name malate dehydrogenase (cytosol)

Reaction equation

$$\mathrm{NADH\_cyt} + \mathrm{OXA\_cyt} \longrightarrow \mathrm{Mal\_cyt} + \mathrm{NAD} \tag{63}$$

Reactants

Table 96: Properties of each reactant.

Id	Name	SBO
NADH_cyt	NADH	
OXA_cyt	oxaloacetate	

Products

Table 97: Properties of each product.

Id	Name	SBO
Mal_cyt	malate	
NAD	NAD	

Kinetic Law

Derived unit contains undeclared units

$$v_{32} = \mathrm{vol}(\mathrm{CYTOPLASM}) \tag{64}$$

$$\cdot \frac{}{\mathrm{kminus1} \cdot (\mathrm{kminus2} + \mathrm{k3}) \cdot \mathrm{k4} + \mathrm{k1} \cdot (\mathrm{kminus2} + \mathrm{k3}) \cdot \mathrm{k4} \cdot [\mathrm{NADH\_cyt}] + \mathrm{kminus1} \cdot (\mathrm{kminus2} + \mathrm{k3}) \cdot \mathrm{kminus4}$$

Table 98: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			$3.4 \cdot 10^7$		☑
k2			$3.5 \cdot 10^7$		☑
k3			4650.000		☑
k4			214.000		☑
kminus1			26.000		☑

Id	Name	SBO	Value	Unit	Constant
kminus2			1400.000		☑
kminus3			570000.000		☑
kminus4			260000.000		☑
v31_MDH	MDH		$3.8617 \cdot 10^{-7}$		☑

6.33 Reaction v32

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

Name aspartate transaminase

Reaction equation

$$\text{Asp\_cyt} + \text{OG\_cyt} \rightleftharpoons \text{OXA\_cyt} + \text{Glu\_cyt} \tag{65}$$

Reactants

Table 99: Properties of each reactant.

Id	Name	SBO
Asp_cyt	aspartate	
OG_cyt	oxoglutarate	

Products

Table 100: Properties of each product.

Id	Name	SBO
OXA_cyt	oxaloacetate	
Glu_cyt	glutamate	

Kinetic Law

Derived unit contains undeclared units

$$v_{33} = \text{vol}(\text{CYTOPLASM}) \tag{66}$$

$$\cdot \frac{\text{KcF} \cdot \text{KcR} \cdot \text{v32\_AspTA} \cdot \left([\text{Asp\_cyt}] \cdot [\text{OG\_cyt}] - \right.}{\text{KcR} \cdot \text{KmS2} \cdot [\text{Asp\_cyt}] + \text{KcR} \cdot \text{KmS1} \cdot [\text{OG\_cyt}] + \frac{\text{KcF} \cdot \text{KmP2} \cdot [\text{OXA\_cyt}]}{\text{Keq}} + \frac{\text{KcF} \cdot \text{KmP1} \cdot [\text{Glu\_cyt}]}{\text{Keq}} + \text{KcR} \cdot [\text{Asp\_cyt}] \cdot [\text{C}}$$

Table 101: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KmS1			$9 \cdot 10^{-4}$		☑
KmS2			10^{-4}		☑
KmP1			$4 \cdot 10^{-5}$		☑
KmP2			0.004		☑
KiS1			0.002		☑
KiP2			0.008		☑
Keq			6.200		☑
KcF			300.000		☑
KcR			1000.000		☑
v32_AspTA	AspTA		$3.8617 \cdot 10^{-7}$		☑

6.34 Reaction v33

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

Name citrate carrier

Reaction equation

$$\text{Cit\_cyt} + \text{Mal} \rightleftharpoons \text{Mal\_cyt} + \text{Cit} \tag{67}$$

Reactants

Table 102: Properties of each reactant.

Id	Name	SBO
Cit_cyt	citrate	
Mal	malate	

Products

Table 103: Properties of each product.

Id	Name	SBO
Mal_cyt	malate	
Cit	citrate	

Kinetic Law

Derived unit contains undeclared units

$$v_{34} = \mathrm{vol}\,(\mathrm{MATRIX}) \cdot \frac{\left(\frac{\frac{[\mathrm{Cit\_cyt}]\cdot[\mathrm{Mal}]}{\mathrm{alpha}}}{\mathrm{KiS1}\cdot\mathrm{KiS2}} \cdot \mathrm{KcF} - \frac{\frac{[\mathrm{Mal\_cyt}]\cdot[\mathrm{Cit}]}{\mathrm{beta}}}{\mathrm{KiP1}\cdot\mathrm{KiP2}} \cdot \mathrm{KcR}\right) \cdot \mathrm{v33\_CIC}}{1 + \frac{[\mathrm{Cit\_cyt}]}{\mathrm{KiS1}} + \frac{[\mathrm{Mal}]}{\mathrm{KiS2}} + \frac{[\mathrm{Mal\_cyt}]}{\mathrm{KiP1}} + \frac{[\mathrm{Cit}]}{\mathrm{KiP2}} + \frac{\frac{[\mathrm{Cit\_cyt}]\cdot[\mathrm{Mal}]}{\mathrm{alpha}}}{\mathrm{KiS1}\cdot\mathrm{KiS2}} + \frac{\frac{[\mathrm{Mal\_cyt}]\cdot[\mathrm{Cit}]}{\mathrm{beta}}}{\mathrm{KiP1}\cdot\mathrm{KiP2}} + \frac{\frac{[\mathrm{Mal}]\cdot[\mathrm{Cit}]}{\mathrm{gamma}}}{\mathrm{KiS2}\cdot\mathrm{KiP2}} + \frac{\frac{[\mathrm{Cit\_cyt}]\cdot[\mathrm{Mal\_cyt}]}{\mathrm{delta}}}{\mathrm{KiS1}\cdot\mathrm{KiP1}}} \tag{68}$$

Table 104: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KiS1			$1.3 \cdot 10^{-4}$		☑
KiS2			$4.4 \cdot 10^{-4}$		☑
KiP1			$3.3 \cdot 10^{-4}$		☑
KiP2			$4.18 \cdot 10^{-5}$		☑
KcF			5.600		☑
KcR			3.500		☑
alpha			1.000		☑
beta			1.000		☑
gamma			1.000		☑
delta			1.000		☑
v33_CIC	CIC		$3.3211 \cdot 10^{-4}$		☑

6.35 Reaction v34

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

Name ETF:Q oxidoreductase

Reaction equation

$$\mathrm{ETFred} + \mathrm{Q} \rightleftharpoons \mathrm{ETFox} + \mathrm{QH2} \tag{69}$$

Reactants

Table 105: Properties of each reactant.

Id	Name	SBO
ETFred	electron transfer flavoprotein (reduced form)	

Id	Name	SBO
Q	ubiquinone	

Products

Table 106: Properties of each product.

Id	Name	SBO
ETFox	electron transfer flavoprotein (oxidised form)	
QH2	ubiquinol	

Kinetic Law

Derived unit contains undeclared units

$$v_{35} = \mathrm{vol}\,(\mathrm{MATRIX}) \tag{70}$$
$$\cdot \frac{\mathrm{KcF} \cdot \mathrm{KcR} \cdot \mathrm{v34\_ETF\_QO} \cdot \left([\mathrm{ETFred}] \cdot [\mathrm{Q}] - \frac{[\mathrm{ETFox}] \cdot [\mathrm{QH2}]}{\mathrm{Keq}}\right.}{\mathrm{KcR} \cdot \mathrm{KmS2} \cdot [\mathrm{ETFred}] + \mathrm{KcR} \cdot \mathrm{KmS1} \cdot [\mathrm{Q}] + \frac{\mathrm{KcF} \cdot \mathrm{KmP2} \cdot [\mathrm{ETFox}]}{\mathrm{Keq}} + \frac{\mathrm{KcF} \cdot \mathrm{KmP1} \cdot [\mathrm{QH2}]}{\mathrm{Keq}} + \mathrm{KcR} \cdot [\mathrm{ETFred}] \cdot [\mathrm{Q}] + \frac{\mathrm{KcF} \cdot \mathrm{Kr}}{}$$

Table 107: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KmS1			$3.1 \cdot 10^{-7}$		☑
KmS2			$3.9 \cdot 10^{-7}$		☑
KmP1			$3.2 \cdot 10^{-7}$		☑
KmP2			$4.2 \cdot 10^{-9}$		☑
KiS1			$3.1 \cdot 10^{-7}$		☑
KiP2			$3 \cdot 10^{-7}$		☑
Keq			0.660		☑
KcF			78.000		☑
KcR			101.000		☑
v34_ETF_QO			$3.3211 \cdot 10^{-5}$		☑

6.36 Reaction v35

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

Name glutathione reductase

Reaction equation

$$\mathrm{FADH2} + \mathrm{ETFox} \rightleftharpoons \mathrm{ETFred} + \mathrm{FAD} \tag{71}$$

Reactants

Table 108: Properties of each reactant.

Id	Name	SBO
FADH2	FADH2	
ETFox	electron transfer flavoprotein (oxidised form)	

Products

Table 109: Properties of each product.

Id	Name	SBO
ETFred	electron transfer flavoprotein (reduced form)	
FAD	FAD	

Kinetic Law

Derived unit contains undeclared units

$$v_{36} = \mathrm{vol}\,(\mathrm{MATRIX}) \cdot \frac{\mathrm{KcF} \cdot \mathrm{KcR} \cdot \mathrm{v}}{\mathrm{KcR} \cdot \mathrm{KiS1} \cdot \mathrm{KmS2} + \mathrm{KcR} \cdot \mathrm{KmS2} \cdot [\mathrm{FADH2}] + \mathrm{KcR} \cdot \mathrm{KmS1} \cdot [\mathrm{ETFox}] + \frac{\mathrm{KcF} \cdot \mathrm{KmP2} \cdot [\mathrm{ETFred}]}{\mathrm{Keq}} + \frac{\mathrm{KcF} \cdot \mathrm{KmP1} \cdot [\mathrm{FAD}]}{\mathrm{Keq}} + \mathrm{I}} \tag{72}$$

Table 110: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KmS1			$3.9 \cdot 10^{-5}$		☑
KmS2			$1.2 \cdot 10^{-7}$		☑
KmP1			$1.08 \cdot 10^{-6}$		☑
KmP2			$2.42 \cdot 10^{-5}$		☑
KiS1			$7.6 \cdot 10^{-5}$		☑
KiS2			$2.4 \cdot 10^{-7}$		☑
KiP1			$7.53 \cdot 10^{-5}$		☑
KiP2			$1.19 \cdot 10^{-5}$		☑
Keq			8.990		☑

Id	Name	SBO	Value	Unit	Constant
KcF			2.180		☑
KcR			0.300		☑
v35_ACD			$3.3211 \cdot 10^{-5}$		☑

6.37 Reaction v36

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

Name pyruvate decarboxylase

Reaction equation

$$\mathrm{ATP} + \mathrm{CO2} + \mathrm{Pyr} \rightleftharpoons \mathrm{Pi} + \mathrm{ADP} + \mathrm{OXA} \tag{73}$$

Reactants

Table 111: Properties of each reactant.

Id	Name	SBO
ATP	adenine triphosphate	
CO2	carbon dioxide	
Pyr	pyruvate	

Products

Table 112: Properties of each product.

Id	Name	SBO
Pi	phosphate	
ADP	adenine diphosphate	
OXA	oxaloacetate	

Kinetic Law

Derived unit contains undeclared units

$$v_{37} = \mathrm{vol}\,(\mathrm{MATRIX}) \tag{74}$$

.

$$\mathrm{Kia} \cdot \mathrm{KmB} \cdot \mathrm{KcR} \cdot [\mathrm{Pyr}] + \mathrm{KmC} \cdot \mathrm{KcR} \cdot [\mathrm{ATP}] \cdot [\mathrm{CO2}] + \mathrm{KmA} \cdot \mathrm{KcR} \cdot [\mathrm{CO2}] \cdot [\mathrm{Pyr}] + \mathrm{KmB} \cdot \mathrm{KcR} \cdot [\mathrm{ATP}] \cdot [\mathrm{Pyr}$$

Table 113: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KmA			$1.1 \cdot 10^{-4}$		☑
KmB			0.002		☑
KmC			$3.7 \cdot 10^{-4}$		☑
KmP			0.016		☑
KmQ			$2.4 \cdot 10^{-4}$		☑
KmR			$5.1 \cdot 10^{-5}$		☑
Keq			9.000		☑
Kia			$1.5 \cdot 10^{-4}$		☑
Kib			0.002		☑
Kic			$1.3 \cdot 10^{-4}$		☑
Kip			0.008		☑
Kiq			$1.9 \cdot 10^{-4}$		☑
Kir			$2.4 \cdot 10^{-4}$		☑
KcF			200.000		☑
KcR			20.000		☑
v36_PC	PC		$3.8617 \cdot 10^{-7}$		☑

6.38 Reaction v37

This is an irreversible reaction of two reactants forming two products.

Name glycerol-3-phosphate dehydrogenase (FAD dependent)

Reaction equation

$$\mathrm{G3P} + \mathrm{FAD} \longrightarrow \mathrm{FADH2} + \mathrm{DHAP} \tag{75}$$

Reactants

Table 114: Properties of each reactant.

Id	Name	SBO
G3P	glycerol-3-phosphate	
FAD	FAD	

Products

Table 115: Properties of each product.

Id	Name	SBO
FADH2	FADH2	
DHAP	dihydrohxyacetone-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{38} = \mathrm{vol}\,(\mathrm{CYTOPLASM}) \cdot \frac{\mathrm{V} \cdot \mathrm{v37\_GUT2P} \cdot [\mathrm{G3P}]}{\mathrm{K} + [\mathrm{G3P}]} \tag{76}$$

Table 116: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K			$3.4 \cdot 10^{-5}$		☑
V			$3.99 \cdot 10^{-8}$		☑
v37_GUT2P	Glycerol-3-phosphate dehydrogenase		0.001		☑

6.39 Reaction v38

This is an irreversible reaction of two reactants forming two products.

Name glycerol-3-phosphate dehydrogenase (NAD+ dependent)

Reaction equation

$$\mathrm{NADH\_cyt} + \mathrm{DHAP} \longrightarrow \mathrm{G3P} + \mathrm{NAD} \tag{77}$$

Reactants

Table 117: Properties of each reactant.

Id	Name	SBO
NADH_cyt	NADH	
DHAP	dihydrohxyacetone-phosphate	

Products

Table 118: Properties of each product.

Id	Name	SBO
G3P	glycerol-3-phosphate	
NAD	NAD	

Kinetic Law

Derived unit contains undeclared units

$$v_{39} = \mathrm{vol}\,(\mathrm{CYTOPLASM}) \cdot \frac{\mathrm{V} \cdot \mathrm{v38\_GUT2P} \cdot [\mathrm{NADH\_cyt}]}{\mathrm{K} + [\mathrm{NADH\_cyt}]} \tag{78}$$

Table 119: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K			34.000		☑
V			0.040		☑
v38_GUT2P	Glycerol-3-phosphate dehydrogenase		0.001		☑

6.40 Reaction v40

This is an irreversible reaction of one reactant forming one product.

Name ATP/ADP carrier

Reaction equation

$$\mathrm{ADP\_cyt} \longrightarrow \mathrm{ADP} \tag{79}$$

Reactant

Table 120: Properties of each reactant.

Id	Name	SBO
ADP_cyt	adenine diphosphate	

Product

Table 121: Properties of each product.

Id	Name	SBO
ADP	adenine diphosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{40} = \text{vol}(\text{MATRIX}) \cdot \frac{\text{V} \cdot \text{v40\_AAC} \cdot [\text{ADP\_cyt}]}{\text{K} + [\text{ADP\_cyt}]} \tag{80}$$

Table 122: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V			0.167		☑
K			0.012		☑
v40_AAC	AAC		$3.3211 \cdot 10^{-4}$		☑

6.41 Reaction v41

This is a reversible reaction of two reactants forming two products influenced by one modifier.

Name cytosolic isocitrate dehydrogenase

Reaction equation

$$\text{IsoCitcyt} + \text{NADP\_cyt} \overset{\text{CO2}}{\rightleftharpoons} \text{OG\_cyt} + \text{NADPH\_cyt} \tag{81}$$

Reactants

Table 123: Properties of each reactant.

Id	Name	SBO
IsoCitcyt	isocitrate	
NADP_cyt	NADP	

Modifier

Table 124: Properties of each modifier.

Id	Name	SBO
CO2	carbon dioxide	

Products

Table 125: Properties of each product.

Id	Name	SBO
OG_cyt	oxoglutarate	
NADPH_cyt	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_{41} = \mathrm{vol}\,(\mathrm{CYTOPLASM}) \cdot \mathrm{v41\_IDHc} \tag{82}$$
$$\cdot \left(\frac{[\mathrm{IsoCitcyt}] \cdot [\mathrm{NADP\_cyt}]}{\mathrm{phi0} \cdot [\mathrm{IsoCitcyt}] \cdot [\mathrm{NADP\_cyt}] + \mathrm{phi1} \cdot [\mathrm{NADP\_cyt}] + \mathrm{phi2} \cdot [\mathrm{IsoCitcyt}] + \mathrm{phi12}} \right.$$
$$\left. - \frac{[\mathrm{OG\_cyt}] \cdot [\mathrm{NADPH\_cyt}]}{\mathrm{phir0} \cdot [\mathrm{OG\_cyt}] \cdot [\mathrm{NADPH\_cyt}] \cdot [\mathrm{CO2}] + \mathrm{phir1} \cdot [\mathrm{NADPH\_cyt}] \cdot [\mathrm{CO2}] + \mathrm{phir2} \cdot [\mathrm{OG\_cyt}] \cdot [\mathrm{CO2}] + \mathrm{phir3} \cdot [\mathrm{O}} \right)$$

Table 126: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
phi0			0.051		☑
phi1			$9.5 \cdot 10^{-8}$		☑
phi2			$9.6 \cdot 10^{-7}$		☑
phi12			$9 \cdot 10^{-8}$		☑
phir0			0.066		☑
phir1			$3.7 \cdot 10^{-7}$		☑
phir2			$2.9 \cdot 10^{-5}$		☑
phir3			$2.5 \cdot 10^{-4}$		☑
phir12			$6 \cdot 10^{-12}$		☑
phir13			$1.3 \cdot 10^{-10}$		☑
phir23			$9.4 \cdot 10^{-8}$		☑
phir123			$4.6 \cdot 10^{-14}$		☑
v41_IDHc	IDHc		$3.8617 \cdot 10^{-7}$		☑

6.42 Reaction v42

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

Name citrate carrier

Reaction equation

$$\mathrm{IsoCitcyt} + \mathrm{Mal} \rightleftharpoons \mathrm{Mal\_cyt} + \mathrm{IsoCit} \tag{83}$$

Reactants

Table 127: Properties of each reactant.

Id	Name	SBO
IsoCitcyt	isocitrate	
Mal	malate	

Products

Table 128: Properties of each product.

Id	Name	SBO
Mal_cyt	malate	
IsoCit	isocitrate	

Kinetic Law

Derived unit contains undeclared units

$$v_{42} = \mathrm{vol}\left(\mathrm{MATRIX}\right) \cdot \frac{\left(\frac{\frac{[\mathrm{IsoCitcyt}]\cdot[\mathrm{Mal}]}{\mathrm{alpha}}}{\mathrm{KiS1}\cdot\mathrm{KiS2}} \cdot \mathrm{KcF} - \frac{\frac{[\mathrm{Mal\_cyt}]\cdot[\mathrm{IsoCit}]}{\mathrm{beta}}}{\mathrm{KiP1}\cdot\mathrm{KiP2}} \cdot \mathrm{KcR}\right) \cdot \mathrm{v42\_CIC}}{1 + \frac{[\mathrm{IsoCitcyt}]}{\mathrm{KiS1}} + \frac{[\mathrm{Mal}]}{\mathrm{KiS2}} + \frac{[\mathrm{Mal\_cyt}]}{\mathrm{KiP1}} + \frac{[\mathrm{IsoCit}]}{\mathrm{KiP2}} + \frac{\frac{[\mathrm{IsoCitcyt}]\cdot[\mathrm{Mal}]}{\mathrm{alpha}}}{\mathrm{KiS1}\cdot\mathrm{KiS2}} + \frac{\frac{[\mathrm{Mal\_cyt}]\cdot[\mathrm{IsoCit}]}{\mathrm{beta}}}{\mathrm{KiP1}\cdot\mathrm{KiP2}} + \frac{\frac{[\mathrm{Mal}]\cdot[\mathrm{IsoCit}]}{\mathrm{gamma}}}{\mathrm{KiS2}\cdot\mathrm{KiP2}} + \frac{\frac{[\mathrm{IsoCitcyt}]\cdot[\mathrm{Mal\_cyt}]}{\mathrm{delta}}}{\mathrm{KiS1}\cdot\mathrm{KiP1}}} \tag{84}$$

Table 129: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KiS1			$1.3 \cdot 10^{-4}$		☑
KiS2			$4.4 \cdot 10^{-4}$		☑

Id	Name	SBO	Value	Unit	Constant
KiP1			$3.3 \cdot 10^{-4}$		☑
KiP2			$4.18 \cdot 10^{-5}$		☑
KcF			5.600		☑
KcR			3.500		☑
alpha			1.000		☑
beta			1.000		☑
gamma			1.000		☑
delta			1.000		☑
v42_CIC	CIC		$3.3211 \cdot 10^{-4}$		☑

6.43 Reaction v43

This is an irreversible reaction of one reactant forming one product.

Name ATP/ADP carrier

Reaction equation

$$\text{ATP} \longrightarrow \text{ATP\_cyt} \tag{85}$$

Reactant

Table 130: Properties of each reactant.

Id	Name	SBO
ATP	adenine triphosphate	

Product

Table 131: Properties of each product.

Id	Name	SBO
ATP_cyt	adenine triphosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{43} = \text{vol}(\text{MATRIX}) \cdot \frac{\text{V} \cdot \text{v43\_AAC} \cdot [\text{ATP}]}{\text{K} + [\text{ATP}]} \tag{86}$$

Table 132: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V			1.117		☑
K			0.005		☑
v43_AAC	AAC		$3.3211 \cdot 10^{-4}$		☑

6.44 Reaction v39

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

Name malate dehydrogenase (oxaloacetate-decarboxylating) (NADP+)

Reaction equation

$$\text{Mal\_cyt} + \text{NADP\_cyt} \rightleftharpoons \text{NADPH\_cyt} + \text{PYR\_cyt} \tag{87}$$

Reactants

Table 133: Properties of each reactant.

Id	Name	SBO
Mal_cyt	malate	
NADP_cyt	NADP	

Products

Table 134: Properties of each product.

Id	Name	SBO
NADPH_cyt	NADPH	
PYR_cyt	pyruvate	

Kinetic Law

Derived unit contains undeclared units

$$v_{44} = \text{vol}(\text{CYTOPLASM}) \cdot \frac{\text{v39\_MDH} \cdot \text{Kcat} \cdot [\text{Mal\_cyt}] \cdot [\text{NADP\_cyt}]}{(\text{Kmal} + [\text{Mal\_cyt}]) \cdot (\text{Knadp} + [\text{NADP\_cyt}])} \tag{88}$$

Table 135: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kcat			0.333		☑
Kmal			$1.25 \cdot 10^{-4}$		☑
Knadp			0.011		☑
v39_MDH	MDH		$3.8617 \cdot 10^{-7}$		☑

6.45 Reaction v44

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

Name malate dehydrogenase (oxaloacetate-decarboxylating) (NADP+)

Reaction equation

$$\mathrm{Mal} + \mathrm{NADP\_p} \rightleftharpoons \mathrm{NADPH} + \mathrm{Pyr} \tag{89}$$

Reactants

Table 136: Properties of each reactant.

Id	Name	SBO
Mal	malate	
NADP_p	NADP+	

Products

Table 137: Properties of each product.

Id	Name	SBO
NADPH	NADPH	
Pyr	pyruvate	

Kinetic Law

Derived unit contains undeclared units

$$v_{45} = \mathrm{vol}\,(\mathrm{MATRIX}) \cdot \frac{\mathrm{v44\_MDH} \cdot \mathrm{Kcat} \cdot [\mathrm{Mal}]}{\mathrm{Km} + [\mathrm{Mal}]} \tag{90}$$

Table 138: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kcat			130.500		☑
Km			0.013		☑
v44_MDH	MDH		$3.8617 \cdot 10^{-7}$		☑

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 GLC

Name glucose

Initial concentration $1.12817 \cdot 10^{-5}$ mol $\cdot$ l^{-1}

This species takes part in two reactions (as a reactant in v1 and as a product in GLCflow).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GLC} = v_1 - v_4 \tag{91}$$

7.2 Species F6P

Name fructose-6-phosphate

Initial concentration $6.5939 \cdot 10^{-4}$ mol $\cdot$ l^{-1}

This species takes part in two reactions (as a reactant in v2 and as a product in v1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{F6P} = v_4 - v_5 \tag{92}$$

7.3 Species FBP

Name fructose-1,6-bisphosphate

Initial concentration $7.70135 \cdot 10^{-6}\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in v3 and as a product in v2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{FBP} = v_5 - v_6 \tag{93}$$

7.4 Species GAP

Name glyceraldehyde 3-phosphate

Initial concentration $1.90919 \cdot 10^{-6}\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in GAPflow, v4 and as a product in v3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GAP} = 2\,v_6 - v_3 - v_7 \tag{94}$$

7.5 Species DPG

Name 1,2-bisphospho-D-glycerate

Initial concentration $2.99109 \cdot 10^{-4}\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in v5 and as a product in v4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DPG} = v_7 - v_8 \tag{95}$$

7.6 Species PEP

Name phosphoenolpyruvate

Initial concentration $2.1125 \cdot 10^{-6}\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in v6 and as a product in v5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PEP} = v_8 - v_9 \tag{96}$$

7.7 Species PYR_cyt

Name pyruvate

Initial concentration $4.22702 \cdot 10^{-6}\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in v7, v8 and as a product in v6, v39).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PYR\_cyt} = v_9 + v_{44} - v_{10} - v_{12} \tag{97}$$

7.8 Species AMP

Name adenine monophosphate

Initial concentration $2.61149 \cdot 10^{-6}$ mol $\cdot$ l^{-1}

This species takes part in two reactions (as a reactant in hidden_1 and as a modifier in v2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AMP} = -v_{11} \tag{98}$$

7.9 Species LAC

Name lactate

Initial concentration $3.3981 \cdot 10^{-4}$ mol $\cdot$ l^{-1}

This species takes part in two reactions (as a reactant in LACflow and as a product in v7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{LAC} = v_{10} - v_{2} \tag{99}$$

7.10 Species G3P

Name glycerol-3-phosphate

Initial concentration 0.0076925 mol $\cdot$ l^{-1}

This species takes part in two reactions (as a reactant in v37 and as a product in v38).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G3P} = v_{39} - v_{38} \tag{100}$$

7.11 Species DHAP

Name dihydrohxyacetone-phosphate

Initial concentration 0.0076925 mol $\cdot$ l^{-1}

This species takes part in two reactions (as a reactant in v38 and as a product in v37).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DHAP} = v_{38} - v_{39} \tag{101}$$

7.12 Species OXA_cyt

Name oxaloacetate

Initial concentration $4 \cdot 10^{-6}$ mol $\cdot$ l^{-1}

This species takes part in three reactions (as a reactant in v31 and as a product in v27, v32).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{OXA\_cyt} = v_{28} + v_{33} - v_{32} \tag{102}$$

7.13 Species Asp_cyt

Name aspartate

Initial concentration $0.00114\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in v32 and as a product in v22).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Asp\_cyt} = v_{24} - v_{33} \tag{103}$$

7.14 Species Glu_cyt

Name glutamate

Initial concentration $0.00303\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in v22 and as a product in v32).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glu\_cyt} = v_{33} - v_{24} \tag{104}$$

7.15 Species OG_cyt

Name oxoglutarate

Initial concentration $2.1\cdot10^{-5}\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in v32 and as a product in v30, v41).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{OG\_cyt} = v_{31} + v_{41} - v_{33} \tag{105}$$

7.16 Species Mal_cyt

Name malate

Initial concentration $5\cdot10^{-4}\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in v30, v39 and as a product in v31, v33, v42).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Mal\_cyt} = v_{32} + v_{34} + v_{42} - v_{31} - v_{44} \tag{106}$$

7.17 Species Acetyl_CoA_cyt

Name acetyl CoA

Initial concentration $3\cdot10^{-5}\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a product in v27).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Acetyl\_CoA\_cyt} = v_{28} \tag{107}$$

7.18 Species CoA_cyt

Name coenzyme A

Initial concentration $2.72 \cdot 10^{-4}$ mol $\cdot$ l^{-1}

This species takes part in one reaction (as a reactant in v27).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CoA\_cyt} = -\,v_{28} \tag{108}$$

7.19 Species IsoCitcyt

Name isocitrate

Initial concentration $4.2 \cdot 10^{-4}$ mol $\cdot$ l^{-1}

This species takes part in three reactions (as a reactant in v41, v42 and as a product in v29).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IsoCitcyt} = v_{30} - v_{41} - v_{42} \tag{109}$$

7.20 Species Cit_cyt

Name citrate

Initial concentration $4.2 \cdot 10^{-4}$ mol $\cdot$ l^{-1}

This species takes part in three reactions (as a reactant in v27, v29, v33).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cit\_cyt} = -\,v_{28} - v_{30} - v_{34} \tag{110}$$

7.21 Species ATP_cyt

Name adenine triphosphate

Initial concentration 0.00449064 mol $\cdot$ l^{-1}

This species takes part in six reactions (as a reactant in v1, v2, hidden_1 and as a product in v5, v6, v43).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATP\_cyt} = v_{8} + v_{9} + v_{43} - v_{4} - v_{5} - v_{11} \tag{111}$$

7.22 Species ADP_cyt

Name adenine diphosphate

Initial concentration $1.08367 \cdot 10^{-4}$ mol · l^{-1}

This species takes part in six reactions (as a reactant in v5, v6, v40 and as a product in v1, v2, hidden_1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADP\_cyt} = v_4 + v_5 + 2\,v_{11} - v_8 - v_9 - v_{40} \tag{112}$$

7.23 Species NAD

Name NAD

Initial concentration 0.00362057 mol · l^{-1}

This species takes part in four reactions (as a reactant in v4 and as a product in v7, v31, v38).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NAD} = v_{10} + v_{32} + v_{39} - v_7 \tag{113}$$

7.24 Species NADH_cyt

Name NADH

Initial concentration $6.16118 \cdot 10^{-4}$ mol · l^{-1}

This species takes part in four reactions (as a reactant in v7, v31, v38 and as a product in v4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADH\_cyt} = v_7 - v_{10} - v_{32} - v_{39} \tag{114}$$

7.25 Species NADP_cyt

Name NADP

Initial concentration 0.00362057 mol · l^{-1}

This species takes part in two reactions (as a reactant in v41, v39).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADP\_cyt} = -v_{41} - v_{44} \tag{115}$$

7.26 Species NADPH_cyt

Name NADPH

Initial concentration $6.16118 \cdot 10^{-4}$ mol · l^{-1}

This species takes part in two reactions (as a product in v41, v39).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADPH\_cyt} = v_{41} + v_{44} \tag{116}$$

7.27 Species Pyr

Name pyruvate

Initial concentration $0.001025\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in v9, v36 and as a product in v8, v20, v44).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pyr} = v_{12} + v_{22} + v_{45} - v_{13} - v_{37} \tag{117}$$

7.28 Species CO2

Name carbon dioxide

Initial concentration $0.00163\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in v36 and as a product in v9, v14 and as a modifier in v41).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CO2} = v_{13} + v_{17} - v_{37} \tag{118}$$

7.29 Species CoA

Name coenzyme A

Initial concentration $2.72\cdot10^{-4}\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in v9, v14 and as a product in v10, v15).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CoA} = v_{14} + v_{18} - v_{13} - v_{17} \tag{119}$$

7.30 Species Acetyl_CoA

Name acetyl CoA

Initial concentration $3\cdot10^{-5}\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in v10 and as a product in v9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Acetyl\_CoA} = v_{13} - v_{14} \tag{120}$$

7.31 Species Pi

Name phosphate

Initial concentration $0.0040\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in v15, v28 and as a product in v36).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pi} = v_{37} - v_{18} - v_{29} \tag{121}$$

7.32 Species Fum

Name fumarate

Initial concentration $6.5\cdot 10^{-5}\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in v17 and as a product in v16).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Fum} = v_{19} - v_{20} \tag{122}$$

7.33 Species SCoA

Name succinyl-CoA

Initial concentration $2.941\cdot 10^{-4}\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in v15 and as a product in v14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{SCoA} = v_{17} - v_{18} \tag{123}$$

7.34 Species Suc

Name succinate

Initial concentration $0.00295\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in v16 and as a product in v15).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Suc} = v_{18} - v_{19} \tag{124}$$

7.35 Species GTP

Name guanosine triphosphate

Initial concentration $0.0045\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a product in v15).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GTP} = v_{18} \tag{125}$$

7.36 Species GDP

Name guanosine diphosphate

Initial concentration $4.5 \cdot 10^{-4}$ mol $\cdot$ l^{-1}

This species takes part in one reaction (as a reactant in v15).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GDP} = -v_{18} \tag{126}$$

7.37 Species Ala

Name slanine

Initial concentration 0.00344 mol $\cdot$ l^{-1}

This species takes part in one reaction (as a reactant in v20).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ala} = -v_{22} \tag{127}$$

7.38 Species Asp

Name aspartate

Initial concentration 0.00114 mol $\cdot$ l^{-1}

This species takes part in two reactions (as a reactant in v22 and as a product in v21).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Asp} = v_{23} - v_{24} \tag{128}$$

7.39 Species Glu

Name glutamate

Initial concentration 0.00303 mol $\cdot$ l^{-1}

This species takes part in three reactions (as a reactant in v21 and as a product in v20, v22).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glu} = v_{22} + v_{24} - v_{23} \tag{129}$$

7.40 Species H2O

Name water

Initial concentration 0.0010 mol $\cdot$ l^{-1}

This species takes part in one reaction (as a product in v28).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{H2O} = v_{29} \tag{130}$$

7.41 Species ETFred

Name electron transfer flavoprotein (reduced form)

Initial concentration $3.1 \cdot 10^{-4}$ mol $\cdot$ l^{-1}

This species takes part in two reactions (as a reactant in v34 and as a product in v35).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ETFred} = v_{36} - v_{35} \tag{131}$$

7.42 Species ETFox

Name electron transfer flavoprotein (oxidised form)

Initial concentration $3.2 \cdot 10^{-4}$ mol $\cdot$ l^{-1}

This species takes part in two reactions (as a reactant in v35 and as a product in v34).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ETFox} = v_{35} - v_{36} \tag{132}$$

7.43 Species FADH2

Name FADH2

Initial concentration $7.2 \cdot 10^{-5}$ mol $\cdot$ l^{-1}

This species takes part in two reactions (as a reactant in v35 and as a product in v37).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{FADH2} = v_{38} - v_{36} \tag{133}$$

7.44 Species FAD

Name FAD

Initial concentration 0.00101 mol $\cdot$ l^{-1}

This species takes part in two reactions (as a reactant in v37 and as a product in v35).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{FAD} = v_{36} - v_{38} \tag{134}$$

7.45 Species OG

Name oxoglutarate

Initial concentration $2.1 \cdot 10^{-5}$ mol $\cdot$ l^{-1}

This species takes part in five reactions (as a reactant in v14, v20, v30 and as a product in v12, v21).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{OG} = v_{16} + v_{23} - v_{17} - v_{22} - v_{31} \tag{135}$$

7.46 Species Mal

Name malate

Initial concentration $5 \cdot 10^{-4}\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in v18, v33, v42, v44 and as a product in v17, v30).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Mal} = v_{20} + v_{31} - v_{21} - v_{34} - v_{42} - v_{45} \tag{136}$$

7.47 Species OXA

Name oxaloacetate

Initial concentration $4 \cdot 10^{-6}\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in v10, v21 and as a product in v18, v36).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{OXA} = v_{21} + v_{37} - v_{14} - v_{23} \tag{137}$$

7.48 Species Cit

Name citrate

Initial concentration $4.2 \cdot 10^{-4}\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in v11 and as a product in v10, v33).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cit} = v_{14} + v_{34} - v_{15} \tag{138}$$

7.49 Species IsoCit

Name isocitrate

Initial concentration $4.2 \cdot 10^{-4}\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in v12 and as a product in v11, v42).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IsoCit} = v_{15} + v_{42} - v_{16} \tag{139}$$

7.50 Species ATP

Name adenine triphosphate

Initial concentration $0.0045\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in v36, v43 and as a product in v28).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATP} = v_{29} - v_{37} - v_{43} \tag{140}$$

7.51 Species ADP

Name adenine diphosphate

Initial concentration $4.5 \cdot 10^{-4}$ mol $\cdot$ l^{-1}

This species takes part in four reactions (as a reactant in v28 and as a product in v36, v40 and as a modifier in v12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADP} = v_{37} + v_{40} - v_{29} \tag{141}$$

7.52 Species NADP_p

Name NADP+

Initial concentration 0.0101 mol $\cdot$ l^{-1}

This species takes part in one reaction (as a reactant in v44).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADP\_p} = -v_{45} \tag{142}$$

7.53 Species NADPH

Name NADPH

Initial concentration $7.2 \cdot 10^{-5}$ mol $\cdot$ l^{-1}

This species takes part in one reaction (as a product in v44).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADPH} = v_{45} \tag{143}$$

7.54 Species NAD_p

Name NAD+

Initial concentration 0.0101 mol $\cdot$ l^{-1}

This species takes part in five reactions (as a reactant in v9, v12, v14, v18 and as a product in v24).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NAD\_p} = v_{25} - v_{13} - v_{16} - v_{17} - v_{21} \tag{144}$$

7.55 Species NADH

Name NADH

Initial concentration $7.2 \cdot 10^{-4}\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in v24 and as a product in v9, v12, v14, v18).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADH} = v_{13} + v_{16} + v_{17} + v_{21} - v_{25} \tag{145}$$

7.56 Species Q

Name ubiquinone

Initial concentration $0.026\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in v16, v24, v34 and as a product in v25).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Q} = v_{26} - v_{19} - v_{25} - v_{35} \tag{146}$$

7.57 Species QH2

Name ubiquinol

Initial concentration $0.028\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in v25 and as a product in v16, v24, v34).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{QH2} = v_{19} + v_{25} + v_{35} - v_{26} \tag{147}$$

7.58 Species Cytc3p

Name ferrocytochrome c

Initial concentration $0.0030\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in v25 and as a product in v26).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cytc3p} = v_{27} - 2\,v_{26} \tag{148}$$

7.59 Species Cytc2p

Name ferricytochrome c

Initial concentration $1.1 \cdot 10^{-4}\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in v26 and as a product in v25).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cytc2p} = 2\,v_{26} - v_{27} \tag{149}$$

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