SBML Model Report

Model name: "Mosca2012 - Central Carbon Metabolism Regulated by AKT"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following three authors: Vijayalakshmi Chelliah[1], Ettore Mosca[2] and Roberta Alfieri[3] at September third 2012 at 3:27 p. m. and last time modified at October nineth 2014 at 5:31 p. m. Table 1 shows 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	1
species types	0	species	34
events	0	constraints	0
reactions	29	function definitions	28
global parameters	86	unit definitions	3
rules	34	initial assignments	0

Model Notes

Mosca2012 - Central Carbon Metabolism Regulated by AKT

The role of the PI3K/Akt/PKB signalling pathway in oncogenesis has been extensively investigated and altered expression or mutations of many components of this pathway have been

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implicated in human cancers. Indeed, expression of constitutively active forms of Akt/PKB can prevent cell death upon growth factor withdrawal. PI3K/Akt/mTOR-mediated survival relies on a profound metabolic adaptation, including aerobic glycolysis. Here, the link between the PI3K/Akt/mTOR pathway, glycolysis, lactic acid production and nucleotide biosynthesis has been modelled, considering two states - high and low PI3K/Akt/mTOR activity. The high PI3K/Akt/mTOR activity represents cancer cell line where PI3K/Akt/mTOR promotes a high rate of glucose metabolism (condition H) and the low PI3K/Akt/mTOR activity is characterised by a lower glycolytic rate due to a reduced PI3K/Akt/mTOR signal (condition L). This model corresponds to the high PI3K/Akt/mTOR signal (condition H).

This model is described in the article:Computational Modelling of the Metabolic States Regulated by the Kinase Akt.Mosca E, Alfieri R, Maj C, Bevilacqua A, Canti G, Milanesi L.Frontiers in Systems Biology. 2012 Oct 13

Abstract:

Signal transduction pathways and gene regulation determine a major reorganization of metabolic activities in order to support cell proliferation. Protein Kinase B (PKB), also known as Akt, participates in the PI3K/Akt/mTOR pathway, a master regulator of aerobic glycolysis and cellular biosynthesis, two activities shown by both normal and cancer proliferating cells. Not surprisingly considering its relevance for cellular metabolism, Akt/PKB is often found hyperactive in cancer cells. In the last decade, many efforts have been made to improve the understanding of the control of glucose metabolism and the identification of a therapeutic window between proliferating cancer cells and proliferating normal cells. In this context, we have modelled the link between the PI3K/Akt/mTOR pathway, glycolysis, lactic acid production and nucleotide biosynthesis. We used a computational model in order to compare two metabolic states generated by the specific variation of the metabolic fluxes regulated by the activity of the PI3K/Akt/mTOR pathway. One of the two states represented the metabolism of a growing cancer cell characterised by aerobic glycolysis and cellular biosynthesis, while the other state represented the same metabolic network with a reduced glycolytic rate and a higher mitochondrial pyruvate metabolism, as reported in literature in relation to the activity of the PI3K/Akt/mTOR. Some steps that link glycolysis and pentose phosphate pathway revealed their importance for controlling the dynamics of cancer glucose metabolism.

This model is hosted on BioModels Database and identified by: MODEL1210150000 .

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 of which two are predefined by SBML and not mentioned in the model.

2.1 Unit volume

Name volume

Definition nl

2.2 Unit time

Name time

Definition 60 s

2.3 Unit substance

Name substance

Definition nmol

2.4 Unit area

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

Definition m^2

2.5 Unit length

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

Definition m

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
compartment_1	compartment		3	1	litre	☑	

3.1 Compartment compartment_1

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

Name compartment

4 Species

This model contains 34 species. The boundary condition of 13 of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 9 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
species_1	GLC	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_2	G6P	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_3	ADP	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☑
species_4	ATP	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_5	F6P	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_6	F16P	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_7	E4P	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_8	PGN	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_9	GLC_e	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☑	☑
species_10	NADP	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☑
species_11	NADPH	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_12	BPG	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_13	RU5P	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_14	X5P	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_15	R5P	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_16	GAP	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_17	S7P	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_18	NADH	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☑
species_19	NAD	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_20	AMP	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☑	☑
species_21	PRPP	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☑	☑

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
species_22	G1P	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_23	Pi	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☑	☑
species_24	GLY	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☑	☑
species_25	CIT	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☑	☑
species_26	F26P	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☑	☑
species_27	DHAP	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_28	PG3	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_29	PG2	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_30	PEP	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_31	PYR	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☐	☐
species_32	LAC	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☑	☑
species_33	CO2	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☑	☑
species_34	O2	compartment_1	$\mathrm{nmol \cdot nl^{-1}}$	☑	☑

5 Parameters

This model contains 86 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
parameter_1	Atot		0.011		☑
parameter_2	NPtot		$1.932 \cdot 10^{-5}$		☑
parameter_3	Ntot		0.001		☑
parameter_4	GPa_Vr		0.018		☐
parameter_5	GPa_Keq		0.420		☑
parameter_6	GPb_Keq		16.620		☑
parameter_7	GPb_Vr		$6.03725213205671 \cdot 10^{-5}$		☐
parameter_8	FBA_Vr		11.560		☐
parameter_9	TPI_Vr		49.208		☐
parameter_10	GAPDH_Vr		135.425		☐
parameter_11	PGK_Vr		71.722		☐
parameter_12	FBA_Keq		0.002		☑
parameter_13	PGI_Vmr		17486.511		☐
parameter_14	PGI_Keq		0.056		☑
parameter_15	PGLM_Vmr		0.204		☐
parameter_16	PGLM_Keq		17.200		☑
parameter_17	scale1e3		1000.000		☑
parameter_18	TPI_Keq		0.381		☑
parameter_19	GAPDH_Keq		0.357		☑
parameter_20	PGK_Keq		11.369		☑
parameter_21	PGYM_Keq		1.649		☑
parameter_22	PGYM_Vr		58.980		☐
parameter_23	ENO_Keq		1.413		☑
parameter_24	ENO_Vr		179.835		☐
parameter_25	LDH_Keq		3452.500		☑
parameter_26	LDH_Vr		54.047		☐
parameter_27	AMP		0.003		☐
parameter_28	AKT		1.000		☑
parameter_29	AKT_MPM		1.000		☑
parameter_30	GLUT_Vf		23.030		☐
parameter_31	HK_Vf		86.850		☐
parameter_32	PGI_Vmf		7778.000		☐
parameter_33	G6PDH_Vf		1.008		☐
parameter_34	PGDH_Vf		31.020		☐
parameter_35	TKL_Vf		1056.000		☐
parameter_36	TKL2_Vf		0.176		☐
parameter_37	FBA_Vf		14.630		☐

Id	Name	SBO	Value	Unit	Constant
parameter_38	TPI_Vf		5.976		⊟
parameter_39	GAPDH_Vf		109.100		⊟
parameter_40	PGK_Vf		73.410		⊟
parameter_41	GS_Vf		32040.000		⊟
parameter_42	PFK_Vf		107.600		⊟
parameter_43	ENO_Vf		160.900		⊟
parameter_44	PK_Vf		27.810		⊟
parameter_45	LDH_Vf		340.300		⊟
parameter_46	DHase_Vf		4982000.000		⊟
parameter_47	DPHase_Vf		127800.000		⊟
parameter_48	MPM_Vf		9801000.000		⊟
parameter_49	PGK_Kp		$1.3 \cdot 10^{-4}$		☑
parameter_50	PGK_Kq		$2.7 \cdot 10^{-4}$		☑
parameter_51	PGK_Ka		$7.9 \cdot 10^{-5}$		☑
parameter_52	PGK_Kb		$4 \cdot 10^{-5}$		☑
parameter_53	ENO_Kmp		$6 \cdot 10^{-5}$		☑
parameter_54	ENO_Kms		$3.8 \cdot 10^{-5}$		☑
parameter_55	PGLM_Vmaxf		7.364		☑
parameter_56	PGLM_KG6P		$3 \cdot 10^{-5}$		☑
parameter_57	PGLM_KG1P		$6.3 \cdot 10^{-5}$		☑
parameter_58	GPa_Vmaxf		0.033		☑
parameter_59	GPa_KiGLYb		$1.5 \cdot 10^{-4}$		☑
parameter_60	GPa_KiG1P		0.010		☑
parameter_61	GPa_KiGLYf		0.002		☑
parameter_62	GPa_KPi		0.004		☑
parameter_63	GPb_Vmaxf		0.010		☑
parameter_64	GPb_KiGLYb		0.004		☑
parameter_65	GPb_KG1P		0.002		☑
parameter_66	GPb_KiGLYf		0.015		☑
parameter_67	GPb_KiPi		0.005		☑
parameter_68	FBA_Kdhap		$8 \cdot 10^{-5}$		☑
parameter_69	FBA_Kg3p		$1.6 \cdot 10^{-4}$		☑
parameter_70	FBA_Kfbp		$9 \cdot 10^{-6}$		☑
parameter_71	TPI_Kmp		0.002		☑
parameter_72	TPI_Kms		$5.1 \cdot 10^{-4}$		☑
parameter_73	GAPDH_Kdpg		$2.2 \cdot 10^{-5}$		☑
parameter_74	GAPDH_Knadh		10^{-5}		☑
parameter_75	GAPDH_Kg3p		$1.9 \cdot 10^{-4}$		☑
parameter_76	GAPDH_Knad		$9 \cdot 10^{-5}$		☑
parameter_77	GAPDH_Kp		0.029		☑
parameter_78	PGYM_Vmf		154.000		☑
parameter_79	PGYM_Kmp		$1.2 \cdot 10^{-4}$		☑

Id	Name	SBO	Value	Unit	Constant
parameter_80	PGYM_Kms		$1.9 \cdot 10^{-4}$		☑
parameter_81	PGI_Kf6p		$5 \cdot 10^{-5}$		☑
parameter_82	PGI_Kg6p		$4 \cdot 10^{-4}$		☑
parameter_83	LDH_Kp		0.005		☑
parameter_84	LDH_Kq		$7 \cdot 10^{-5}$		☑
parameter_85	LDH_Ka		$2 \cdot 10^{-6}$		☑
parameter_86	LDH_Kb		$3 \cdot 10^{-4}$		☑

6 Function definitions

This is an overview of 28 function definitions.

6.1 Function definition RUPE

Name RUPE

Arguments Vmax, RU5P, X5P, Keq_RUPE, KRu5P, KX5P

Mathematical Expression

$$\frac{\mathrm{Vmax} \cdot \left(\mathrm{RU5P} - \frac{\mathrm{X5P}}{\mathrm{Keq\_RUPE}}\right)}{\mathrm{RU5P} + \mathrm{KRu5P} \cdot \left(1 + \frac{\mathrm{X5P}}{\mathrm{KX5P}}\right)} \tag{1}$$

6.2 Function definition PGDH

Name PGDH

Arguments Vmax, K6PG1, KNADP, PGN, NADP, RU5P, NADPH, Kapp, BPG, KPGA23, ATP, KATP, K6PG2, KNADPH

Mathematical Expression

$$\frac{\frac{\mathrm{Vmax}}{\frac{\mathrm{K6PG1}}{\mathrm{KNADP}}} \cdot \left(\mathrm{PGN} \cdot \mathrm{NADP} - \frac{\mathrm{RU5P} \cdot \mathrm{NADPH}}{\mathrm{Kapp}}\right)}{\left(1 + \frac{\mathrm{NADP}}{\mathrm{KNADP}}\right) \cdot \left(1 + \frac{\mathrm{PGN}}{\mathrm{K6PG1}} + \frac{\mathrm{BPG}}{\mathrm{KPGA23}}\right) + \frac{\mathrm{ATP}}{\mathrm{KATP}} + \frac{\mathrm{NADPH} \cdot \left(1 + \frac{\mathrm{PGN}}{\mathrm{K6PG2}}\right)}{\mathrm{KNADPH}}} \tag{2}$$

6.3 Function definition G6PDH

Name G6PDH

Arguments Vmax, KG6P, KNADP, G6P, NADP, PGN, NADPH, Kapp, ATP, KATP, KNADPH, BPG, KPGA23

Mathematical Expression

$$\frac{\frac{\text{Vmax}}{\text{KG6P}} \cdot \left(\text{G6P} \cdot \text{NADP} - \frac{\text{PGN} \cdot \text{NADPH}}{\text{Kapp}}\right)}{1 + \frac{\text{NADP} \cdot \left(1 + \frac{\text{G6P}}{\text{KG6P}}\right)}{\text{KNADP}} + \frac{\text{ATP}}{\text{KATP}} + \frac{\text{NADPH}}{\text{KNADPH}} + \frac{\text{BPG}}{\text{KPGA23}}} \tag{3}$$

6.4 Function definition TKL

Name TKL

Arguments Vmax, R5P, X5P, GAP, S7P, Keq_TKL, K1, K2, K6, K3, K5, K4, K7

Mathematical Expression

$$\frac{\text{Vmax} \cdot \left(\text{R5P} \cdot \text{X5P} - \frac{\text{GAP} \cdot \text{S7P}}{\text{Keq\_TKL}}\right)}{(\text{K1} + \text{R5P}) \cdot \text{X5P} + (\text{K2} + \text{K6} \cdot \text{S7P}) \cdot \text{R5P} + (\text{K3} + \text{K5} \cdot \text{S7P}) \cdot \text{GAP} + \text{K4} \cdot \text{S7P} + \text{K7} \cdot \text{X5P} \cdot \text{GAP}} \tag{4}$$

6.5 Function definition PGI

Name PGI

Arguments Vmf, A, Kg6p, Vmr, P, Kf6p, E4P, Kery4p, F16P, Kfbp, PGN, Kpg

Mathematical Expression

$$\frac{\frac{\text{Vmf} \cdot \text{A}}{\text{Kg6p}} - \frac{\text{Vmr} \cdot \text{P}}{\text{Kf6p}}}{1 + \frac{\text{A}}{\text{Kg6p}} + \frac{\text{P}}{\text{Kf6p}} + \frac{\text{E4P}}{\text{Kery4p}} + \frac{\text{F16P}}{\text{Kfbp}} + \frac{\text{PGN}}{\text{Kpg}}} \tag{5}$$

6.6 Function definition TKL2

Name TKL2

Arguments Vmax, E4P, X5P, GAP, F6P, Keq_TKL2, K1, K2, K6, K3, K5, K4, K7

Mathematical Expression

$$\frac{\text{Vmax} \cdot \left(\text{E4P} \cdot \text{X5P} - \frac{\text{GAP} \cdot \text{F6P}}{\text{Keq\_TKL2}}\right)}{(\text{K1} + \text{E4P}) \cdot \text{X5P} + (\text{K2} + \text{K6} \cdot \text{F6P}) \cdot \text{E4P} + (\text{K3} + \text{K5} \cdot \text{F6P}) \cdot \text{GAP} + \text{K4} \cdot \text{F6P} + \text{K7} \cdot \text{X5P} \cdot \text{GAP}} \tag{6}$$

6.7 Function definition HK

Name HK

Arguments Vmf, Ka, Kb, A, B, P, Q, Kapp, Kp, Kq

Mathematical Expression

$$\frac{\frac{\mathrm{Vmf}}{\mathrm{Ka}\cdot\mathrm{Kb}}\cdot\left(\mathrm{A}\cdot\mathrm{B}-\frac{\mathrm{P}\cdot\mathrm{Q}}{\mathrm{Kapp}}\right)}{1+\frac{\mathrm{A}}{\mathrm{Ka}}+\frac{\mathrm{B}}{\mathrm{Kb}}+\frac{\mathrm{A}\cdot\mathrm{B}}{\mathrm{Ka}\cdot\mathrm{Kb}}+\frac{\mathrm{P}}{\mathrm{Kp}}+\frac{\mathrm{Q}}{\mathrm{Kq}}+\frac{\mathrm{P}\cdot\mathrm{Q}}{\mathrm{Kp}\cdot\mathrm{Kq}}+\frac{\mathrm{A}\cdot\mathrm{Q}}{\mathrm{Ka}\cdot\mathrm{Kq}}+\frac{\mathrm{P}\cdot\mathrm{B}}{\mathrm{Kp}\cdot\mathrm{Kb}}} \tag{7}$$

6.8 Function definition R5PI

Name R5PI

Arguments Vmax, RU5P, R5P, Keq_R5PI, KRu5P, KR5P

Mathematical Expression

$$\frac{\mathrm{Vmax}\cdot\left(\mathrm{RU5P}-\frac{\mathrm{R5P}}{\mathrm{Keq\_R5PI}}\right)}{\mathrm{RU5P}+\mathrm{KRu5P}\cdot\left(1+\frac{\mathrm{R5P}}{\mathrm{KR5P}}\right)} \tag{8}$$

6.9 Function definition GLUT

Name GLUT

Arguments Vmaxf, GLC_e, GLC, keq, KGlc_e, KGlc

Mathematical Expression

$$\frac{\mathrm{Vmaxf}\cdot\left(\mathrm{GLC\_e}-\frac{\mathrm{GLC}}{\mathrm{keq}}\right)}{\mathrm{KGlc\_e}\cdot\left(1+\frac{\mathrm{GLC}}{\mathrm{KGlc}}\right)+\mathrm{GLC\_e}} \tag{9}$$

6.10 Function definition TAL

Name TAL

Arguments Vmax, S7P, GAP, E4P, F6P, Keq_TAL, K1, K2, K6, K3, K5, K4, K7

Mathematical Expression

$$\frac{\mathrm{Vmax}\cdot\left(\mathrm{S7P}\cdot\mathrm{GAP}-\frac{\mathrm{E4P}\cdot\mathrm{F6P}}{\mathrm{Keq\_TAL}}\right)}{(\mathrm{K1}+\mathrm{GAP})\cdot\mathrm{S7P}+(\mathrm{K2}+\mathrm{K6}\cdot\mathrm{F6P})\cdot\mathrm{GAP}+(\mathrm{K3}+\mathrm{K5}\cdot\mathrm{F6P})\cdot\mathrm{E4P}+\mathrm{K4}\cdot\mathrm{F6P}+\mathrm{K7}\cdot\mathrm{S7P}\cdot\mathrm{E4P}} \tag{10}$$

6.11 Function definition PGLM

Name PGLM

Arguments Vmaxf, G1P, KG1P, Vmaxr, G6P, KG6P

Mathematical Expression

$$\frac{\frac{\text{Vmaxf}\cdot\text{G1P}}{\text{KG1P}} - \frac{\text{Vmaxr}\cdot\text{G6P}}{\text{KG6P}}}{1 + \frac{\text{G1P}}{\text{KG1P}} + \frac{\text{G6P}}{\text{KG6P}}} \tag{11}$$

6.12 Function definition PRPPS

Name PRPPS

Arguments Vmax, R5P, ATP, PRPP, AMP, Kapp, KATP, KR5P

Mathematical Expression

$$\frac{\text{Vmax}\cdot\left(\text{R5P}\cdot\text{ATP} - \frac{\text{PRPP}\cdot\text{AMP}}{\text{Kapp}}\right)}{(\text{KATP}+\text{ATP})\cdot(\text{KR5P}+\text{R5P})} \tag{12}$$

6.13 Function definition GPa

Name GPa

Arguments Vmaxf, GLY, Pi, KiGLYf, KPi, Vmaxr, G1P, KGLYb, KiG1P, KiPi, KiGLYb

Mathematical Expression

$$\frac{\text{Vmaxf}\cdot\frac{\text{GLY}\cdot\text{Pi}}{\text{KiGLYf}\cdot\text{KPi}} - \text{Vmaxr}\cdot\frac{\text{GLY}\cdot\text{G1P}}{\text{KGLYb}\cdot\text{KiG1P}}}{1 + \frac{\text{GLY}}{\text{KiGLYf}} + \frac{\text{Pi}}{\text{KiPi}} + \frac{\text{GLY}}{\text{KiGLYb}} + \frac{\text{G1P}}{\text{KiG1P}} + \frac{\text{GLY}\cdot\text{Pi}}{\text{KiGLYf}\cdot\text{KiPi}} + \frac{\text{GLY}\cdot\text{G1P}}{\text{KiGLYb}\cdot\text{KiG1P}}} \tag{13}$$

6.14 Function definition GPb

Name GPb

Arguments Vmaxf, GLY, Pi, KiGLYf, KPi, Vmaxr, G1P, KiGLYb, KG1P, KiPi, KiG1P, AMP, nH, Kamp

Mathematical Expression

$$\frac{\frac{\text{Vmaxf}\cdot\frac{\text{GLY}\cdot\text{Pi}}{\text{KiGLYf}\cdot\text{KPi}} - \text{Vmaxr}\cdot\frac{\text{GLY}\cdot\text{G1P}}{\text{KiGLYb}\cdot\text{KG1P}}}{1 + \frac{\text{GLY}}{\text{KiGLYf}} + \frac{\text{Pi}}{\text{KiPi}} + \frac{\text{GLY}}{\text{KiGLYb}} + \frac{\text{G1P}}{\text{KiG1P}} + \frac{\text{GLY}\cdot\text{Pi}}{\text{KiGLYf}\cdot\text{KPi}} + \frac{\text{GLY}\cdot\text{G1P}}{\text{KiGLYb}\cdot\text{KG1P}}} \cdot \frac{\text{AMP}^{\text{nH}}}{\text{Kamp}}}{1 + \frac{\text{AMP}^{\text{nH}}}{\text{Kamp}}} \tag{14}$$

6.15 Function definition FBA

Name FBA

Arguments Vmf, A, Kfbp, Vmr, P, Q, Kdhap, Kg3p

Mathematical Expression

$$\frac{\frac{\mathrm{Vmf}\cdot\mathrm{A}}{\mathrm{Kfbp}} - \frac{\mathrm{Vmr}\cdot\mathrm{P}\cdot\mathrm{Q}}{\mathrm{Kdhap}\cdot\mathrm{Kg3p}}}{1 + \frac{\mathrm{A}}{\mathrm{Kfbp}} + \frac{\mathrm{P}}{\mathrm{Kdhap}} + \frac{\mathrm{Q}}{\mathrm{Kg3p}} + \frac{\mathrm{P}\cdot\mathrm{Q}}{\mathrm{Kdhap}\cdot\mathrm{Kg3p}}} \tag{15}$$

6.16 Function definition TPI

Name TPI

Arguments Vf, GAP, Kms, Vr, DHAP, Kmp

Mathematical Expression

$$\frac{\frac{\mathrm{Vf}\cdot\mathrm{GAP}}{\mathrm{Kms}} - \frac{\mathrm{Vr}\cdot\mathrm{DHAP}}{\mathrm{Kmp}}}{1 + \frac{\mathrm{GAP}}{\mathrm{Kms}} + \frac{\mathrm{DHAP}}{\mathrm{Kmp}}} \tag{16}$$

6.17 Function definition GAPDH

Name GAPDH

Arguments Vmf, A, B, C, Knad, Kg3p, Kp, Vmr, P, Q, Kdpg, Knadh

Mathematical Expression

$$\frac{\frac{\mathrm{Vmf}\cdot\mathrm{A}\cdot\mathrm{B}\cdot\mathrm{C}}{\mathrm{Knad}\cdot\mathrm{Kg3p}\cdot\mathrm{Kp}} - \frac{\mathrm{Vmr}\cdot\mathrm{P}\cdot\mathrm{Q}}{\mathrm{Kdpg}\cdot\mathrm{Knadh}}}{1 + \frac{\mathrm{A}}{\mathrm{Knad}} + \frac{\mathrm{A}\cdot\mathrm{B}}{\mathrm{Knad}\cdot\mathrm{Kg3p}} + \frac{\mathrm{A}\cdot\mathrm{B}\cdot\mathrm{C}}{\mathrm{Knad}\cdot\mathrm{Kg3p}\cdot\mathrm{Kp}} + \frac{\mathrm{P}\cdot\mathrm{Q}}{\mathrm{Kdpg}\cdot\mathrm{Knadh}} + \frac{\mathrm{Q}}{\mathrm{Knadh}}} \tag{17}$$

6.18 Function definition PGK

Name PGK

Arguments Vmf, A, B, alfa, Ka, Kb, Vmr, P, Q, beta, Kp, Kq

Mathematical Expression

$$\frac{\frac{\mathrm{Vmf}\cdot\mathrm{A}\cdot\mathrm{B}}{\mathrm{alfa}\cdot\mathrm{Ka}\cdot\mathrm{Kb}} - \frac{\mathrm{Vmr}\cdot\mathrm{P}\cdot\mathrm{Q}}{\mathrm{beta}\cdot\mathrm{Kp}\cdot\mathrm{Kq}}}{1 + \frac{\mathrm{A}}{\mathrm{Ka}} + \frac{\mathrm{B}}{\mathrm{Kb}} + \frac{\mathrm{A}\cdot\mathrm{B}}{\mathrm{alfa}\cdot\mathrm{Ka}\cdot\mathrm{Kb}} + \frac{\mathrm{P}\cdot\mathrm{Q}}{\mathrm{beta}\cdot\mathrm{Kp}\cdot\mathrm{Kq}} + \frac{\mathrm{P}}{\mathrm{Kp}} + \frac{\mathrm{Q}}{\mathrm{Kq}}} \tag{18}$$

6.19 Function definition PFK

Name PFK

Arguments Vm, a, B, Katp, beta, F26P, alfa, Kf26bp, A, Kf6p, L, CIT, Kcit, Kiatp, Q, P, Kadp, Kfbp, Kapp

Mathematical Expression

$$\mathrm{Vm}\cdot\frac{\frac{\mathrm{a\cdot B}}{\mathrm{Katp}}}{1+\frac{\mathrm{a\cdot B}}{\mathrm{Katp}}}\cdot\frac{1+\frac{\mathrm{beta\cdot a\cdot F26P}}{\mathrm{alfa\cdot Kf26bp}}}{1+\frac{\mathrm{a\cdot F26P}}{\mathrm{alfa\cdot Kf26bp}}}\cdot\left(\frac{\frac{\mathrm{a\cdot A}\cdot\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{alfa\cdot Kf26bp}}\right)}{\mathrm{Kf6p}\cdot\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{Kf26bp}}\right)}\cdot\left(1+\frac{\mathrm{a\cdot A}\cdot\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{alfa\cdot Kf26bp}}\right)}{\mathrm{Kf6p}\cdot\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{Kf26bp}}\right)}\right)^{3}}{\frac{\mathrm{L}\cdot\left(1+\frac{\mathrm{a\cdot CIT}}{\mathrm{Kcit}}\right)^{4}\cdot\left(1+\frac{\mathrm{a\cdot B}}{\mathrm{Kiatp}}\right)^{4}}{\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{Kf26bp}}\right)^{4}}+\left(1+\frac{\mathrm{a\cdot A}\cdot\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{alfa\cdot Kf26bp}}\right)}{\mathrm{Kf6p}\cdot\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{Kf26bp}}\right)}\right)^{4}}-\frac{\frac{\mathrm{a\cdot Q\cdot a\cdot P}}{\mathrm{Kadp\cdot Kfbp\cdot Kapp}}}{\frac{\mathrm{a\cdot Q}}{\mathrm{Kadp}}+\frac{\mathrm{a\cdot P}}{\mathrm{Kfbp}}+\frac{\mathrm{a\cdot Q\cdot a\cdot P}}{\mathrm{Kadp\cdot Kfbp}}+1}\right) \tag{19}$$

6.20 Function definition function_1

Name PGYM [1]

Arguments Vmf, PG3, Kms, Vmr, PG2, Kmp

Mathematical Expression

$$\frac{\frac{\mathrm{Vmf\cdot PG3}}{\mathrm{Kms}}-\frac{\mathrm{Vmr\cdot PG2}}{\mathrm{Kmp}}}{1+\frac{\mathrm{PG3}}{\mathrm{Kms}}+\frac{\mathrm{PG2}}{\mathrm{Kmp}}} \tag{20}$$

6.21 Function definition GS

Name GS

Arguments Vmaxf, Kf, a, G1P, ATP, GLY, Pi, ADP, Keq, Kr

Mathematical Expression

$$\frac{\frac{\mathrm{Vmaxf}}{\mathrm{Kf}}\cdot\mathrm{a}\cdot\mathrm{G1P}\cdot\mathrm{a}\cdot\mathrm{ATP}\cdot\mathrm{a}\cdot\mathrm{GLY}\cdot\left(1-\frac{(\mathrm{a\cdot Pi})^{2}\cdot\mathrm{a\cdot ADP}}{\mathrm{a\cdot G1P\cdot a\cdot ATP\cdot Keq}}\right)}{1+\frac{\mathrm{a\cdot G1P\cdot a\cdot ATP\cdot a\cdot GLY}}{\mathrm{Kf}}+\frac{\mathrm{a\cdot GLY}\cdot(\mathrm{a\cdot Pi})^{2}\cdot\mathrm{a\cdot ADP}}{\mathrm{Kr}}} \tag{21}$$

6.22 Function definition function_2

Name ENO [1]

Arguments Vmf, PG2, Kms, Vmr, PEP, Kmp

Mathematical Expression

$$\frac{\frac{\mathrm{Vmf}\cdot\mathrm{PG2}}{\mathrm{Kms}} - \frac{\mathrm{Vmr}\cdot\mathrm{PEP}}{\mathrm{Kmp}}}{1 + \frac{\mathrm{PG2}}{\mathrm{Kms}} + \frac{\mathrm{PEP}}{\mathrm{Kmp}}} \tag{22}$$

6.23 Function definition function_3

Name PK [1]

Arguments Vm, B, Kadp, A, Kpep, L, Q, Kiatp, F16P, Kfbp, P, Katp, Kpyr, Kapp, a

Mathematical Expression

$$\mathrm{Vm}\cdot\left(\frac{\frac{\mathrm{a}\cdot\mathrm{B}}{\mathrm{Kadp}}}{1+\frac{\mathrm{a}\cdot\mathrm{B}}{\mathrm{Kadp}}}\cdot\frac{\frac{\mathrm{a}\cdot\mathrm{A}}{\mathrm{Kpep}}\cdot\left(1+\frac{\mathrm{a}\cdot\mathrm{A}}{\mathrm{Kpep}}\right)^3}{\frac{\mathrm{L}\cdot\left(1+\frac{\mathrm{a}\cdot\mathrm{Q}}{\mathrm{Kiatp}}\right)^4}{\left(1+\frac{\mathrm{a}\cdot\mathrm{F16P}}{\mathrm{Kfbp}}\right)^4}+\left(1+\frac{\mathrm{a}\cdot\mathrm{A}}{\mathrm{Kpep}}\right)^4}-\frac{\frac{\mathrm{a}\cdot\mathrm{Q}\cdot\mathrm{a}\cdot\mathrm{P}}{\mathrm{Katp}\cdot\mathrm{Kpyr}\cdot\mathrm{Kapp}}}{\frac{\mathrm{a}\cdot\mathrm{Q}}{\mathrm{Katp}}+\frac{\mathrm{a}\cdot\mathrm{P}}{\mathrm{Kpyr}}+\frac{\mathrm{a}\cdot\mathrm{Q}\cdot\mathrm{a}\cdot\mathrm{P}}{\mathrm{Katp}\cdot\mathrm{Kpyr}}+1}\right) \tag{23}$$

6.24 Function definition function_4

Name LDH [1]

Arguments Vmf, A, B, alfa, Ka, Kb, Vmr, P, Q, beta, Kp, Kq

Mathematical Expression

$$\frac{\frac{\mathrm{Vmf}\cdot\mathrm{A}\cdot\mathrm{B}}{\mathrm{alfa}\cdot\mathrm{Ka}\cdot\mathrm{Kb}} - \frac{\mathrm{Vmr}\cdot\mathrm{P}\cdot\mathrm{Q}}{\mathrm{beta}\cdot\mathrm{Kp}\cdot\mathrm{Kq}}}{1+\frac{\mathrm{A}}{\mathrm{Ka}}+\frac{\mathrm{B}}{\mathrm{Kb}}+\frac{\mathrm{A}\cdot\mathrm{B}}{\mathrm{alfa}\cdot\mathrm{Ka}\cdot\mathrm{Kb}}+\frac{\mathrm{P}\cdot\mathrm{Q}}{\mathrm{beta}\cdot\mathrm{Kp}\cdot\mathrm{Kq}}+\frac{\mathrm{P}}{\mathrm{Kp}}+\frac{\mathrm{Q}}{\mathrm{Kq}}} \tag{24}$$

6.25 Function definition function_5

Name AK [1]

Arguments Vf, ADP, ATP, AMP, Keq

Mathematical Expression

$$\frac{\mathrm{Vf}\cdot\mathrm{ADP}^2\cdot\left(1-\frac{\mathrm{ATP}\cdot\mathrm{AMP}}{\mathrm{Keq}}\right)}{(1+\mathrm{ADP})^2+(1+\mathrm{ATP})\cdot(1+\mathrm{AMP})-1} \tag{25}$$

6.26 Function definition function_6

Name DHase [1]

Arguments Vf, NADH, NAD, Keq

Mathematical Expression

$$\frac{\mathrm{Vf} \cdot \mathrm{NADH} \cdot \left(1 - \frac{\mathrm{NAD}}{\mathrm{NADH} \cdot \mathrm{Keq}}\right)}{1 + \mathrm{NADH} + 1 + \mathrm{NAD} - 1} \tag{26}$$

6.27 Function definition function_7

Name DPHase [1]

Arguments Vf, NADPH, NADP, Keq

Mathematical Expression

$$\frac{\mathrm{Vf} \cdot \mathrm{NADPH} \cdot \left(1 - \frac{\mathrm{NADP}}{\mathrm{NADPH} \cdot \mathrm{Keq}}\right)}{1 + \mathrm{NADPH} + 1 + \mathrm{NADP} - 1} \tag{27}$$

6.28 Function definition function_8

Name MPM [1]

Arguments Vmf, PYR, y, Pi, ADP, O2, ATP, CO2, Keq

Mathematical Expression

$$\frac{\mathrm{Vmf} \cdot \mathrm{PYR}^{\frac{1}{\mathrm{y}}} \cdot \mathrm{Pi} \cdot \mathrm{ADP} \cdot \mathrm{O2}^{\frac{5}{2 \cdot \mathrm{y}}} \cdot \left(1 - \frac{\mathrm{ATP} \cdot \mathrm{CO2}^{\frac{3}{\mathrm{y}}}}{\mathrm{PYR}^{\frac{1}{\mathrm{y}}} \cdot \mathrm{O2}^{\frac{5}{2 \cdot \mathrm{y}}} \cdot \mathrm{Pi} \cdot \mathrm{ADP} \cdot \mathrm{Keq}}\right)}{(1 + \mathrm{PYR})^{\frac{1}{\mathrm{y}}} \cdot (1 + \mathrm{O2})^{\frac{5}{2 \cdot \mathrm{y}}} \cdot (1 + \mathrm{Pi}) \cdot (1 + \mathrm{ADP}) + (1 + \mathrm{ATP}) \cdot (1 + \mathrm{CO2})^{\frac{3}{\mathrm{y}}} - 1} \tag{28}$$

7 Rules

This is an overview of 34 rules.

7.1 Rule parameter_35

Rule parameter_35 is an assignment rule for parameter parameter_35:

$$\mathrm{parameter\_35} = 1056 \cdot \mathrm{parameter\_28} \tag{29}$$

7.2 Rule parameter_36

Rule parameter_36 is an assignment rule for parameter parameter_36:

$$\text{parameter\_36} = 0.1761 \cdot \text{parameter\_28} \tag{30}$$

7.3 Rule parameter_40

Rule parameter_40 is an assignment rule for parameter parameter_40:

$$\text{parameter\_40} = 73.41 \cdot \text{parameter\_28} \tag{31}$$

7.4 Rule parameter_44

Rule parameter_44 is an assignment rule for parameter parameter_44:

$$\text{parameter\_44} = 27.81 \cdot \text{parameter\_28} \tag{32}$$

7.5 Rule parameter_30

Rule parameter_30 is an assignment rule for parameter parameter_30:

$$\text{parameter\_30} = 23.03 \cdot \text{parameter\_28} \tag{33}$$

7.6 Rule parameter_42

Rule parameter_42 is an assignment rule for parameter parameter_42:

$$\text{parameter\_42} = 107.6 \cdot \text{parameter\_28} \tag{34}$$

7.7 Rule parameter_11

Rule parameter_11 is an assignment rule for parameter parameter_11:

$$\text{parameter\_11} = \frac{\text{parameter\_40} \cdot \text{parameter\_49} \cdot \text{parameter\_50}}{\text{parameter\_51} \cdot \text{parameter\_52} \cdot \text{parameter\_20}} \tag{35}$$

7.8 Rule parameter_48

Rule parameter_48 is an assignment rule for parameter parameter_48:

$$\text{parameter\_48} = 9801000 \cdot \text{parameter\_29} \tag{36}$$

7.9 Rule parameter_34

Rule parameter_34 is an assignment rule for parameter parameter_34:

$$\text{parameter\_34} = 31.02 \cdot \text{parameter\_28} \tag{37}$$

7.10 Rule parameter_43

Rule parameter_43 is an assignment rule for parameter parameter_43:

$$\text{parameter\_43} = 160.9 \cdot \text{parameter\_28} \tag{38}$$

7.11 Rule parameter_24

Rule parameter_24 is an assignment rule for parameter parameter_24:

$$\text{parameter\_24} = \frac{\text{parameter\_43} \cdot \text{parameter\_53}}{\text{parameter\_54} \cdot \text{parameter\_23}} \tag{39}$$

7.12 Rule parameter_15

Rule parameter_15 is an assignment rule for parameter parameter_15:

$$\text{parameter\_15} = \frac{\text{parameter\_55} \cdot \text{parameter\_56}}{\text{parameter\_57} \cdot \text{parameter\_16}} \tag{40}$$

7.13 Rule parameter_47

Rule parameter_47 is an assignment rule for parameter parameter_47:

$$\text{parameter\_47} = 127800 \cdot \text{parameter\_28} \tag{41}$$

7.14 Rule species_10

Rule species_10 is an assignment rule for species species_10:

$$\text{species\_10} = \text{parameter\_2} - [\text{species\_11}] \tag{42}$$

7.15 Rule species_3

Rule species_3 is an assignment rule for species species_3:

$$\text{species\_3} = \text{parameter\_1} - [\text{species\_4}] \tag{43}$$

7.16 Rule species_18

Rule species_18 is an assignment rule for species species_18:

$$\text{species\_18} = \text{parameter\_3} - [\text{species\_19}] \tag{44}$$

7.17 Rule parameter_4

Rule parameter_4 is an assignment rule for parameter parameter_4:

$$\text{parameter\_4} = \frac{\text{parameter\_58} \cdot \text{parameter\_59} \cdot \text{parameter\_60}}{\text{parameter\_61} \cdot \text{parameter\_62} \cdot \text{parameter\_5}} \tag{45}$$

7.18 Rule parameter_7

Rule parameter_7 is an assignment rule for parameter parameter_7:

$$\text{parameter\_7} = \frac{\text{parameter\_63} \cdot \text{parameter\_64} \cdot \text{parameter\_65}}{\text{parameter\_66} \cdot \text{parameter\_67} \cdot \text{parameter\_6}} \tag{46}$$

7.19 Rule parameter_37

Rule parameter_37 is an assignment rule for parameter parameter_37:

$$\text{parameter\_37} = 14.63 \cdot \text{parameter\_28} \tag{47}$$

7.20 Rule parameter_8

Rule parameter_8 is an assignment rule for parameter parameter_8:

$$\text{parameter\_8} = \frac{\text{parameter\_37} \cdot \text{parameter\_68} \cdot \text{parameter\_69}}{\text{parameter\_12} \cdot \text{parameter\_70}} \tag{48}$$

7.21 Rule parameter_38

Rule parameter_38 is an assignment rule for parameter parameter_38:

$$\text{parameter\_38} = 5.976 \cdot \text{parameter\_28} \tag{49}$$

7.22 Rule parameter_9

Rule parameter_9 is an assignment rule for parameter parameter_9:

$$\text{parameter\_9} = \frac{\text{parameter\_38} \cdot \text{parameter\_71}}{\text{parameter\_72} \cdot \text{parameter\_18}} \tag{50}$$

7.23 Rule parameter_39

Rule parameter_39 is an assignment rule for parameter parameter_39:

$$\text{parameter\_39} = 109.1 \cdot \text{parameter\_28} \tag{51}$$

7.24 Rule parameter_10

Rule parameter_10 is an assignment rule for parameter parameter_10:

$$\text{parameter\_10} = \frac{\text{parameter\_39} \cdot \text{parameter\_73} \cdot \text{parameter\_74}}{\text{parameter\_75} \cdot \text{parameter\_76} \cdot \text{parameter\_77} \cdot \text{parameter\_19}} \tag{52}$$

7.25 Rule parameter_41

Rule parameter_41 is an assignment rule for parameter parameter_41:

$$\text{parameter\_41} = 32040 \cdot \text{parameter\_28} \tag{53}$$

7.26 Rule parameter_46

Rule parameter_46 is an assignment rule for parameter parameter_46:

$$\text{parameter\_46} = 4982000 \cdot \text{parameter\_28} \tag{54}$$

7.27 Rule parameter_22

Rule parameter_22 is an assignment rule for parameter parameter_22:

$$\text{parameter\_22} = \frac{\text{parameter\_78} \cdot \text{parameter\_79}}{\text{parameter\_80} \cdot \text{parameter\_21}} \tag{55}$$

7.28 Rule parameter_31

Rule parameter_31 is an assignment rule for parameter parameter_31:

$$\text{parameter\_31} = 86.85 \cdot \text{parameter\_28} \tag{56}$$

7.29 Rule parameter_33

Rule parameter_33 is an assignment rule for parameter parameter_33:

$$\text{parameter\_33} = 1.008 \cdot \text{parameter\_28} \tag{57}$$

7.30 Rule parameter_32

Rule parameter_32 is an assignment rule for parameter parameter_32:

$$\text{parameter\_32} = 7778 \cdot \text{parameter\_28} \tag{58}$$

7.31 Rule parameter_13

Rule parameter_13 is an assignment rule for parameter parameter_13:

$$\text{parameter\_13} = \text{parameter\_32} \cdot \frac{\text{parameter\_81}}{\text{parameter\_82} \cdot \text{parameter\_14}} \tag{59}$$

7.32 Rule parameter_27

Rule parameter_27 is an assignment rule for parameter parameter_27:

$$\text{parameter\_27} = [\text{species\_20}] \tag{60}$$

Derived unit $\text{nmol} \cdot \text{nl}^{-1}$

7.33 Rule parameter_45

Rule parameter_45 is an assignment rule for parameter parameter_45:

$$\text{parameter\_45} = 340.3 \cdot \text{parameter\_28} \tag{61}$$

7.34 Rule parameter_26

Rule parameter_26 is an assignment rule for parameter parameter_26:

$$\text{parameter\_26} = \frac{\text{parameter\_45} \cdot \text{parameter\_83} \cdot \text{parameter\_84}}{\text{parameter\_85} \cdot \text{parameter\_86} \cdot \text{parameter\_25}} \tag{62}$$

8 Reactions

This model contains 29 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	reaction_1	GLUT	$\text{species\_9} \xrightleftharpoons{\text{species\_9, species\_1}} \text{species\_1}$	
2	reaction_2	HK	$\text{species\_1} + \text{species\_4} \xrightleftharpoons{\text{species\_1, species\_4, species\_2, species\_3}} \text{species\_2} + \text{species\_3}$	
3	reaction_3	PGI	$\text{species\_2} \xrightleftharpoons{\text{species\_7, species\_6, species\_8, species\_2, species\_5, species\_7, species\_6, sp}}$	
4	reaction_4	G6PDH	$\text{species\_2} + \text{species\_10} \xrightleftharpoons{\text{species\_4, species\_12, species\_2, species\_10, species\_8, species\_}} \text{species\_11}$	
5	reaction_5	PGDH	$\text{species\_8} + \text{species\_10} \xrightleftharpoons{\text{species\_12, species\_4, species\_8, species\_10, species\_13, specie}} \text{species\_11}$	
6	reaction_6	RUPE	$\text{species\_13} \xrightleftharpoons{\text{species\_13, species\_14}} \text{species\_14}$	
7	reaction_7	R5PI	$\text{species\_13} \xrightleftharpoons{\text{species\_13, species\_15}} \text{species\_15}$	
8	reaction_8	TKL	$\text{species\_15} + \text{species\_14} \xrightleftharpoons{\text{species\_15, species\_14, species\_16, species\_17}} \text{species\_16} + \text{species\_17}$	
9	reaction_9	TKL2	$\text{species\_14} + \text{species\_7} \xrightleftharpoons{\text{species\_7, species\_14, species\_16, species\_5}} \text{species\_16} + \text{species\_5}$	
10	reaction_10	TAL	$\text{species\_17} + \text{species\_16} \xrightleftharpoons{\text{species\_17, species\_16, species\_7, species\_5}} \text{species\_5} + \text{species\_7}$	

№	Id	Name	Reaction Equation	SBO
11	reaction_11	PRPPS	species_15 + species_4 $\overset{\text{species\_15, species\_4, species\_21, species\_20}}{\rightleftharpoons}$ species_20 + species_21	
12	reaction_12	PGLM	species_22 $\overset{\text{species\_22, species\_2}}{\rightleftharpoons}$ species_2	
13	reaction_13	GPa	species_24 + species_23 $\overset{\text{species\_24, species\_23, species\_22}}{\rightleftharpoons}$ species_24 + species_22	
14	reaction_14	FBA	species_6 $\overset{\text{species\_6, species\_27, species\_16}}{\rightleftharpoons}$ species_16 + species_27	
15	reaction_15	TPI	species_16 $\overset{\text{species\_16, species\_27}}{\rightleftharpoons}$ species_27	
16	reaction_16	GAPDH	species_16 + species_19 + species_23 $\overset{\text{species\_19, species\_16, species\_23, species\_12, species\_18}}{\rightleftharpoons}$ species_12 + species_18	
17	reaction_17	PGK	species_12 + species_3 $\overset{\text{species\_12, species\_3, species\_28, species\_4}}{\rightleftharpoons}$ species_28 + species_4	
18	reaction_18	GPb	species_24 + species_23 $\overset{\text{species\_24, species\_23, species\_22}}{\rightleftharpoons}$ species_24 + species_22	
19	reaction_19	GS	species_22 + species_4 $\overset{\text{species\_22, species\_4, species\_24, species\_23, species\_3}}{\rightleftharpoons}$ species_3 + 2 species_23	
20	reaction_20	PFK	species_5 + species_4 $\overset{\text{species\_26, species\_25, species\_4, species\_26, species\_5, species\_}}{\rightleftharpoons}$ species_3	
21	reaction_21	PGYM	species_28 $\overset{\text{species\_28, species\_29}}{\rightleftharpoons}$ species_29	
22	reaction_22	ENO	species_29 $\overset{\text{species\_29, species\_30}}{\rightleftharpoons}$ species_30	

№	Id	Name	Reaction Equation	SBO
23	reaction_23	PK	$\text{species\_30} + \text{species\_3} \xrightleftharpoons{\text{species\_6, species\_3, species\_30, species\_4, species\_6, species\_3}} \text{species\_4}$	
24	reaction_24	LDH	$\text{species\_31} + \text{species\_18} \xrightleftharpoons{\text{species\_18, species\_31, species\_32, species\_19}} \text{species\_32} + \text{species\_19}$	
25	reaction_25	AK	$2\,\text{species\_3} \xrightleftharpoons{\text{species\_3, species\_4, species\_20}} \text{species\_4} + \text{species\_20}$	
26	reaction_26	DHase	$\text{species\_18} \xrightleftharpoons{\text{species\_18, species\_19}} \text{species\_19}$	
27	reaction_27	DPHase	$\text{species\_11} \xrightleftharpoons{\text{species\_11, species\_10}} \text{species\_10}$	
28	reaction_28	MPM	$0 \cdot 08\,\text{species\_31} + 0 \cdot 2\,\text{species\_34} + \text{species\_23} + \text{species\_3} \xrightleftharpoons{\text{species\_31, species\_23, species\_3, species\_34, species\_4, species\_33}} 0 \cdot 24\,\text{sp} \text{species\_4}$	
29	reaction_29	ATPase	$\text{species\_4} \xrightarrow{\text{species\_4}} \text{species\_3} + \text{species\_23}$	

8.1 Reaction reaction_1

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

Name GLUT

Reaction equation

$$\text{species\_9} \xrightleftharpoons{\text{species\_9, species\_1}} \text{species\_1} \tag{63}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
species_9	GLC_e	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
species_9	GLC_e	
species_1	GLC	

Product

Table 8: Properties of each product.

Id	Name	SBO
species_1	GLC	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}\left(\text{compartment\_1}\right) \cdot \text{GLUT}\left(\text{parameter\_30}, [\text{species\_9}], [\text{species\_1}], \text{keq}, \text{KGlc\_e}, \text{KGlc}\right) \tag{64}$$

$$\text{GLUT}\left(\text{Vmaxf}, \text{GLC\_e}, \text{GLC}, \text{keq}, \text{KGlc\_e}, \text{KGlc}\right) = \frac{\text{Vmaxf} \cdot \left(\text{GLC\_e} - \frac{\text{GLC}}{\text{keq}}\right)}{\text{KGlc\_e} \cdot \left(1 + \frac{\text{GLC}}{\text{KGlc}}\right) + \text{GLC\_e}} \tag{65}$$

$$\mathrm{GLUT}\left(\mathrm{Vmaxf}, \mathrm{GLC\_e}, \mathrm{GLC}, \mathrm{keq}, \mathrm{KGlc\_e}, \mathrm{KGlc}\right) = \frac{\mathrm{Vmaxf} \cdot \left(\mathrm{GLC\_e} - \frac{\mathrm{GLC}}{\mathrm{keq}}\right)}{\mathrm{KGlc\_e} \cdot \left(1 + \frac{\mathrm{GLC}}{\mathrm{KGlc}}\right) + \mathrm{GLC\_e}} \quad (66)$$

Table 9: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`keq`	keq		1.000		☑
`KGlc_e`	KGlc_e		0.010		☑
`KGlc`	KGlc		0.009		☑

8.2 Reaction `reaction_2`

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

Name HK

Reaction equation

$$\mathrm{species\_1} + \mathrm{species\_4} \xrightleftharpoons{\mathrm{species\_1},\ \mathrm{species\_4},\ \mathrm{species\_2},\ \mathrm{species\_3}} \mathrm{species\_2} + \mathrm{species\_3} \quad (67)$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
`species_1`	GLC	
`species_4`	ATP	

Modifiers

Table 11: Properties of each modifier.

Id	Name	SBO
`species_1`	GLC	
`species_4`	ATP	
`species_2`	G6P	
`species_3`	ADP	

Products

Table 12: Properties of each product.

Id	Name	SBO
species_2	G6P	
species_3	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{HK}\left(\mathrm{parameter\_31}, \mathrm{Ka}, \mathrm{Kb}, [\mathrm{species\_1}], [\mathrm{species\_4}], [\mathrm{species\_2}], [\mathrm{species\_3}], \mathrm{Kapp}, \mathrm{Kp}, \mathrm{Kq}\right) \tag{68}$$

$$\mathrm{HK}\left(\mathrm{Vmf}, \mathrm{Ka}, \mathrm{Kb}, \mathrm{A}, \mathrm{B}, \mathrm{P}, \mathrm{Q}, \mathrm{Kapp}, \mathrm{Kp}, \mathrm{Kq}\right) = \frac{\frac{\mathrm{Vmf}}{\mathrm{Ka}\cdot\mathrm{Kb}} \cdot \left(\mathrm{A}\cdot\mathrm{B} - \frac{\mathrm{P}\cdot\mathrm{Q}}{\mathrm{Kapp}}\right)}{1 + \frac{\mathrm{A}}{\mathrm{Ka}} + \frac{\mathrm{B}}{\mathrm{Kb}} + \frac{\mathrm{A}\cdot\mathrm{B}}{\mathrm{Ka}\cdot\mathrm{Kb}} + \frac{\mathrm{P}}{\mathrm{Kp}} + \frac{\mathrm{Q}}{\mathrm{Kq}} + \frac{\mathrm{P}\cdot\mathrm{Q}}{\mathrm{Kp}\cdot\mathrm{Kq}} + \frac{\mathrm{A}\cdot\mathrm{Q}}{\mathrm{Ka}\cdot\mathrm{Kq}} + \frac{\mathrm{P}\cdot\mathrm{B}}{\mathrm{Kp}\cdot\mathrm{Kb}}} \tag{69}$$

$$\mathrm{HK}\left(\mathrm{Vmf}, \mathrm{Ka}, \mathrm{Kb}, \mathrm{A}, \mathrm{B}, \mathrm{P}, \mathrm{Q}, \mathrm{Kapp}, \mathrm{Kp}, \mathrm{Kq}\right) = \frac{\frac{\mathrm{Vmf}}{\mathrm{Ka}\cdot\mathrm{Kb}} \cdot \left(\mathrm{A}\cdot\mathrm{B} - \frac{\mathrm{P}\cdot\mathrm{Q}}{\mathrm{Kapp}}\right)}{1 + \frac{\mathrm{A}}{\mathrm{Ka}} + \frac{\mathrm{B}}{\mathrm{Kb}} + \frac{\mathrm{A}\cdot\mathrm{B}}{\mathrm{Ka}\cdot\mathrm{Kb}} + \frac{\mathrm{P}}{\mathrm{Kp}} + \frac{\mathrm{Q}}{\mathrm{Kq}} + \frac{\mathrm{P}\cdot\mathrm{Q}}{\mathrm{Kp}\cdot\mathrm{Kq}} + \frac{\mathrm{A}\cdot\mathrm{Q}}{\mathrm{Ka}\cdot\mathrm{Kq}} + \frac{\mathrm{P}\cdot\mathrm{B}}{\mathrm{Kp}\cdot\mathrm{Kb}}} \tag{70}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Ka	Ka		10^{-4}		☑
Kb	Kb		0.001		☑
Kapp	Kapp		651.000		☑
Kp	Kp		$2 \cdot 10^{-5}$		☑
Kq	Kq		0.004		☑

8.3 Reaction reaction_3

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

Name PGI

Reaction equation

$$\text{species\_2} \xrightleftharpoons{\text{species\_7, species\_6, species\_8, species\_2, species\_5, species\_7, species\_6, species\_8}} \text{species\_5} \tag{71}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
species_2	G6P	

Modifiers

Table 15: Properties of each modifier.

Id	Name	SBO
species_7	E4P	
species_6	F16P	
species_8	PGN	
species_2	G6P	
species_5	F6P	
species_7	E4P	
species_6	F16P	
species_8	PGN	

Product

Table 16: Properties of each product.

Id	Name	SBO
species_5	F6P	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}\left(\text{compartment\_1}\right) \cdot \text{PGI}\left(\text{parameter\_32}, [\text{species\_2}], \text{parameter\_82}, \text{parameter\_13}, [\text{species\_5}], \text{parameter\_81}, [\text{species\_7}], \text{Kery4p}, [\text{species\_6}], \text{Kfbp}, [\text{species\_8}], \text{Kpg}\right) \tag{72}$$

$$\begin{aligned}&\mathrm{PGI}\left(\mathrm{Vmf},\mathrm{A},\mathrm{Kg6p},\mathrm{Vmr},\mathrm{P},\mathrm{Kf6p},\mathrm{E4P},\mathrm{Kery4p},\mathrm{F16P},\mathrm{Kfbp},\mathrm{PGN},\mathrm{Kpg}\right)\\&=\frac{\frac{\mathrm{Vmf}\cdot\mathrm{A}}{\mathrm{Kg6p}}-\frac{\mathrm{Vmr}\cdot\mathrm{P}}{\mathrm{Kf6p}}}{1+\frac{\mathrm{A}}{\mathrm{Kg6p}}+\frac{\mathrm{P}}{\mathrm{Kf6p}}+\frac{\mathrm{E4P}}{\mathrm{Kery4p}}+\frac{\mathrm{F16P}}{\mathrm{Kfbp}}+\frac{\mathrm{PGN}}{\mathrm{Kpg}}}\end{aligned}\tag{73}$$

$$\begin{aligned}&\mathrm{PGI}\left(\mathrm{Vmf},\mathrm{A},\mathrm{Kg6p},\mathrm{Vmr},\mathrm{P},\mathrm{Kf6p},\mathrm{E4P},\mathrm{Kery4p},\mathrm{F16P},\mathrm{Kfbp},\mathrm{PGN},\mathrm{Kpg}\right)\\&=\frac{\frac{\mathrm{Vmf}\cdot\mathrm{A}}{\mathrm{Kg6p}}-\frac{\mathrm{Vmr}\cdot\mathrm{P}}{\mathrm{Kf6p}}}{1+\frac{\mathrm{A}}{\mathrm{Kg6p}}+\frac{\mathrm{P}}{\mathrm{Kf6p}}+\frac{\mathrm{E4P}}{\mathrm{Kery4p}}+\frac{\mathrm{F16P}}{\mathrm{Kfbp}}+\frac{\mathrm{PGN}}{\mathrm{Kpg}}}\end{aligned}\tag{74}$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Kery4p`	Kery4p		10^{-6}		☑
`Kfbp`	Kfbp		$6\cdot10^{-5}$		☑
`Kpg`	Kpg		$1.5\cdot10^{-5}$		☑

8.4 Reaction `reaction_4`

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

Name G6PDH

Reaction equation

$$\mathrm{species\_2}+\mathrm{species\_10}\xrightleftharpoons{\mathrm{species\_4},\ \mathrm{species\_12},\ \mathrm{species\_2},\ \mathrm{species\_10},\ \mathrm{species\_8},\ \mathrm{species\_11},\ \mathrm{species\_4},\ \mathrm{species\_12}}\ \mathrm{sp}\tag{75}$$

Reactants

Table 18: Properties of each reactant.

Id	Name	SBO
`species_2`	G6P	
`species_10`	NADP	

Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
species_4	ATP	
species_12	BPG	
species_2	G6P	
species_10	NADP	
species_8	PGN	
species_11	NADPH	
species_4	ATP	
species_12	BPG	

Products

Table 20: Properties of each product.

Id	Name	SBO
species_8	PGN	
species_11	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{G6PDH}\left(\mathrm{parameter\_33}, \mathrm{KG6P}, \mathrm{KNADP}, [\mathrm{species\_2}], [\mathrm{species\_10}], [\mathrm{species\_8}], [\mathrm{species\_11}], \mathrm{Kapp}, [\mathrm{species\_4}], \mathrm{KATP}, \mathrm{KNADPH}, [\mathrm{species\_12}], \mathrm{KPGA23}\right) \tag{76}$$

$$\mathrm{G6PDH}\left(\mathrm{Vmax}, \mathrm{KG6P}, \mathrm{KNADP}, \mathrm{G6P}, \mathrm{NADP}, \mathrm{PGN}, \mathrm{NADPH}, \mathrm{Kapp}, \mathrm{ATP}, \mathrm{KATP}, \mathrm{KNADPH}, \mathrm{BPG}, \mathrm{KPGA23}\right) = \frac{\frac{\frac{\mathrm{Vmax}}{\mathrm{KG6P}}}{\mathrm{KNADP}} \cdot \left(\mathrm{G6P} \cdot \mathrm{NADP} - \frac{\mathrm{PGN} \cdot \mathrm{NADPH}}{\mathrm{Kapp}}\right)}{1 + \frac{\mathrm{NADP} \cdot \left(1 + \frac{\mathrm{G6P}}{\mathrm{KG6P}}\right)}{\mathrm{KNADP}} + \frac{\mathrm{ATP}}{\mathrm{KATP}} + \frac{\mathrm{NADPH}}{\mathrm{KNADPH}} + \frac{\mathrm{BPG}}{\mathrm{KPGA23}}} \tag{77}$$

$$\mathrm{G6PDH}\left(\mathrm{Vmax}, \mathrm{KG6P}, \mathrm{KNADP}, \mathrm{G6P}, \mathrm{NADP}, \mathrm{PGN}, \mathrm{NADPH}, \mathrm{Kapp}, \mathrm{ATP}, \mathrm{KATP}, \mathrm{KNADPH}, \mathrm{BPG}, \mathrm{KPGA23}\right) = \frac{\frac{\frac{\mathrm{Vmax}}{\mathrm{KG6P}}}{\mathrm{KNADP}} \cdot \left(\mathrm{G6P} \cdot \mathrm{NADP} - \frac{\mathrm{PGN} \cdot \mathrm{NADPH}}{\mathrm{Kapp}}\right)}{1 + \frac{\mathrm{NADP} \cdot \left(1 + \frac{\mathrm{G6P}}{\mathrm{KG6P}}\right)}{\mathrm{KNADP}} + \frac{\mathrm{ATP}}{\mathrm{KATP}} + \frac{\mathrm{NADPH}}{\mathrm{KNADPH}} + \frac{\mathrm{BPG}}{\mathrm{KPGA23}}} \tag{78}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KG6P	KG6P		$6.67 \cdot 10^{-8}$		☑
KNADP	KNADP		$3.67 \cdot 10^{-9}$		☑
Kapp	Kapp		2000.000		☑
KATP	KATP		$7.49 \cdot 10^{-7}$		☑
KNADPH	KNADPH		$3.12 \cdot 10^{-9}$		☑
KPGA23	KPGA23		$2.289 \cdot 10^{-6}$		☑

8.5 Reaction reaction_5

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

Name PGDH

Reaction equation

$$\text{species\_8} + \text{species\_10} \xrightleftharpoons{\text{species\_12, species\_4, species\_8, species\_10, species\_13, species\_11, species\_12, species\_4}} \text{s} \tag{79}$$

Reactants

Table 22: Properties of each reactant.

Id	Name	SBO
species_8	PGN	
species_10	NADP	

Modifiers

Table 23: Properties of each modifier.

Id	Name	SBO
species_12	BPG	
species_4	ATP	
species_8	PGN	
species_10	NADP	
species_13	RU5P	
species_11	NADPH	
species_12	BPG	
species_4	ATP	

Id	Name	SBO

Products

Table 24: Properties of each product.

Id	Name	SBO
species_13	RU5P	
species_11	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{PGDH}\left(\mathrm{parameter\_34}, \mathrm{K6PG1}, \mathrm{KNADP}, [\mathrm{species\_8}], [\mathrm{species\_10}], [\mathrm{species\_13}], [\mathrm{species\_11}], \mathrm{Kapp}, [\mathrm{species\_12}], \mathrm{KPGA23}, [\mathrm{species\_4}], \mathrm{KATP}, \mathrm{K6PG2}, \mathrm{KNADPH}\right) \tag{80}$$

$$\mathrm{PGDH}\left(\mathrm{Vmax}, \mathrm{K6PG1}, \mathrm{KNADP}, \mathrm{PGN}, \mathrm{NADP}, \mathrm{RU5P}, \mathrm{NADPH}, \mathrm{Kapp}, \mathrm{BPG}, \mathrm{KPGA23}, \mathrm{ATP}, \mathrm{KATP}, \mathrm{K6PG2}, \mathrm{KNADPH}\right) = \frac{\frac{\frac{\mathrm{Vmax}}{\mathrm{K6PG1}}}{\mathrm{KNADP}} \cdot \left(\mathrm{PGN} \cdot \mathrm{NADP} - \frac{\mathrm{RU5P} \cdot \mathrm{NADPH}}{\mathrm{Kapp}}\right)}{\left(1 + \frac{\mathrm{NADP}}{\mathrm{KNADP}}\right) \cdot \left(1 + \frac{\mathrm{PGN}}{\mathrm{K6PG1}} + \frac{\mathrm{BPG}}{\mathrm{KPGA23}}\right) + \frac{\mathrm{ATP}}{\mathrm{KATP}} + \frac{\mathrm{NADPH} \cdot \left(1 + \frac{\mathrm{PGN}}{\mathrm{K6PG2}}\right)}{\mathrm{KNADPH}}} \tag{81}$$

$$\mathrm{PGDH}\left(\mathrm{Vmax}, \mathrm{K6PG1}, \mathrm{KNADP}, \mathrm{PGN}, \mathrm{NADP}, \mathrm{RU5P}, \mathrm{NADPH}, \mathrm{Kapp}, \mathrm{BPG}, \mathrm{KPGA23}, \mathrm{ATP}, \mathrm{KATP}, \mathrm{K6PG2}, \mathrm{KNADPH}\right) = \frac{\frac{\frac{\mathrm{Vmax}}{\mathrm{K6PG1}}}{\mathrm{KNADP}} \cdot \left(\mathrm{PGN} \cdot \mathrm{NADP} - \frac{\mathrm{RU5P} \cdot \mathrm{NADPH}}{\mathrm{Kapp}}\right)}{\left(1 + \frac{\mathrm{NADP}}{\mathrm{KNADP}}\right) \cdot \left(1 + \frac{\mathrm{PGN}}{\mathrm{K6PG1}} + \frac{\mathrm{BPG}}{\mathrm{KPGA23}}\right) + \frac{\mathrm{ATP}}{\mathrm{KATP}} + \frac{\mathrm{NADPH} \cdot \left(1 + \frac{\mathrm{PGN}}{\mathrm{K6PG2}}\right)}{\mathrm{KNADPH}}} \tag{82}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K6PG1	K6PG1		10^{-8}		☑
KNADP	KNADP		$1.8 \cdot 10^{-8}$		☑
Kapp	Kapp		141.700		☑
KPGA23	KPGA23		$1.2 \cdot 10^{-7}$		☑
KATP	KATP		$1.54 \cdot 10^{-7}$		☑
K6PG2	K6PG2		$5.8 \cdot 10^{-8}$		☑
KNADPH	KNADPH		$4.5 \cdot 10^{-9}$		☑

8.6 Reaction reaction_6

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

Name RUPE

Reaction equation

$$\text{species\_13} \xrightleftharpoons{\text{species\_13, species\_14}} \text{species\_14} \tag{83}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
species_13	RU5P	

Modifiers

Table 27: Properties of each modifier.

Id	Name	SBO
species_13	RU5P	
species_14	X5P	

Product

Table 28: Properties of each product.

Id	Name	SBO
species_14	X5P	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{vol}(\text{compartment\_1}) \cdot \text{RUPE}(\text{Vmax}, [\text{species\_13}], [\text{species\_14}], \text{Keq\_RUPE}, \text{KRu5P}, \text{KX5P}) \tag{84}$$

$$\text{RUPE}(\text{Vmax}, \text{RU5P}, \text{X5P}, \text{Keq\_RUPE}, \text{KRu5P}, \text{KX5P}) = \frac{\text{Vmax} \cdot \left(\text{RU5P} - \frac{\text{X5P}}{\text{Keq\_RUPE}}\right)}{\text{RU5P} + \text{KRu5P} \cdot \left(1 + \frac{\text{X5P}}{\text{KX5P}}\right)} \tag{85}$$

$$\mathrm{RUPE}\left(\mathrm{Vmax}, \mathrm{RU5P}, \mathrm{X5P}, \mathrm{Keq\_RUPE}, \mathrm{KRu5P}, \mathrm{KX5P}\right) = \frac{\mathrm{Vmax} \cdot \left(\mathrm{RU5P} - \frac{\mathrm{X5P}}{\mathrm{Keq\_RUPE}}\right)}{\mathrm{RU5P} + \mathrm{KRu5P} \cdot \left(1 + \frac{\mathrm{X5P}}{\mathrm{KX5P}}\right)} \quad (86)$$

Table 29: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Vmax`	Vmax		1.471		☑
`Keq_RUPE`	Keq_RUPE		2.700		☑
`KRu5P`	KRu5P		$1.9 \cdot 10^{-7}$		☑
`KX5P`	KX5P		$5 \cdot 10^{-7}$		☑

8.7 Reaction `reaction_7`

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

Name R5PI

Reaction equation

$$\mathrm{species\_13} \xrightleftharpoons{\mathrm{species\_13},\ \mathrm{species\_15}} \mathrm{species\_15} \quad (87)$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
`species_13`	RU5P	

Modifiers

Table 31: Properties of each modifier.

Id	Name	SBO
`species_13`	RU5P	
`species_15`	R5P	

Product

Table 32: Properties of each product.

Id	Name	SBO
species_15	R5P	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{R5PI}\left(\mathrm{Vmax}, [\mathrm{species\_13}], [\mathrm{species\_15}], \mathrm{Keq\_R5PI}, \mathrm{KRu5P}, \mathrm{KR5P}\right) \tag{88}$$

$$\mathrm{R5PI}\left(\mathrm{Vmax}, \mathrm{RU5P}, \mathrm{R5P}, \mathrm{Keq\_R5PI}, \mathrm{KRu5P}, \mathrm{KR5P}\right) = \frac{\mathrm{Vmax} \cdot \left(\mathrm{RU5P} - \frac{\mathrm{R5P}}{\mathrm{Keq\_R5PI}}\right)}{\mathrm{RU5P} + \mathrm{KRu5P} \cdot \left(1 + \frac{\mathrm{R5P}}{\mathrm{KR5P}}\right)} \tag{89}$$

$$\mathrm{R5PI}\left(\mathrm{Vmax}, \mathrm{RU5P}, \mathrm{R5P}, \mathrm{Keq\_R5PI}, \mathrm{KRu5P}, \mathrm{KR5P}\right) = \frac{\mathrm{Vmax} \cdot \left(\mathrm{RU5P} - \frac{\mathrm{R5P}}{\mathrm{Keq\_R5PI}}\right)}{\mathrm{RU5P} + \mathrm{KRu5P} \cdot \left(1 + \frac{\mathrm{R5P}}{\mathrm{KR5P}}\right)} \tag{90}$$

Table 33: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax	Vmax		0.765		☑
Keq_R5PI	Keq_R5PI		3.000		☑
KRu5P	KRu5P		$7.8 \cdot 10^{-7}$		☑
KR5P	KR5P		$2.2 \cdot 10^{-6}$		☑

8.8 Reaction reaction_8

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

Name TKL

Reaction equation

$$\mathrm{species\_15} + \mathrm{species\_14} \xrightleftharpoons{\mathrm{species\_15},\ \mathrm{species\_14},\ \mathrm{species\_16},\ \mathrm{species\_17}} \mathrm{species\_16} + \mathrm{species\_17} \tag{91}$$

Reactants

Table 34: Properties of each reactant.

Id	Name	SBO
species_15	R5P	
species_14	X5P	

Modifiers

Table 35: Properties of each modifier.

Id	Name	SBO
species_15	R5P	
species_14	X5P	
species_16	GAP	
species_17	S7P	

Products

Table 36: Properties of each product.

Id	Name	SBO
species_16	GAP	
species_17	S7P	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{TKL}\,(\mathrm{parameter\_35}, [\mathrm{species\_15}], [\mathrm{species\_14}], [\mathrm{species\_16}], [\mathrm{species\_17}], \mathrm{Keq\_TKL}, \mathrm{K1}, \mathrm{K2}, \mathrm{K6}, \mathrm{K3}, \mathrm{K5}, \mathrm{K4}, \mathrm{K7}) \tag{92}$$

$$\mathrm{TKL}\,(\mathrm{Vmax}, \mathrm{R5P}, \mathrm{X5P}, \mathrm{GAP}, \mathrm{S7P}, \mathrm{Keq\_TKL}, \mathrm{K1}, \mathrm{K2}, \mathrm{K6}, \mathrm{K3}, \mathrm{K5}, \mathrm{K4}, \mathrm{K7}) \tag{93}$$
$$= \frac{\mathrm{Vmax} \cdot \left(\mathrm{R5P} \cdot \mathrm{X5P} - \frac{\mathrm{GAP} \cdot \mathrm{S7P}}{\mathrm{Keq\_TKL}}\right)}{(\mathrm{K1} + \mathrm{R5P}) \cdot \mathrm{X5P} + (\mathrm{K2} + \mathrm{K6} \cdot \mathrm{S7P}) \cdot \mathrm{R5P} + (\mathrm{K3} + \mathrm{K5} \cdot \mathrm{S7P}) \cdot \mathrm{GAP} + \mathrm{K4} \cdot \mathrm{S7P} + \mathrm{K7} \cdot \mathrm{X5P} \cdot \mathrm{GAP}}$$

$$\mathrm{TKL}\,(\mathrm{Vmax}, \mathrm{R5P}, \mathrm{X5P}, \mathrm{GAP}, \mathrm{S7P}, \mathrm{Keq\_TKL}, \mathrm{K1}, \mathrm{K2}, \mathrm{K6}, \mathrm{K3}, \mathrm{K5}, \mathrm{K4}, \mathrm{K7}) \tag{94}$$
$$= \frac{\mathrm{Vmax} \cdot \left(\mathrm{R5P} \cdot \mathrm{X5P} - \frac{\mathrm{GAP} \cdot \mathrm{S7P}}{\mathrm{Keq\_TKL}}\right)}{(\mathrm{K1} + \mathrm{R5P}) \cdot \mathrm{X5P} + (\mathrm{K2} + \mathrm{K6} \cdot \mathrm{S7P}) \cdot \mathrm{R5P} + (\mathrm{K3} + \mathrm{K5} \cdot \mathrm{S7P}) \cdot \mathrm{GAP} + \mathrm{K4} \cdot \mathrm{S7P} + \mathrm{K7} \cdot \mathrm{X5P} \cdot \mathrm{GAP}}$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Keq_TKL	Keq_TKL		2.080		☑
K1	K1		$4.177 \cdot 10^{-7}$		☑
K2	K2		$3.055 \cdot 10^{-7}$		☑
K6	K6		0.008		☑
K3	K3		$1.2432 \cdot 10^{-5}$		☑
K5	K5		0.411		☑
K4	K4		$4.96 \cdot 10^{-9}$		☑
K7	K7		48.800		☑

8.9 Reaction reaction_9

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

Name TKL2

Reaction equation

$$\text{species\_14} + \text{species\_7} \xrightleftharpoons{\text{species\_7, species\_14, species\_16, species\_5}} \text{species\_16} + \text{species\_5} \tag{95}$$

Reactants

Table 38: Properties of each reactant.

Id	Name	SBO
species_14	X5P	
species_7	E4P	

Modifiers

Table 39: Properties of each modifier.

Id	Name	SBO
species_7	E4P	
species_14	X5P	
species_16	GAP	
species_5	F6P	

Products

Table 40: Properties of each product.

Id	Name	SBO
species_16	GAP	
species_5	F6P	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{TKL2}\left(\mathrm{parameter\_36}, [\mathrm{species\_7}], [\mathrm{species\_14}], [\mathrm{species\_16}], [\mathrm{species\_5}], \mathrm{Keq\_TKL2}, \mathrm{K1}, \mathrm{K2}, \mathrm{K6}, \mathrm{K3}, \mathrm{K5}, \mathrm{K4}, \mathrm{K7}\right) \tag{96}$$

$$\mathrm{TKL2}\left(\mathrm{Vmax}, \mathrm{E4P}, \mathrm{X5P}, \mathrm{GAP}, \mathrm{F6P}, \mathrm{Keq\_TKL2}, \mathrm{K1}, \mathrm{K2}, \mathrm{K6}, \mathrm{K3}, \mathrm{K5}, \mathrm{K4}, \mathrm{K7}\right) \tag{97}$$
$$= \frac{\mathrm{Vmax} \cdot \left(\mathrm{E4P} \cdot \mathrm{X5P} - \frac{\mathrm{GAP} \cdot \mathrm{F6P}}{\mathrm{Keq\_TKL2}}\right)}{(\mathrm{K1} + \mathrm{E4P}) \cdot \mathrm{X5P} + (\mathrm{K2} + \mathrm{K6} \cdot \mathrm{F6P}) \cdot \mathrm{E4P} + (\mathrm{K3} + \mathrm{K5} \cdot \mathrm{F6P}) \cdot \mathrm{GAP} + \mathrm{K4} \cdot \mathrm{F6P} + \mathrm{K7} \cdot \mathrm{X5P} \cdot \mathrm{GAP}}$$

$$\mathrm{TKL2}\left(\mathrm{Vmax}, \mathrm{E4P}, \mathrm{X5P}, \mathrm{GAP}, \mathrm{F6P}, \mathrm{Keq\_TKL2}, \mathrm{K1}, \mathrm{K2}, \mathrm{K6}, \mathrm{K3}, \mathrm{K5}, \mathrm{K4}, \mathrm{K7}\right) \tag{98}$$
$$= \frac{\mathrm{Vmax} \cdot \left(\mathrm{E4P} \cdot \mathrm{X5P} - \frac{\mathrm{GAP} \cdot \mathrm{F6P}}{\mathrm{Keq\_TKL2}}\right)}{(\mathrm{K1} + \mathrm{E4P}) \cdot \mathrm{X5P} + (\mathrm{K2} + \mathrm{K6} \cdot \mathrm{F6P}) \cdot \mathrm{E4P} + (\mathrm{K3} + \mathrm{K5} \cdot \mathrm{F6P}) \cdot \mathrm{GAP} + \mathrm{K4} \cdot \mathrm{F6P} + \mathrm{K7} \cdot \mathrm{X5P} \cdot \mathrm{GAP}}$$

Table 41: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Keq_TKL2	Keq_TKL2		29.700		☑
K1	K1		$1.84 \cdot 10^{-9}$		☑
K2	K2		$3.055 \cdot 10^{-7}$		☑
K6	K6		0.122		☑
K3	K3		$5.48 \cdot 10^{-8}$		☑
K5	K5		0.029		☑
K4	K4		$3 \cdot 10^{-10}$		☑
K7	K7		0.215		☑

8.10 Reaction reaction_10

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

Name TAL

Reaction equation

$$\text{species\_17} + \text{species\_16} \xrightleftharpoons{\text{species\_17, species\_16, species\_7, species\_5}} \text{species\_5} + \text{species\_7} \tag{99}$$

Reactants

Table 42: Properties of each reactant.

Id	Name	SBO
species_17	S7P	
species_16	GAP	

Modifiers

Table 43: Properties of each modifier.

Id	Name	SBO
species_17	S7P	
species_16	GAP	
species_7	E4P	
species_5	F6P	

Products

Table 44: Properties of each product.

Id	Name	SBO
species_5	F6P	
species_7	E4P	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{vol}\left(\text{compartment\_1}\right) \cdot \text{TAL}\left(\text{Vmax}, [\text{species\_17}], [\text{species\_16}], [\text{species\_7}], [\text{species\_5}], \text{Keq\_TAL}, \text{K1}, \text{K2}, \text{K6}, \text{K3}, \text{K5}, \text{K4}, \text{K7}\right) \tag{100}$$

$$\mathrm{TAL}\left(\mathrm{Vmax}, \mathrm{S7P}, \mathrm{GAP}, \mathrm{E4P}, \mathrm{F6P}, \mathrm{Keq\_TAL}, \mathrm{K1}, \mathrm{K2}, \mathrm{K6}, \mathrm{K3}, \mathrm{K5}, \mathrm{K4}, \mathrm{K7}\right) \tag{101}$$
$$= \frac{\mathrm{Vmax} \cdot \left(\mathrm{S7P} \cdot \mathrm{GAP} - \frac{\mathrm{E4P} \cdot \mathrm{F6P}}{\mathrm{Keq\_TAL}}\right)}{(\mathrm{K1} + \mathrm{GAP}) \cdot \mathrm{S7P} + (\mathrm{K2} + \mathrm{K6} \cdot \mathrm{F6P}) \cdot \mathrm{GAP} + (\mathrm{K3} + \mathrm{K5} \cdot \mathrm{F6P}) \cdot \mathrm{E4P} + \mathrm{K4} \cdot \mathrm{F6P} + \mathrm{K7} \cdot \mathrm{S7P} \cdot \mathrm{E4P}}$$

$$\mathrm{TAL}\left(\mathrm{Vmax}, \mathrm{S7P}, \mathrm{GAP}, \mathrm{E4P}, \mathrm{F6P}, \mathrm{Keq\_TAL}, \mathrm{K1}, \mathrm{K2}, \mathrm{K6}, \mathrm{K3}, \mathrm{K5}, \mathrm{K4}, \mathrm{K7}\right) \tag{102}$$
$$= \frac{\mathrm{Vmax} \cdot \left(\mathrm{S7P} \cdot \mathrm{GAP} - \frac{\mathrm{E4P} \cdot \mathrm{F6P}}{\mathrm{Keq\_TAL}}\right)}{(\mathrm{K1} + \mathrm{GAP}) \cdot \mathrm{S7P} + (\mathrm{K2} + \mathrm{K6} \cdot \mathrm{F6P}) \cdot \mathrm{GAP} + (\mathrm{K3} + \mathrm{K5} \cdot \mathrm{F6P}) \cdot \mathrm{E4P} + \mathrm{K4} \cdot \mathrm{F6P} + \mathrm{K7} \cdot \mathrm{S7P} \cdot \mathrm{E4P}}$$

Table 45: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Vmax`	Vmax		58.270		☑
`Keq_TAL`	Keq_TAL		2.703		☑
`K1`	K1		$8.23 \cdot 10^{-9}$		☑
`K2`	K2		$4.765 \cdot 10^{-8}$		☑
`K6`	K6		0.465		☑
`K3`	K3		$1.733 \cdot 10^{-7}$		☑
`K5`	K5		0.868		☑
`K4`	K4		$6.095 \cdot 10^{-9}$		☑
`K7`	K7		2.524		☑

8.11 Reaction `reaction_11`

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

Name PRPPS

Reaction equation

$$\mathrm{species\_15} + \mathrm{species\_4} \xrightleftharpoons{\mathrm{species\_15},\ \mathrm{species\_4},\ \mathrm{species\_21},\ \mathrm{species\_20}} \mathrm{species\_20} + \mathrm{species\_21} \tag{103}$$

Reactants

Table 46: Properties of each reactant.

Id	Name	SBO
`species_15`	R5P	
`species_4`	ATP	

Modifiers

Table 47: Properties of each modifier.

Id	Name	SBO
species_15	R5P	
species_4	ATP	
species_21	PRPP	
species_20	AMP	

Products

Table 48: Properties of each product.

Id	Name	SBO
species_20	AMP	
species_21	PRPP	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{PRPPS}\left(\mathrm{Vmax}, [\mathrm{species\_15}], [\mathrm{species\_4}], [\mathrm{species\_21}], [\mathrm{species\_20}], \mathrm{Kapp}, \mathrm{KATP}, \mathrm{KR5P}\right) \tag{104}$$

$$\begin{aligned} &\mathrm{PRPPS}\left(\mathrm{Vmax}, \mathrm{R5P}, \mathrm{ATP}, \mathrm{PRPP}, \mathrm{AMP}, \mathrm{Kapp}, \mathrm{KATP}, \mathrm{KR5P}\right) \\ &= \frac{\mathrm{Vmax} \cdot \left(\mathrm{R5P} \cdot \mathrm{ATP} - \frac{\mathrm{PRPP} \cdot \mathrm{AMP}}{\mathrm{Kapp}}\right)}{\left(\mathrm{KATP} + \mathrm{ATP}\right) \cdot \left(\mathrm{KR5P} + \mathrm{R5P}\right)} \end{aligned} \tag{105}$$

$$\begin{aligned} &\mathrm{PRPPS}\left(\mathrm{Vmax}, \mathrm{R5P}, \mathrm{ATP}, \mathrm{PRPP}, \mathrm{AMP}, \mathrm{Kapp}, \mathrm{KATP}, \mathrm{KR5P}\right) \\ &= \frac{\mathrm{Vmax} \cdot \left(\mathrm{R5P} \cdot \mathrm{ATP} - \frac{\mathrm{PRPP} \cdot \mathrm{AMP}}{\mathrm{Kapp}}\right)}{\left(\mathrm{KATP} + \mathrm{ATP}\right) \cdot \left(\mathrm{KR5P} + \mathrm{R5P}\right)} \end{aligned} \tag{106}$$

Table 49: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax	Vmax		0.510		☑
Kapp	Kapp		100000.000		☑
KATP	KATP		$3 \cdot 10^{-8}$		☑
KR5P	KR5P		$5.7 \cdot 10^{-7}$		☑

8.12 Reaction reaction_12

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

Name PGLM

Reaction equation

$$\text{species\_22} \xrightleftharpoons{\text{species\_22, species\_2}} \text{species\_2} \tag{107}$$

Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
species_22	G1P	

Modifiers

Table 51: Properties of each modifier.

Id	Name	SBO
species_22	G1P	
species_2	G6P	

Product

Table 52: Properties of each product.

Id	Name	SBO
species_2	G6P	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \text{vol}(\text{compartment\_1}) \cdot \text{PGLM}(\text{parameter\_55}, [\text{species\_22}], \text{parameter\_57}, \text{parameter\_15}, [\text{species\_2}], \text{parameter\_56}) \tag{108}$$

$$\text{PGLM}(\text{Vmaxf}, \text{G1P}, \text{KG1P}, \text{Vmaxr}, \text{G6P}, \text{KG6P}) = \frac{\frac{\text{Vmaxf}\cdot\text{G1P}}{\text{KG1P}} - \frac{\text{Vmaxr}\cdot\text{G6P}}{\text{KG6P}}}{1 + \frac{\text{G1P}}{\text{KG1P}} + \frac{\text{G6P}}{\text{KG6P}}} \tag{109}$$

$$\mathrm{PGLM}\left(\mathrm{Vmaxf},\mathrm{G1P},\mathrm{KG1P},\mathrm{Vmaxr},\mathrm{G6P},\mathrm{KG6P}\right) = \frac{\frac{\mathrm{Vmaxf}\cdot\mathrm{G1P}}{\mathrm{KG1P}} - \frac{\mathrm{Vmaxr}\cdot\mathrm{G6P}}{\mathrm{KG6P}}}{1 + \frac{\mathrm{G1P}}{\mathrm{KG1P}} + \frac{\mathrm{G6P}}{\mathrm{KG6P}}} \tag{110}$$

8.13 Reaction `reaction_13`

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

Name GPa

Reaction equation

$$\mathrm{species\_24} + \mathrm{species\_23} \xrightleftharpoons{\mathrm{species\_24},\ \mathrm{species\_23},\ \mathrm{species\_22}} \mathrm{species\_24} + \mathrm{species\_22} \tag{111}$$

Reactants

Table 53: Properties of each reactant.

Id	Name	SBO
`species_24`	GLY	
`species_23`	Pi	

Modifiers

Table 54: Properties of each modifier.

Id	Name	SBO
`species_24`	GLY	
`species_23`	Pi	
`species_22`	G1P	

Products

Table 55: Properties of each product.

Id	Name	SBO
`species_24`	GLY	
`species_22`	G1P	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{GPa}\,(\mathrm{parameter\_58}, [\mathrm{species\_24}], [\mathrm{species\_23}], \mathrm{parameter\_61}, \mathrm{parameter\_62}, \mathrm{parameter\_4}, [\mathrm{species\_22}], \mathrm{KGLYb}, \mathrm{parameter\_60}, \mathrm{KiPi}, \mathrm{parameter\_59}) \tag{112}$$

$$\mathrm{GPa}\,(\mathrm{Vmaxf}, \mathrm{GLY}, \mathrm{Pi}, \mathrm{KiGLYf}, \mathrm{KPi}, \mathrm{Vmaxr}, \mathrm{G1P}, \mathrm{KGLYb}, \mathrm{KiG1P}, \mathrm{KiPi}, \mathrm{KiGLYb}) = \frac{\mathrm{Vmaxf} \cdot \frac{\mathrm{GLY} \cdot \mathrm{Pi}}{\mathrm{KiGLYf} \cdot \mathrm{KPi}} - \mathrm{Vmaxr} \cdot \frac{\mathrm{GLY} \cdot \mathrm{G1P}}{\mathrm{KGLYb} \cdot \mathrm{KiG1P}}}{1 + \frac{\mathrm{GLY}}{\mathrm{KiGLYf}} + \frac{\mathrm{Pi}}{\mathrm{KiPi}} + \frac{\mathrm{GLY}}{\mathrm{KiGLYb}} + \frac{\mathrm{G1P}}{\mathrm{KiG1P}} + \frac{\mathrm{GLY} \cdot \mathrm{Pi}}{\mathrm{KiGLYf} \cdot \mathrm{KiPi}} + \frac{\mathrm{GLY} \cdot \mathrm{G1P}}{\mathrm{KiGLYb} \cdot \mathrm{KiG1P}}} \tag{113}$$

$$\mathrm{GPa}\,(\mathrm{Vmaxf}, \mathrm{GLY}, \mathrm{Pi}, \mathrm{KiGLYf}, \mathrm{KPi}, \mathrm{Vmaxr}, \mathrm{G1P}, \mathrm{KGLYb}, \mathrm{KiG1P}, \mathrm{KiPi}, \mathrm{KiGLYb}) = \frac{\mathrm{Vmaxf} \cdot \frac{\mathrm{GLY} \cdot \mathrm{Pi}}{\mathrm{KiGLYf} \cdot \mathrm{KPi}} - \mathrm{Vmaxr} \cdot \frac{\mathrm{GLY} \cdot \mathrm{G1P}}{\mathrm{KGLYb} \cdot \mathrm{KiG1P}}}{1 + \frac{\mathrm{GLY}}{\mathrm{KiGLYf}} + \frac{\mathrm{Pi}}{\mathrm{KiPi}} + \frac{\mathrm{GLY}}{\mathrm{KiGLYb}} + \frac{\mathrm{G1P}}{\mathrm{KiG1P}} + \frac{\mathrm{GLY} \cdot \mathrm{Pi}}{\mathrm{KiGLYf} \cdot \mathrm{KiPi}} + \frac{\mathrm{GLY} \cdot \mathrm{G1P}}{\mathrm{KiGLYb} \cdot \mathrm{KiG1P}}} \tag{114}$$

Table 56: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KGLYb	KGLYb		$1.5 \cdot 10^{-4}$		☑
KiPi	KiPi		0.005		☑

8.14 Reaction reaction_14

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

Name FBA

Reaction equation

$$\mathrm{species\_6} \xrightleftharpoons{\mathrm{species\_6,\ species\_27,\ species\_16}} \mathrm{species\_16} + \mathrm{species\_27} \tag{115}$$

Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
species_6	F16P	

Modifiers

Table 58: Properties of each modifier.

Id	Name	SBO
species_6	F16P	
species_27	DHAP	
species_16	GAP	

Products

Table 59: Properties of each product.

Id	Name	SBO
species_16	GAP	
species_27	DHAP	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{FBA}\left(\mathrm{parameter\_37}, [\mathrm{species\_6}], \mathrm{parameter\_70}, \mathrm{parameter\_8}, [\mathrm{species\_27}], [\mathrm{species\_16}], \mathrm{parameter\_68}, \mathrm{parameter\_69}\right) \tag{116}$$

$$\mathrm{FBA}\left(\mathrm{Vmf}, \mathrm{A}, \mathrm{Kfbp}, \mathrm{Vmr}, \mathrm{P}, \mathrm{Q}, \mathrm{Kdhap}, \mathrm{Kg3p}\right) = \frac{\frac{\mathrm{Vmf} \cdot \mathrm{A}}{\mathrm{Kfbp}} - \frac{\mathrm{Vmr} \cdot \mathrm{P} \cdot \mathrm{Q}}{\mathrm{Kdhap} \cdot \mathrm{Kg3p}}}{1 + \frac{\mathrm{A}}{\mathrm{Kfbp}} + \frac{\mathrm{P}}{\mathrm{Kdhap}} + \frac{\mathrm{Q}}{\mathrm{Kg3p}} + \frac{\mathrm{P} \cdot \mathrm{Q}}{\mathrm{Kdhap} \cdot \mathrm{Kg3p}}} \tag{117}$$

$$\mathrm{FBA}\left(\mathrm{Vmf}, \mathrm{A}, \mathrm{Kfbp}, \mathrm{Vmr}, \mathrm{P}, \mathrm{Q}, \mathrm{Kdhap}, \mathrm{Kg3p}\right) = \frac{\frac{\mathrm{Vmf} \cdot \mathrm{A}}{\mathrm{Kfbp}} - \frac{\mathrm{Vmr} \cdot \mathrm{P} \cdot \mathrm{Q}}{\mathrm{Kdhap} \cdot \mathrm{Kg3p}}}{1 + \frac{\mathrm{A}}{\mathrm{Kfbp}} + \frac{\mathrm{P}}{\mathrm{Kdhap}} + \frac{\mathrm{Q}}{\mathrm{Kg3p}} + \frac{\mathrm{P} \cdot \mathrm{Q}}{\mathrm{Kdhap} \cdot \mathrm{Kg3p}}} \tag{118}$$

8.15 Reaction reaction_15

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

Name TPI

Reaction equation

$$\mathrm{species\_16} \xrightleftharpoons{\mathrm{species\_16},\ \mathrm{species\_27}} \mathrm{species\_27} \tag{119}$$

Reactant

Table 60: Properties of each reactant.

Id	Name	SBO
species_16	GAP	

Modifiers

Table 61: Properties of each modifier.

Id	Name	SBO
species_16	GAP	
species_27	DHAP	

Product

Table 62: Properties of each product.

Id	Name	SBO
species_27	DHAP	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{TPI}\left(\mathrm{parameter\_38}, [\mathrm{species\_16}], \mathrm{parameter\_72}, \mathrm{parameter\_9}, [\mathrm{species\_27}], \mathrm{parameter\_71}\right) \tag{120}$$

$$\mathrm{TPI}\left(\mathrm{Vf}, \mathrm{GAP}, \mathrm{Kms}, \mathrm{Vr}, \mathrm{DHAP}, \mathrm{Kmp}\right) = \frac{\frac{\mathrm{Vf}\cdot\mathrm{GAP}}{\mathrm{Kms}} - \frac{\mathrm{Vr}\cdot\mathrm{DHAP}}{\mathrm{Kmp}}}{1 + \frac{\mathrm{GAP}}{\mathrm{Kms}} + \frac{\mathrm{DHAP}}{\mathrm{Kmp}}} \tag{121}$$

$$\mathrm{TPI}\left(\mathrm{Vf}, \mathrm{GAP}, \mathrm{Kms}, \mathrm{Vr}, \mathrm{DHAP}, \mathrm{Kmp}\right) = \frac{\frac{\mathrm{Vf}\cdot\mathrm{GAP}}{\mathrm{Kms}} - \frac{\mathrm{Vr}\cdot\mathrm{DHAP}}{\mathrm{Kmp}}}{1 + \frac{\mathrm{GAP}}{\mathrm{Kms}} + \frac{\mathrm{DHAP}}{\mathrm{Kmp}}} \tag{122}$$

8.16 Reaction reaction_16

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

Name GAPDH

Reaction equation

$$\text{species\_16} + \text{species\_19} + \text{species\_23} \xrightleftharpoons{\text{species\_19, species\_16, species\_23, species\_12, species\_18}} \text{species\_12} + \text{speci} \tag{123}$$

Reactants

Table 63: Properties of each reactant.

Id	Name	SBO
species_16	GAP	
species_19	NAD	
species_23	Pi	

Modifiers

Table 64: Properties of each modifier.

Id	Name	SBO
species_19	NAD	
species_16	GAP	
species_23	Pi	
species_12	BPG	
species_18	NADH	

Products

Table 65: Properties of each product.

Id	Name	SBO
species_12	BPG	
species_18	NADH	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \text{vol}(\text{compartment\_1}) \cdot \text{GAPDH}(\text{parameter\_39}, [\text{species\_19}], [\text{species\_16}], [\text{species\_23}], \text{parameter\_76}, \text{parameter\_75}, \text{parameter\_77}, \text{parameter\_10}, [\text{species\_12}], [\text{species\_18}], \text{parameter\_73}, \text{parameter\_74}) \tag{124}$$

$$\mathrm{GAPDH}\left(\mathrm{Vmf},\mathrm{A},\mathrm{B},\mathrm{C},\mathrm{Knad},\mathrm{Kg3p},\mathrm{Kp},\mathrm{Vmr},\mathrm{P},\mathrm{Q},\mathrm{Kdpg},\mathrm{Knadh}\right) = \frac{\frac{\mathrm{Vmf}\cdot\mathrm{A}\cdot\mathrm{B}\cdot\mathrm{C}}{\mathrm{Knad}\cdot\mathrm{Kg3p}\cdot\mathrm{Kp}} - \frac{\mathrm{Vmr}\cdot\mathrm{P}\cdot\mathrm{Q}}{\mathrm{Kdpg}\cdot\mathrm{Knadh}}}{1 + \frac{\mathrm{A}}{\mathrm{Knad}} + \frac{\mathrm{A}\cdot\mathrm{B}}{\mathrm{Knad}\cdot\mathrm{Kg3p}} + \frac{\mathrm{A}\cdot\mathrm{B}\cdot\mathrm{C}}{\mathrm{Knad}\cdot\mathrm{Kg3p}\cdot\mathrm{Kp}} + \frac{\mathrm{P}\cdot\mathrm{Q}}{\mathrm{Kdpg}\cdot\mathrm{Knadh}} + \frac{\mathrm{Q}}{\mathrm{Knadh}}} \tag{125}$$

$$\mathrm{GAPDH}\left(\mathrm{Vmf},\mathrm{A},\mathrm{B},\mathrm{C},\mathrm{Knad},\mathrm{Kg3p},\mathrm{Kp},\mathrm{Vmr},\mathrm{P},\mathrm{Q},\mathrm{Kdpg},\mathrm{Knadh}\right) = \frac{\frac{\mathrm{Vmf}\cdot\mathrm{A}\cdot\mathrm{B}\cdot\mathrm{C}}{\mathrm{Knad}\cdot\mathrm{Kg3p}\cdot\mathrm{Kp}} - \frac{\mathrm{Vmr}\cdot\mathrm{P}\cdot\mathrm{Q}}{\mathrm{Kdpg}\cdot\mathrm{Knadh}}}{1 + \frac{\mathrm{A}}{\mathrm{Knad}} + \frac{\mathrm{A}\cdot\mathrm{B}}{\mathrm{Knad}\cdot\mathrm{Kg3p}} + \frac{\mathrm{A}\cdot\mathrm{B}\cdot\mathrm{C}}{\mathrm{Knad}\cdot\mathrm{Kg3p}\cdot\mathrm{Kp}} + \frac{\mathrm{P}\cdot\mathrm{Q}}{\mathrm{Kdpg}\cdot\mathrm{Knadh}} + \frac{\mathrm{Q}}{\mathrm{Knadh}}} \tag{126}$$

8.17 Reaction `reaction_17`

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

Name PGK

Reaction equation

$$\mathrm{species\_12} + \mathrm{species\_3} \xrightleftharpoons{\mathrm{species\_12},\ \mathrm{species\_3},\ \mathrm{species\_28},\ \mathrm{species\_4}} \mathrm{species\_28} + \mathrm{species\_4} \tag{127}$$

Reactants

Table 66: Properties of each reactant.

Id	Name	SBO
`species_12`	BPG	
`species_3`	ADP	

Modifiers

Table 67: Properties of each modifier.

Id	Name	SBO
`species_12`	BPG	
`species_3`	ADP	
`species_28`	PG3	
`species_4`	ATP	

Products

Table 68: Properties of each product.

Id	Name	SBO
species_28	PG3	
species_4	ATP	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{PGK}\,(\mathrm{parameter\_40}, [\mathrm{species\_12}], [\mathrm{species\_3}], \mathrm{alfa}, \mathrm{parameter\_51}, \mathrm{parameter\_52}, \mathrm{parameter\_11}, [\mathrm{species\_28}], [\mathrm{species\_4}], \mathrm{beta}, \mathrm{parameter\_49}, \mathrm{parameter\_50}) \tag{128}$$

$$\mathrm{PGK}\,(\mathrm{Vmf}, \mathrm{A}, \mathrm{B}, \mathrm{alfa}, \mathrm{Ka}, \mathrm{Kb}, \mathrm{Vmr}, \mathrm{P}, \mathrm{Q}, \mathrm{beta}, \mathrm{Kp}, \mathrm{Kq}) = \frac{\frac{\mathrm{Vmf}\cdot\mathrm{A}\cdot\mathrm{B}}{\mathrm{alfa}\cdot\mathrm{Ka}\cdot\mathrm{Kb}} - \frac{\mathrm{Vmr}\cdot\mathrm{P}\cdot\mathrm{Q}}{\mathrm{beta}\cdot\mathrm{Kp}\cdot\mathrm{Kq}}}{1 + \frac{\mathrm{A}}{\mathrm{Ka}} + \frac{\mathrm{B}}{\mathrm{Kb}} + \frac{\mathrm{A}\cdot\mathrm{B}}{\mathrm{alfa}\cdot\mathrm{Ka}\cdot\mathrm{Kb}} + \frac{\mathrm{P}\cdot\mathrm{Q}}{\mathrm{beta}\cdot\mathrm{Kp}\cdot\mathrm{Kq}} + \frac{\mathrm{P}}{\mathrm{Kp}} + \frac{\mathrm{Q}}{\mathrm{Kq}}} \tag{129}$$

$$\mathrm{PGK}\,(\mathrm{Vmf}, \mathrm{A}, \mathrm{B}, \mathrm{alfa}, \mathrm{Ka}, \mathrm{Kb}, \mathrm{Vmr}, \mathrm{P}, \mathrm{Q}, \mathrm{beta}, \mathrm{Kp}, \mathrm{Kq}) = \frac{\frac{\mathrm{Vmf}\cdot\mathrm{A}\cdot\mathrm{B}}{\mathrm{alfa}\cdot\mathrm{Ka}\cdot\mathrm{Kb}} - \frac{\mathrm{Vmr}\cdot\mathrm{P}\cdot\mathrm{Q}}{\mathrm{beta}\cdot\mathrm{Kp}\cdot\mathrm{Kq}}}{1 + \frac{\mathrm{A}}{\mathrm{Ka}} + \frac{\mathrm{B}}{\mathrm{Kb}} + \frac{\mathrm{A}\cdot\mathrm{B}}{\mathrm{alfa}\cdot\mathrm{Ka}\cdot\mathrm{Kb}} + \frac{\mathrm{P}\cdot\mathrm{Q}}{\mathrm{beta}\cdot\mathrm{Kp}\cdot\mathrm{Kq}} + \frac{\mathrm{P}}{\mathrm{Kp}} + \frac{\mathrm{Q}}{\mathrm{Kq}}} \tag{130}$$

Table 69: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
alfa	alfa		1.0		☑
beta	beta		1.0		☑

8.18 Reaction reaction_18

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

Name GPb

Reaction equation

$$\mathrm{species\_24} + \mathrm{species\_23} \xrightleftharpoons{\mathrm{species\_24},\ \mathrm{species\_23},\ \mathrm{species\_22}} \mathrm{species\_24} + \mathrm{species\_22} \tag{131}$$

Reactants

Table 70: Properties of each reactant.

Id	Name	SBO
species_24	GLY	
species_23	Pi	

Modifiers

Table 71: Properties of each modifier.

Id	Name	SBO
species_24	GLY	
species_23	Pi	
species_22	G1P	

Products

Table 72: Properties of each product.

Id	Name	SBO
species_24	GLY	
species_22	G1P	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{GPb}\left(\mathrm{parameter\_63}, [\mathrm{species\_24}], [\mathrm{species\_23}], \mathrm{parameter\_66}, \mathrm{KPi}, \mathrm{parameter\_7}, [\mathrm{species\_22}], \mathrm{parameter\_64}, \mathrm{parameter\_65}, \mathrm{parameter\_67}, \mathrm{KiG1P}, \mathrm{parameter\_27}, \mathrm{nH}, \mathrm{Kamp}\right) \tag{132}$$

$$\mathrm{GPb}\left(\mathrm{Vmaxf}, \mathrm{GLY}, \mathrm{Pi}, \mathrm{KiGLYf}, \mathrm{KPi}, \mathrm{Vmaxr}, \mathrm{G1P}, \mathrm{KiGLYb}, \mathrm{KG1P}, \mathrm{KiPi}, \mathrm{KiG1P}, \mathrm{AMP}, \mathrm{nH}, \mathrm{Kamp}\right) = \frac{\frac{\mathrm{Vmaxf} \cdot \frac{\mathrm{GLY} \cdot \mathrm{Pi}}{\mathrm{KiGLYf} \cdot \mathrm{KPi}} - \mathrm{Vmaxr} \cdot \frac{\mathrm{GLY} \cdot \mathrm{G1P}}{\mathrm{KiGLYb} \cdot \mathrm{KG1P}}}{1 + \frac{\mathrm{GLY}}{\mathrm{KiGLYf}} + \frac{\mathrm{Pi}}{\mathrm{KiPi}} + \frac{\mathrm{GLY}}{\mathrm{KiGLYb}} + \frac{\mathrm{G1P}}{\mathrm{KiG1P}} + \frac{\mathrm{GLY} \cdot \mathrm{Pi}}{\mathrm{KiGLYf} \cdot \mathrm{KPi}} + \frac{\mathrm{GLY} \cdot \mathrm{G1P}}{\mathrm{KiGLYb} \cdot \mathrm{KG1P}}} \cdot \frac{\mathrm{AMP}^{\mathrm{nH}}}{\mathrm{Kamp}}}{1 + \frac{\mathrm{AMP}^{\mathrm{nH}}}{\mathrm{Kamp}}} \tag{133}$$

$$\mathrm{GPb}\left(\mathrm{Vmaxf}, \mathrm{GLY}, \mathrm{Pi}, \mathrm{KiGLYf}, \mathrm{KPi}, \mathrm{Vmaxr}, \mathrm{G1P}, \mathrm{KiGLYb}, \mathrm{KG1P}, \mathrm{KiPi}, \mathrm{KiG1P}, \mathrm{AMP}, \mathrm{nH}, \mathrm{Kamp}\right) = \frac{\frac{\mathrm{Vmaxf} \cdot \frac{\mathrm{GLY} \cdot \mathrm{Pi}}{\mathrm{KiGLYf} \cdot \mathrm{KPi}} - \mathrm{Vmaxr} \cdot \frac{\mathrm{GLY} \cdot \mathrm{G1P}}{\mathrm{KiGLYb} \cdot \mathrm{KG1P}}}{1 + \frac{\mathrm{GLY}}{\mathrm{KiGLYf}} + \frac{\mathrm{Pi}}{\mathrm{KiPi}} + \frac{\mathrm{GLY}}{\mathrm{KiGLYb}} + \frac{\mathrm{G1P}}{\mathrm{KiG1P}} + \frac{\mathrm{GLY} \cdot \mathrm{Pi}}{\mathrm{KiGLYf} \cdot \mathrm{KPi}} + \frac{\mathrm{GLY} \cdot \mathrm{G1P}}{\mathrm{KiGLYb} \cdot \mathrm{KG1P}}} \cdot \frac{\mathrm{AMP}^{\mathrm{nH}}}{\mathrm{Kamp}}}{1 + \frac{\mathrm{AMP}^{\mathrm{nH}}}{\mathrm{Kamp}}} \tag{134}$$

Table 73: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KPi	KPi		$2 \cdot 10^{-4}$		☑
KiG1P	KiG1P		0.007		☑
nH	nH		1.750		☑
Kamp	Kamp		$1.9 \cdot 10^{-12}$		☑

8.19 Reaction reaction_19

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

Name GS

Reaction equation

$$\mathrm{species\_22} + \mathrm{species\_4} \xrightleftharpoons{\mathrm{species\_22},\ \mathrm{species\_4},\ \mathrm{species\_24},\ \mathrm{species\_23},\ \mathrm{species\_3}} \mathrm{species\_24} + \mathrm{species\_3} + 2\,\mathrm{species\_2} \tag{135}$$

Reactants

Table 74: Properties of each reactant.

Id	Name	SBO
species_22	G1P	
species_4	ATP	

Modifiers

Table 75: Properties of each modifier.

Id	Name	SBO
species_22	G1P	
species_4	ATP	
species_24	GLY	

Id	Name	SBO
species_23	Pi	
species_3	ADP	

Products

Table 76: Properties of each product.

Id	Name	SBO
species_24	GLY	
species_3	ADP	
species_23	Pi	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{GS}\left(\mathrm{parameter\_41}, \mathrm{Kf}, \mathrm{parameter\_17}, [\mathrm{species\_22}], [\mathrm{species\_4}], [\mathrm{species\_24}], [\mathrm{species\_23}], [\mathrm{species\_3}], \mathrm{Keq}, \mathrm{Kr}\right) \tag{136}$$

$$\begin{aligned} &\mathrm{GS}\left(\mathrm{Vmaxf}, \mathrm{Kf}, \mathrm{a}, \mathrm{G1P}, \mathrm{ATP}, \mathrm{GLY}, \mathrm{Pi}, \mathrm{ADP}, \mathrm{Keq}, \mathrm{Kr}\right) \\ &= \frac{\frac{\mathrm{Vmaxf}}{\mathrm{Kf}} \cdot \mathrm{a} \cdot \mathrm{G1P} \cdot \mathrm{a} \cdot \mathrm{ATP} \cdot \mathrm{a} \cdot \mathrm{GLY} \cdot \left(1 - \frac{(\mathrm{a}\cdot\mathrm{Pi})^2 \cdot \mathrm{a}\cdot\mathrm{ADP}}{\mathrm{a}\cdot\mathrm{G1P}\cdot\mathrm{a}\cdot\mathrm{ATP}\cdot\mathrm{Keq}}\right)}{1 + \frac{\mathrm{a}\cdot\mathrm{G1P}\cdot\mathrm{a}\cdot\mathrm{ATP}\cdot\mathrm{a}\cdot\mathrm{GLY}}{\mathrm{Kf}} + \frac{\mathrm{a}\cdot\mathrm{GLY}\cdot(\mathrm{a}\cdot\mathrm{Pi})^2\cdot\mathrm{a}\cdot\mathrm{ADP}}{\mathrm{Kr}}} \end{aligned} \tag{137}$$

$$\begin{aligned} &\mathrm{GS}\left(\mathrm{Vmaxf}, \mathrm{Kf}, \mathrm{a}, \mathrm{G1P}, \mathrm{ATP}, \mathrm{GLY}, \mathrm{Pi}, \mathrm{ADP}, \mathrm{Keq}, \mathrm{Kr}\right) \\ &= \frac{\frac{\mathrm{Vmaxf}}{\mathrm{Kf}} \cdot \mathrm{a} \cdot \mathrm{G1P} \cdot \mathrm{a} \cdot \mathrm{ATP} \cdot \mathrm{a} \cdot \mathrm{GLY} \cdot \left(1 - \frac{(\mathrm{a}\cdot\mathrm{Pi})^2 \cdot \mathrm{a}\cdot\mathrm{ADP}}{\mathrm{a}\cdot\mathrm{G1P}\cdot\mathrm{a}\cdot\mathrm{ATP}\cdot\mathrm{Keq}}\right)}{1 + \frac{\mathrm{a}\cdot\mathrm{G1P}\cdot\mathrm{a}\cdot\mathrm{ATP}\cdot\mathrm{a}\cdot\mathrm{GLY}}{\mathrm{Kf}} + \frac{\mathrm{a}\cdot\mathrm{GLY}\cdot(\mathrm{a}\cdot\mathrm{Pi})^2\cdot\mathrm{a}\cdot\mathrm{ADP}}{\mathrm{Kr}}} \end{aligned} \tag{138}$$

Table 77: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kf	Kf		17400.0		☑
Keq	Keq		267100.0		☑
Kr	Kr		158.0		☑

8.20 Reaction `reaction_20`

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

Name PFK

Reaction equation

$$\text{species\_5} + \text{species\_4} \xrightleftharpoons{\text{species\_26, species\_25, species\_4, species\_26, species\_5, species\_25, species\_3, species\_6}} \text{spec} \tag{139}$$

Reactants

Table 78: Properties of each reactant.

Id	Name	SBO
`species_5`	F6P	
`species_4`	ATP	

Modifiers

Table 79: Properties of each modifier.

Id	Name	SBO
`species_26`	F26P	
`species_25`	CIT	
`species_4`	ATP	
`species_26`	F26P	
`species_5`	F6P	
`species_25`	CIT	
`species_3`	ADP	
`species_6`	F16P	

Products

Table 80: Properties of each product.

Id	Name	SBO
`species_6`	F16P	
`species_3`	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{PFK}\,(\mathrm{parameter\_42}, \mathrm{parameter\_17}, [\mathrm{species\_4}], \mathrm{Katp}, \mathrm{beta}, [\mathrm{species\_26}], \mathrm{alfa}, \mathrm{Kf26bp}, [\mathrm{species\_5}], \mathrm{Kf6p}, \mathrm{L}, [\mathrm{species\_25}], \mathrm{Kcit}, \mathrm{Kiatp}, [\mathrm{species\_3}], [\mathrm{species\_6}], \mathrm{Kadp}, \mathrm{Kfbp}, \mathrm{Kapp}) \tag{140}$$

$$\mathrm{PFK}\,(\mathrm{Vm}, \mathrm{a}, \mathrm{B}, \mathrm{Katp}, \mathrm{beta}, \mathrm{F26P}, \mathrm{alfa}, \mathrm{Kf26bp}, \mathrm{A}, \mathrm{Kf6p}, \mathrm{L}, \mathrm{CIT}, \mathrm{Kcit}, \mathrm{Kiatp}, \mathrm{Q}, \mathrm{P}, \mathrm{Kadp}, \mathrm{Kfbp}, \mathrm{Kapp}) = \mathrm{Vm} \cdot \frac{\frac{\mathrm{a\cdot B}}{\mathrm{Katp}}}{1 + \frac{\mathrm{a\cdot B}}{\mathrm{Katp}}} \cdot \frac{1 + \frac{\mathrm{beta\cdot a\cdot F26P}}{\mathrm{alfa\cdot Kf26bp}}}{1 + \frac{\mathrm{a\cdot F26P}}{\mathrm{alfa\cdot Kf26bp}}} \cdot \left(\frac{\frac{\mathrm{a\cdot A}\cdot\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{alfa\cdot Kf26bp}}\right)}{\mathrm{Kf6p}\cdot\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{Kf26bp}}\right)} \cdot \left(1 + \frac{\mathrm{a\cdot A}\cdot\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{alfa\cdot Kf26bp}}\right)}{\mathrm{Kf6p}\cdot\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{Kf26bp}}\right)}\right)^3}{\frac{\mathrm{L}\cdot\left(1+\frac{\mathrm{a\cdot CIT}}{\mathrm{Kcit}}\right)^4\cdot\left(1+\frac{\mathrm{a\cdot B}}{\mathrm{Kiatp}}\right)^4}{\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{Kf26bp}}\right)^4} + \left(1 + \frac{\mathrm{a\cdot A}\cdot\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{alfa\cdot Kf26bp}}\right)}{\mathrm{Kf6p}\cdot\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{Kf26bp}}\right)}\right)^4} - \frac{\frac{\mathrm{a\cdot Q\cdot a\cdot P}}{\mathrm{Kadp\cdot Kfbp\cdot Kapp}}}{\frac{\mathrm{a\cdot Q}}{\mathrm{Kadp}} + \frac{\mathrm{a\cdot P}}{\mathrm{Kfbp}} + \frac{\mathrm{a\cdot Q\cdot a\cdot P}}{\mathrm{Kadp\cdot Kfbp}} + 1} \right) \tag{141}$$

$$\mathrm{PFK}\,(\mathrm{Vm}, \mathrm{a}, \mathrm{B}, \mathrm{Katp}, \mathrm{beta}, \mathrm{F26P}, \mathrm{alfa}, \mathrm{Kf26bp}, \mathrm{A}, \mathrm{Kf6p}, \mathrm{L}, \mathrm{CIT}, \mathrm{Kcit}, \mathrm{Kiatp}, \mathrm{Q}, \mathrm{P}, \mathrm{Kadp}, \mathrm{Kfbp}, \mathrm{Kapp}) = \mathrm{Vm} \cdot \frac{\frac{\mathrm{a\cdot B}}{\mathrm{Katp}}}{1 + \frac{\mathrm{a\cdot B}}{\mathrm{Katp}}} \cdot \frac{1 + \frac{\mathrm{beta\cdot a\cdot F26P}}{\mathrm{alfa\cdot Kf26bp}}}{1 + \frac{\mathrm{a\cdot F26P}}{\mathrm{alfa\cdot Kf26bp}}} \cdot \left(\frac{\frac{\mathrm{a\cdot A}\cdot\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{alfa\cdot Kf26bp}}\right)}{\mathrm{Kf6p}\cdot\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{Kf26bp}}\right)} \cdot \left(1 + \frac{\mathrm{a\cdot A}\cdot\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{alfa\cdot Kf26bp}}\right)}{\mathrm{Kf6p}\cdot\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{Kf26bp}}\right)}\right)^3}{\frac{\mathrm{L}\cdot\left(1+\frac{\mathrm{a\cdot CIT}}{\mathrm{Kcit}}\right)^4\cdot\left(1+\frac{\mathrm{a\cdot B}}{\mathrm{Kiatp}}\right)^4}{\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{Kf26bp}}\right)^4} + \left(1 + \frac{\mathrm{a\cdot A}\cdot\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{alfa\cdot Kf26bp}}\right)}{\mathrm{Kf6p}\cdot\left(1+\frac{\mathrm{a\cdot F26P}}{\mathrm{Kf26bp}}\right)}\right)^4} - \frac{\frac{\mathrm{a\cdot Q\cdot a\cdot P}}{\mathrm{Kadp\cdot Kfbp\cdot Kapp}}}{\frac{\mathrm{a\cdot Q}}{\mathrm{Kadp}} + \frac{\mathrm{a\cdot P}}{\mathrm{Kfbp}} + \frac{\mathrm{a\cdot Q\cdot a\cdot P}}{\mathrm{Kadp\cdot Kfbp}} + 1} \right) \tag{142}$$

Table 81: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Katp	Katp		$2.1 \cdot 10^{-5}$		☑
beta	beta		0.980		☑
alfa	alfa		0.320		☑
Kf26bp	Kf26bp		$8.4 \cdot 10^{-7}$		☑
Kf6p	Kf6p		1.000		☑
L	L		4.100		☑
Kcit	Kcit		6.800		☑
Kiatp	Kiatp		20.000		☑
Kadp	Kadp		5.000		☑
Kfbp	Kfbp		5.000		☑
Kapp	Kapp		247.000		☑

8.21 Reaction reaction_21

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

Name PGYM

Reaction equation

$$\text{species\_28} \xrightleftharpoons{\text{species\_28, species\_29}} \text{species\_29} \tag{143}$$

Reactant

Table 82: Properties of each reactant.

Id	Name	SBO
species_28	PG3	

Modifiers

Table 83: Properties of each modifier.

Id	Name	SBO
species_28	PG3	
species_29	PG2	

Product

Table 84: Properties of each product.

Id	Name	SBO
species_29	PG2	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \text{vol}\left(\text{compartment\_1}\right) \cdot \text{function\_1}\left(\text{parameter\_78}, [\text{species\_28}], \text{parameter\_80}, \text{parameter\_22}, [\text{species\_29}], \text{parameter\_79}\right) \tag{144}$$

$$\text{function\_1}\left(\text{Vmf}, \text{PG3}, \text{Kms}, \text{Vmr}, \text{PG2}, \text{Kmp}\right) = \frac{\frac{\text{Vmf}\cdot\text{PG3}}{\text{Kms}} - \frac{\text{Vmr}\cdot\text{PG2}}{\text{Kmp}}}{1 + \frac{\text{PG3}}{\text{Kms}} + \frac{\text{PG2}}{\text{Kmp}}} \tag{145}$$

$$\text{function\_1}\left(\text{Vmf},\text{PG3},\text{Kms},\text{Vmr},\text{PG2},\text{Kmp}\right) = \frac{\frac{\text{Vmf}\cdot\text{PG3}}{\text{Kms}} - \frac{\text{Vmr}\cdot\text{PG2}}{\text{Kmp}}}{1 + \frac{\text{PG3}}{\text{Kms}} + \frac{\text{PG2}}{\text{Kmp}}} \tag{146}$$

8.22 Reaction `reaction_22`

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

Name ENO

Reaction equation

$$\text{species\_29} \xrightleftharpoons{\text{species\_29, species\_30}} \text{species\_30} \tag{147}$$

Reactant

Table 85: Properties of each reactant.

Id	Name	SBO
`species_29`	PG2	

Modifiers

Table 86: Properties of each modifier.

Id	Name	SBO
`species_29`	PG2	
`species_30`	PEP	

Product

Table 87: Properties of each product.

Id	Name	SBO
`species_30`	PEP	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \text{vol}\left(\text{compartment\_1}\right) \cdot \text{function\_2}\left(\text{parameter\_43}, [\text{species\_29}], \text{parameter\_54}, \text{parameter\_24}, [\text{species\_30}], \text{parameter\_53}\right) \tag{148}$$

$$\text{function\_2}\left(\text{Vmf}, \text{PG2}, \text{Kms}, \text{Vmr}, \text{PEP}, \text{Kmp}\right) = \frac{\frac{\text{Vmf} \cdot \text{PG2}}{\text{Kms}} - \frac{\text{Vmr} \cdot \text{PEP}}{\text{Kmp}}}{1 + \frac{\text{PG2}}{\text{Kms}} + \frac{\text{PEP}}{\text{Kmp}}} \tag{149}$$

$$\text{function\_2}\left(\text{Vmf}, \text{PG2}, \text{Kms}, \text{Vmr}, \text{PEP}, \text{Kmp}\right) = \frac{\frac{\text{Vmf} \cdot \text{PG2}}{\text{Kms}} - \frac{\text{Vmr} \cdot \text{PEP}}{\text{Kmp}}}{1 + \frac{\text{PG2}}{\text{Kms}} + \frac{\text{PEP}}{\text{Kmp}}} \tag{150}$$

8.23 Reaction `reaction_23`

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

Name PK

Reaction equation

$$\text{species\_30} + \text{species\_3} \xrightleftharpoons{\text{species\_6, species\_3, species\_30, species\_4, species\_6, species\_31}} \text{species\_31} + \text{species\_4} \tag{151}$$

Reactants

Table 88: Properties of each reactant.

Id	Name	SBO
`species_30`	PEP	
`species_3`	ADP	

Modifiers

Table 89: Properties of each modifier.

Id	Name	SBO
`species_6`	F16P	
`species_3`	ADP	
`species_30`	PEP	
`species_4`	ATP	
`species_6`	F16P	
`species_31`	PYR	

Products

Table 90: Properties of each product.

Id	Name	SBO
species_31	PYR	
species_4	ATP	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{function\_3}\,(\mathrm{parameter\_44}, [\mathrm{species\_3}], \mathrm{Kadp}, [\mathrm{species\_30}], \mathrm{Kpep}, \mathrm{L}, [\mathrm{species\_4}], \mathrm{Kiatp}, [\mathrm{species\_6}], \mathrm{Kfbp}, [\mathrm{species\_31}], \mathrm{Katp}, \mathrm{Kpyr}, \mathrm{Kapp}, \mathrm{parameter\_17}) \tag{152}$$

$$\mathrm{function\_3}\,(\mathrm{Vm}, \mathrm{B}, \mathrm{Kadp}, \mathrm{A}, \mathrm{Kpep}, \mathrm{L}, \mathrm{Q}, \mathrm{Kiatp}, \mathrm{F16P}, \mathrm{Kfbp}, \mathrm{P}, \mathrm{Katp}, \mathrm{Kpyr}, \mathrm{Kapp}, \mathrm{a}) = \mathrm{Vm} \cdot \left(\frac{\frac{\mathrm{a\cdot B}}{\mathrm{Kadp}}}{1 + \frac{\mathrm{a\cdot B}}{\mathrm{Kadp}}} \cdot \frac{\frac{\mathrm{a\cdot A}}{\mathrm{Kpep}} \cdot \left(1 + \frac{\mathrm{a\cdot A}}{\mathrm{Kpep}}\right)^3}{\frac{\mathrm{L}\cdot\left(1+\frac{\mathrm{a\cdot Q}}{\mathrm{Kiatp}}\right)^4}{\left(1+\frac{\mathrm{a\cdot F16P}}{\mathrm{Kfbp}}\right)^4} + \left(1 + \frac{\mathrm{a\cdot A}}{\mathrm{Kpep}}\right)^4} - \frac{\frac{\mathrm{a\cdot Q\cdot a\cdot P}}{\mathrm{Katp\cdot Kpyr\cdot Kapp}}}{\frac{\mathrm{a\cdot Q}}{\mathrm{Katp}} + \frac{\mathrm{a\cdot P}}{\mathrm{Kpyr}} + \frac{\mathrm{a\cdot Q\cdot a\cdot P}}{\mathrm{Katp\cdot Kpyr}} + 1} \right) \tag{153}$$

$$\mathrm{function\_3}\,(\mathrm{Vm}, \mathrm{B}, \mathrm{Kadp}, \mathrm{A}, \mathrm{Kpep}, \mathrm{L}, \mathrm{Q}, \mathrm{Kiatp}, \mathrm{F16P}, \mathrm{Kfbp}, \mathrm{P}, \mathrm{Katp}, \mathrm{Kpyr}, \mathrm{Kapp}, \mathrm{a}) = \mathrm{Vm} \cdot \left(\frac{\frac{\mathrm{a\cdot B}}{\mathrm{Kadp}}}{1 + \frac{\mathrm{a\cdot B}}{\mathrm{Kadp}}} \cdot \frac{\frac{\mathrm{a\cdot A}}{\mathrm{Kpep}} \cdot \left(1 + \frac{\mathrm{a\cdot A}}{\mathrm{Kpep}}\right)^3}{\frac{\mathrm{L}\cdot\left(1+\frac{\mathrm{a\cdot Q}}{\mathrm{Kiatp}}\right)^4}{\left(1+\frac{\mathrm{a\cdot F16P}}{\mathrm{Kfbp}}\right)^4} + \left(1 + \frac{\mathrm{a\cdot A}}{\mathrm{Kpep}}\right)^4} - \frac{\frac{\mathrm{a\cdot Q\cdot a\cdot P}}{\mathrm{Katp\cdot Kpyr\cdot Kapp}}}{\frac{\mathrm{a\cdot Q}}{\mathrm{Katp}} + \frac{\mathrm{a\cdot P}}{\mathrm{Kpyr}} + \frac{\mathrm{a\cdot Q\cdot a\cdot P}}{\mathrm{Katp\cdot Kpyr}} + 1} \right) \tag{154}$$

Table 91: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kadp	Kadp		0.400		☑
Kpep	Kpep		0.014		☑
L	L		1.000		☑
Kiatp	Kiatp		2.500		☑
Kfbp	Kfbp		$4 \cdot 10^{-4}$		☑
Katp	Katp		0.860		☑
Kpyr	Kpyr		10.000		☑
Kapp	Kapp		195172.000		☑

8.24 Reaction reaction_24

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

Name LDH

Reaction equation

$$\text{species\_31} + \text{species\_18} \xrightleftharpoons{\text{species\_18, species\_31, species\_32, species\_19}} \text{species\_32} + \text{species\_19} \tag{155}$$

Reactants

Table 92: Properties of each reactant.

Id	Name	SBO
species_31	PYR	
species_18	NADH	

Modifiers

Table 93: Properties of each modifier.

Id	Name	SBO
species_18	NADH	
species_31	PYR	
species_32	LAC	
species_19	NAD	

Products

Table 94: Properties of each product.

Id	Name	SBO
species_32	LAC	
species_19	NAD	

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{function\_4}\,(\mathrm{parameter\_45}, [\mathrm{species\_18}], [\mathrm{species\_31}], \mathrm{alfa}, \mathrm{parameter\_85}, \mathrm{parameter\_86}, \mathrm{parameter\_26}, [\mathrm{species\_32}], [\mathrm{species\_19}], \mathrm{beta}, \mathrm{parameter\_83}, \mathrm{parameter\_84}) \tag{156}$$

$$\mathrm{function\_4}\,(\mathrm{Vmf}, \mathrm{A}, \mathrm{B}, \mathrm{alfa}, \mathrm{Ka}, \mathrm{Kb}, \mathrm{Vmr}, \mathrm{P}, \mathrm{Q}, \mathrm{beta}, \mathrm{Kp}, \mathrm{Kq}) = \frac{\frac{\mathrm{Vmf}\cdot\mathrm{A}\cdot\mathrm{B}}{\mathrm{alfa}\cdot\mathrm{Ka}\cdot\mathrm{Kb}} - \frac{\mathrm{Vmr}\cdot\mathrm{P}\cdot\mathrm{Q}}{\mathrm{beta}\cdot\mathrm{Kp}\cdot\mathrm{Kq}}}{1 + \frac{\mathrm{A}}{\mathrm{Ka}} + \frac{\mathrm{B}}{\mathrm{Kb}} + \frac{\mathrm{A}\cdot\mathrm{B}}{\mathrm{alfa}\cdot\mathrm{Ka}\cdot\mathrm{Kb}} + \frac{\mathrm{P}\cdot\mathrm{Q}}{\mathrm{beta}\cdot\mathrm{Kp}\cdot\mathrm{Kq}} + \frac{\mathrm{P}}{\mathrm{Kp}} + \frac{\mathrm{Q}}{\mathrm{Kq}}} \tag{157}$$

$$\mathrm{function\_4}\,(\mathrm{Vmf}, \mathrm{A}, \mathrm{B}, \mathrm{alfa}, \mathrm{Ka}, \mathrm{Kb}, \mathrm{Vmr}, \mathrm{P}, \mathrm{Q}, \mathrm{beta}, \mathrm{Kp}, \mathrm{Kq}) = \frac{\frac{\mathrm{Vmf}\cdot\mathrm{A}\cdot\mathrm{B}}{\mathrm{alfa}\cdot\mathrm{Ka}\cdot\mathrm{Kb}} - \frac{\mathrm{Vmr}\cdot\mathrm{P}\cdot\mathrm{Q}}{\mathrm{beta}\cdot\mathrm{Kp}\cdot\mathrm{Kq}}}{1 + \frac{\mathrm{A}}{\mathrm{Ka}} + \frac{\mathrm{B}}{\mathrm{Kb}} + \frac{\mathrm{A}\cdot\mathrm{B}}{\mathrm{alfa}\cdot\mathrm{Ka}\cdot\mathrm{Kb}} + \frac{\mathrm{P}\cdot\mathrm{Q}}{\mathrm{beta}\cdot\mathrm{Kp}\cdot\mathrm{Kq}} + \frac{\mathrm{P}}{\mathrm{Kp}} + \frac{\mathrm{Q}}{\mathrm{Kq}}} \tag{158}$$

Table 95: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`alfa`	alfa		1.0		☑
`beta`	beta		1.0		☑

8.25 Reaction `reaction_25`

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

Name AK

Reaction equation

$$2\,\mathrm{species\_3} \xrightleftharpoons{\mathrm{species\_3},\ \mathrm{species\_4},\ \mathrm{species\_20}} \mathrm{species\_4} + \mathrm{species\_20} \tag{159}$$

Reactant

Table 96: Properties of each reactant.

Id	Name	SBO
`species_3`	ADP	

Modifiers

Table 97: Properties of each modifier.

Id	Name	SBO
species_3	ADP	
species_4	ATP	
species_20	AMP	

Products

Table 98: Properties of each product.

Id	Name	SBO
species_4	ATP	
species_20	AMP	

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{function\_5}\,(\mathrm{Vf}, [\mathrm{species\_3}], [\mathrm{species\_4}], [\mathrm{species\_20}], \mathrm{Keq}) \quad (160)$$

$$\mathrm{function\_5}\,(\mathrm{Vf}, \mathrm{ADP}, \mathrm{ATP}, \mathrm{AMP}, \mathrm{Keq}) = \frac{\mathrm{Vf} \cdot \mathrm{ADP}^2 \cdot \left(1 - \frac{\mathrm{ATP} \cdot \mathrm{AMP}}{\mathrm{Keq}}\right)}{(1 + \mathrm{ADP})^2 + (1 + \mathrm{ATP}) \cdot (1 + \mathrm{AMP}) - 1} \quad (161)$$

$$\mathrm{function\_5}\,(\mathrm{Vf}, \mathrm{ADP}, \mathrm{ATP}, \mathrm{AMP}, \mathrm{Keq}) = \frac{\mathrm{Vf} \cdot \mathrm{ADP}^2 \cdot \left(1 - \frac{\mathrm{ATP} \cdot \mathrm{AMP}}{\mathrm{Keq}}\right)}{(1 + \mathrm{ADP})^2 + (1 + \mathrm{ATP}) \cdot (1 + \mathrm{AMP}) - 1} \quad (162)$$

Table 99: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vf	Vf		141.20		☑
Keq	Keq		2.26		☑

8.26 Reaction reaction_26

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

Name DHase

Reaction equation

$$\text{species\_18} \xrightleftharpoons{\text{species\_18, species\_19}} \text{species\_19} \tag{163}$$

Reactant

Table 100: Properties of each reactant.

Id	Name	SBO
species_18	NADH	

Modifiers

Table 101: Properties of each modifier.

Id	Name	SBO
species_18	NADH	
species_19	NAD	

Product

Table 102: Properties of each product.

Id	Name	SBO
species_19	NAD	

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = \text{vol}\left(\text{compartment\_1}\right) \cdot \text{function\_6}\left(\text{parameter\_46}, [\text{species\_18}], [\text{species\_19}], \text{Keq}\right) \tag{164}$$

$$\text{function\_6}\left(\text{Vf}, \text{NADH}, \text{NAD}, \text{Keq}\right) = \frac{\text{Vf} \cdot \text{NADH} \cdot \left(1 - \frac{\text{NAD}}{\text{NADH} \cdot \text{Keq}}\right)}{1 + \text{NADH} + 1 + \text{NAD} - 1} \tag{165}$$

$$\text{function\_6}\left(\text{Vf}, \text{NADH}, \text{NAD}, \text{Keq}\right) = \frac{\text{Vf} \cdot \text{NADH} \cdot \left(1 - \frac{\text{NAD}}{\text{NADH} \cdot \text{Keq}}\right)}{1 + \text{NADH} + 1 + \text{NAD} - 1} \tag{166}$$

Table 103: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Keq	Keq		300.0		☑

8.27 Reaction reaction_27

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

Name DPHase

Reaction equation

$$\text{species\_11} \xrightleftharpoons{\text{species\_11, species\_10}} \text{species\_10} \tag{167}$$

Reactant

Table 104: Properties of each reactant.

Id	Name	SBO
species_11	NADPH	

Modifiers

Table 105: Properties of each modifier.

Id	Name	SBO
species_11	NADPH	
species_10	NADP	

Product

Table 106: Properties of each product.

Id	Name	SBO
species_10	NADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{27} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_7}\left(\mathrm{parameter\_47}, [\mathrm{species\_11}], [\mathrm{species\_10}], \mathrm{Keq}\right) \quad (168)$$

$$\mathrm{function\_7}\left(\mathrm{Vf}, \mathrm{NADPH}, \mathrm{NADP}, \mathrm{Keq}\right) = \frac{\mathrm{Vf} \cdot \mathrm{NADPH} \cdot \left(1 - \frac{\mathrm{NADP}}{\mathrm{NADPH} \cdot \mathrm{Keq}}\right)}{1 + \mathrm{NADPH} + 1 + \mathrm{NADP} - 1} \quad (169)$$

$$\mathrm{function\_7}\left(\mathrm{Vf}, \mathrm{NADPH}, \mathrm{NADP}, \mathrm{Keq}\right) = \frac{\mathrm{Vf} \cdot \mathrm{NADPH} \cdot \left(1 - \frac{\mathrm{NADP}}{\mathrm{NADPH} \cdot \mathrm{Keq}}\right)}{1 + \mathrm{NADPH} + 1 + \mathrm{NADP} - 1} \quad (170)$$

Table 107: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Keq	Keq		0.2		☑

8.28 Reaction reaction_28

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

Name MPM

Reaction equation

$$0{\cdot}08\,\mathrm{species\_31} + 0{\cdot}2\,\mathrm{species\_34} + \mathrm{species\_23} + \mathrm{species\_3} \xleftrightarrow{\mathrm{species\_31},\ \mathrm{species\_23},\ \mathrm{species\_3},\ \mathrm{species\_34},\ \mathrm{species\_4},} \quad (171)$$

Reactants

Table 108: Properties of each reactant.

Id	Name	SBO
species_31	PYR	
species_34	O2	
species_23	Pi	
species_3	ADP	

Modifiers

Table 109: Properties of each modifier.

Id	Name	SBO
species_31	PYR	
species_23	Pi	
species_3	ADP	
species_34	O2	
species_4	ATP	
species_33	CO2	

Products

Table 110: Properties of each product.

Id	Name	SBO
species_33	CO2	
species_4	ATP	

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_8}\left(\mathrm{parameter\_48}, [\mathrm{species\_31}], \mathrm{y}, [\mathrm{species\_23}], [\mathrm{species\_3}], [\mathrm{species\_34}], [\mathrm{species\_4}], [\mathrm{species\_33}], \mathrm{Keq}\right) \tag{172}$$

$$\begin{aligned}&\mathrm{function\_8}\left(\mathrm{Vmf}, \mathrm{PYR}, \mathrm{y}, \mathrm{Pi}, \mathrm{ADP}, \mathrm{O2}, \mathrm{ATP}, \mathrm{CO2}, \mathrm{Keq}\right)\\ &= \frac{\mathrm{Vmf} \cdot \mathrm{PYR}^{\frac{1}{\mathrm{y}}} \cdot \mathrm{Pi} \cdot \mathrm{ADP} \cdot \mathrm{O2}^{\frac{5}{2 \cdot \mathrm{y}}} \cdot \left(1 - \frac{\mathrm{ATP} \cdot \mathrm{CO2}^{\frac{3}{\mathrm{y}}}}{\mathrm{PYR}^{\frac{1}{\mathrm{y}}} \cdot \mathrm{O2}^{\frac{5}{2 \cdot \mathrm{y}}} \cdot \mathrm{Pi} \cdot \mathrm{ADP} \cdot \mathrm{Keq}}\right)}{\left(1 + \mathrm{PYR}\right)^{\frac{1}{\mathrm{y}}} \cdot \left(1 + \mathrm{O2}\right)^{\frac{5}{2 \cdot \mathrm{y}}} \cdot \left(1 + \mathrm{Pi}\right) \cdot \left(1 + \mathrm{ADP}\right) + \left(1 + \mathrm{ATP}\right) \cdot \left(1 + \mathrm{CO2}\right)^{\frac{3}{\mathrm{y}}} - 1}\end{aligned} \tag{173}$$

$$\begin{aligned}&\mathrm{function\_8}\left(\mathrm{Vmf}, \mathrm{PYR}, \mathrm{y}, \mathrm{Pi}, \mathrm{ADP}, \mathrm{O2}, \mathrm{ATP}, \mathrm{CO2}, \mathrm{Keq}\right)\\ &= \frac{\mathrm{Vmf} \cdot \mathrm{PYR}^{\frac{1}{\mathrm{y}}} \cdot \mathrm{Pi} \cdot \mathrm{ADP} \cdot \mathrm{O2}^{\frac{5}{2 \cdot \mathrm{y}}} \cdot \left(1 - \frac{\mathrm{ATP} \cdot \mathrm{CO2}^{\frac{3}{\mathrm{y}}}}{\mathrm{PYR}^{\frac{1}{\mathrm{y}}} \cdot \mathrm{O2}^{\frac{5}{2 \cdot \mathrm{y}}} \cdot \mathrm{Pi} \cdot \mathrm{ADP} \cdot \mathrm{Keq}}\right)}{\left(1 + \mathrm{PYR}\right)^{\frac{1}{\mathrm{y}}} \cdot \left(1 + \mathrm{O2}\right)^{\frac{5}{2 \cdot \mathrm{y}}} \cdot \left(1 + \mathrm{Pi}\right) \cdot \left(1 + \mathrm{ADP}\right) + \left(1 + \mathrm{ATP}\right) \cdot \left(1 + \mathrm{CO2}\right)^{\frac{3}{\mathrm{y}}} - 1}\end{aligned} \tag{174}$$

Table 111: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
y	y		12.5		☑
Keq	Keq		1000000.0		☑

8.29 Reaction reaction_29

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

Name ATPase

Reaction equation

$$\text{species\_4} \xrightarrow{\text{species\_4}} \text{species\_3} + \text{species\_23} \tag{175}$$

Reactant

Table 112: Properties of each reactant.

Id	Name	SBO
species_4	ATP	

Modifier

Table 113: Properties of each modifier.

Id	Name	SBO
species_4	ATP	

Products

Table 114: Properties of each product.

Id	Name	SBO
species_3	ADP	
species_23	Pi	

Kinetic Law

Derived unit contains undeclared units

$$v_{29} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_4}] \tag{176}$$

Table 115: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		6210.0		☑

9 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.

9.1 Species species_1

Name GLC

SBO:0000247 simple chemical

Initial concentration $8.97 \cdot 10^{-4}$ nmol $\cdot$ nl^{-1}

This species takes part in four reactions (as a reactant in reaction_2 and as a product in reaction_1 and as a modifier in reaction_1, reaction_2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_1} = v_1 - v_2 \tag{177}$$

9.2 Species species_2

Name G6P

SBO:0000247 simple chemical

Initial concentration 0.00109 nmol $\cdot$ nl^{-1}

This species takes part in eight reactions (as a reactant in reaction_3, reaction_4 and as a product in reaction_2, reaction_12 and as a modifier in reaction_2, reaction_3, reaction_4, reaction_12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_2} = v_2 + v_{12} - v_3 - v_4 \tag{178}$$

9.3 Species species_3

Name ADP

SBO:0000247 simple chemical

Initial concentration $0.0027\ \mathrm{nmol} \cdot \mathrm{nl}^{-1}$

Involved in rule species_3

This species takes part in 15 reactions (as a reactant in reaction_17, reaction_23, reaction_25, reaction_28 and as a product in reaction_2, reaction_19, reaction_20, reaction_29 and as a modifier in reaction_2, reaction_17, reaction_19, reaction_20, reaction_23, reaction_25, reaction_28). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

9.4 Species species_4

Name ATP

SBO:0000247 simple chemical

Initial concentration $0.0087\ \mathrm{nmol} \cdot \mathrm{nl}^{-1}$

This species takes part in 22 reactions (as a reactant in reaction_2, reaction_11, reaction_19, reaction_20, reaction_29 and as a product in reaction_17, reaction_23, reaction_25, reaction_28 and as a modifier in reaction_2, reaction_4, reaction_4, reaction_5, reaction_5, reaction_11, reaction_17, reaction_19, reaction_20, reaction_23, reaction_25, reaction_28, reaction_29).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_4} = v_{17} + v_{23} + v_{25} + v_{28} - v_2 - v_{11} - v_{19} - v_{20} - v_{29} \tag{179}$$

9.5 Species species_5

Name F6P

SBO:0000247 simple chemical

Initial concentration $3.62 \cdot 10^{-5}\ \mathrm{nmol} \cdot \mathrm{nl}^{-1}$

This species takes part in eight reactions (as a reactant in reaction_20 and as a product in reaction_3, reaction_9, reaction_10 and as a modifier in reaction_3, reaction_9, reaction_10, reaction_20).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_5} = v_3 + v_9 + v_{10} - v_{20} \tag{180}$$

9.6 Species species_6

Name F16P

SBO:0000247 simple chemical

Initial concentration $3.67 \cdot 10^{-4}$ nmol $\cdot$ nl^{-1}

This species takes part in eight reactions (as a reactant in reaction_14 and as a product in reaction_20 and as a modifier in reaction_3, reaction_3, reaction_14, reaction_20, reaction_23, reaction_23).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_6} = v_{20} - v_{14} \tag{181}$$

9.7 Species species_7

Name E4P

SBO:0000247 simple chemical

Initial concentration $9.3 \cdot 10^{-4}$ nmol $\cdot$ nl^{-1}

This species takes part in six reactions (as a reactant in reaction_9 and as a product in reaction_10 and as a modifier in reaction_3, reaction_3, reaction_9, reaction_10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_7} = v_{10} - v_{9} \tag{182}$$

9.8 Species species_8

Name PGN

SBO:0000247 simple chemical

Initial concentration 10^{-4} nmol $\cdot$ nl^{-1}

This species takes part in six reactions (as a reactant in reaction_5 and as a product in reaction_4 and as a modifier in reaction_3, reaction_3, reaction_4, reaction_5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_8} = v_{4} - v_{5} \tag{183}$$

9.9 Species species_9

Name GLC_e

SBO:0000247 simple chemical

Initial concentration $0.01\ \mathrm{nmol \cdot nl^{-1}}$

This species takes part in two reactions (as a reactant in reaction_1 and as a modifier in reaction_1), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_9} = 0 \tag{184}$$

9.10 Species species_10

Name NADP

SBO:0000247 simple chemical

Initial concentration $6.118 \cdot 10^{-7}\ \mathrm{nmol \cdot nl^{-1}}$

Involved in rule species_10

This species takes part in six reactions (as a reactant in reaction_4, reaction_5 and as a product in reaction_27 and as a modifier in reaction_4, reaction_5, reaction_27). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

9.11 Species species_11

Name NADPH

SBO:0000247 simple chemical

Initial concentration $1.87082 \cdot 10^{-5}\ \mathrm{nmol \cdot nl^{-1}}$

This species takes part in six reactions (as a reactant in reaction_27 and as a product in reaction_4, reaction_5 and as a modifier in reaction_4, reaction_5, reaction_27).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_11} = v_4 + v_5 - v_{27} \tag{185}$$

9.12 Species species_12

Name BPG

SBO:0000247 simple chemical

Initial concentration $6.29 \cdot 10^{-5}$ nmol $\cdot$ nl^{-1}

This species takes part in eight reactions (as a reactant in reaction_17 and as a product in reaction_16 and as a modifier in reaction_4, reaction_4, reaction_5, reaction_5, reaction_16, reaction_17).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_12} = v_{16} - v_{17} \tag{186}$$

9.13 Species species_13

Name RU5P

SBO:0000247 simple chemical

Initial concentration $1.43 \cdot 10^{-4}$ nmol $\cdot$ nl^{-1}

This species takes part in six reactions (as a reactant in reaction_6, reaction_7 and as a product in reaction_5 and as a modifier in reaction_5, reaction_6, reaction_7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_13} = v_5 - v_6 - v_7 \tag{187}$$

9.14 Species species_14

Name X5P

SBO:0000247 simple chemical

Initial concentration $2.42 \cdot 10^{-4}$ nmol $\cdot$ nl^{-1}

This species takes part in six reactions (as a reactant in reaction_8, reaction_9 and as a product in reaction_6 and as a modifier in reaction_6, reaction_8, reaction_9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_14} = v_6 - v_8 - v_9 \tag{188}$$

9.15 Species species_15

Name R5P

SBO:0000247 simple chemical

Initial concentration $2.74 \cdot 10^{-5}$ nmol $\cdot$ nl^{-1}

This species takes part in six reactions (as a reactant in reaction_8, reaction_11 and as a product in reaction_7 and as a modifier in reaction_7, reaction_8, reaction_11).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_15} = v_7 - v_8 - v_{11} \tag{189}$$

9.16 Species species_16

Name GAP

SBO:0000247 simple chemical

Initial concentration $1.53 \cdot 10^{-4}$ nmol $\cdot$ nl^{-1}

This species takes part in twelve reactions (as a reactant in reaction_10, reaction_15, reaction_16 and as a product in reaction_8, reaction_9, reaction_14 and as a modifier in reaction_8, reaction_9, reaction_10, reaction_14, reaction_15, reaction_16).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_16} = v_8 + v_9 + v_{14} - v_{10} - v_{15} - v_{16} \tag{190}$$

9.17 Species species_17

Name S7P

SBO:0000247 simple chemical

Initial concentration $8.58 \cdot 10^{-5}$ nmol $\cdot$ nl^{-1}

This species takes part in four reactions (as a reactant in reaction_10 and as a product in reaction_8 and as a modifier in reaction_8, reaction_10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_17} = v_8 - v_{10} \tag{191}$$

9.18 Species species_18

Name NADH

SBO:0000247 simple chemical

Initial concentration $5.00000000000001 \cdot 10^{-6}\ \mathrm{nmol} \cdot \mathrm{nl}^{-1}$

Involved in rule species_18

This species takes part in six reactions (as a reactant in reaction_24, reaction_26 and as a product in reaction_16 and as a modifier in reaction_16, reaction_24, reaction_26). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

9.19 Species species_19

Name NAD

SBO:0000247 simple chemical

Initial concentration $0.00134\ \mathrm{nmol} \cdot \mathrm{nl}^{-1}$

This species takes part in six reactions (as a reactant in reaction_16 and as a product in reaction_24, reaction_26 and as a modifier in reaction_16, reaction_24, reaction_26).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_19} = v_{24} + v_{26} - v_{16} \tag{192}$$

9.20 Species species_20

Name AMP

SBO:0000247 simple chemical

Initial concentration $0.00311\ \mathrm{nmol} \cdot \mathrm{nl}^{-1}$

This species takes part in four reactions (as a product in reaction_11, reaction_25 and as a modifier in reaction_11, reaction_25), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_20} = 0 \tag{193}$$

9.21 Species species_21

Name PRPP

SBO:0000247 simple chemical

Initial concentration $0.0010\ \mathrm{nmol \cdot nl^{-1}}$

This species takes part in two reactions (as a product in reaction_11 and as a modifier in reaction_11), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_21} = 0 \tag{194}$$

9.22 Species species_22

Name G1P

SBO:0000247 simple chemical

Initial concentration $3.41 \cdot 10^{-5}\ \mathrm{nmol \cdot nl^{-1}}$

This species takes part in eight reactions (as a reactant in reaction_12, reaction_19 and as a product in reaction_13, reaction_18 and as a modifier in reaction_12, reaction_13, reaction_18, reaction_19).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_22} = v_{13} + v_{18} - v_{12} - v_{19} \tag{195}$$

9.23 Species species_23

Name Pi

SBO:0000247 simple chemical

Initial concentration $0.02\ \mathrm{nmol \cdot nl^{-1}}$

This species takes part in eleven reactions (as a reactant in reaction_13, reaction_16, reaction_18, reaction_28 and as a product in reaction_19, reaction_29 and as a modifier in reaction_13, reaction_16, reaction_18, reaction_19, reaction_28), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_23} = 0 \tag{196}$$

9.24 Species species_24

Name GLY

SBO:0000247 simple chemical

Initial concentration $0.208403745497308\ \mathrm{nmol \cdot nl^{-1}}$

This species takes part in eight reactions (as a reactant in reaction_13, reaction_18 and as a product in reaction_13, reaction_18, reaction_19 and as a modifier in reaction_13, reaction_18, reaction_19), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_24} = 0 \tag{197}$$

9.25 Species species_25

Name CIT

SBO:0000247 simple chemical

Initial concentration $0.00108\ \mathrm{nmol \cdot nl^{-1}}$

This species takes part in two reactions (as a modifier in reaction_20, reaction_20), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_25} = 0 \tag{198}$$

9.26 Species species_26

Name F26P

SBO:0000247 simple chemical

Initial concentration $3.67 \cdot 10^{-6}\ \mathrm{nmol \cdot nl^{-1}}$

This species takes part in two reactions (as a modifier in reaction_20, reaction_20), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_26} = 0 \tag{199}$$

9.27 Species species_27

Name DHAP

SBO:0000247 simple chemical

Initial concentration $5.53 \cdot 10^{-4}$ nmol · nl^{-1}

This species takes part in four reactions (as a product in reaction_14, reaction_15 and as a modifier in reaction_14, reaction_15).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_27} = v_{14} + v_{15} \tag{200}$$

9.28 Species species_28

Name PG3

SBO:0000247 simple chemical

Initial concentration $3.07 \cdot 10^{-5}$ nmol · nl^{-1}

This species takes part in four reactions (as a reactant in reaction_21 and as a product in reaction_17 and as a modifier in reaction_17, reaction_21).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_28} = v_{17} - v_{21} \tag{201}$$

9.29 Species species_29

Name PG2

SBO:0000247 simple chemical

Initial concentration $4.98 \cdot 10^{-6}$ nmol · nl^{-1}

This species takes part in four reactions (as a reactant in reaction_22 and as a product in reaction_21 and as a modifier in reaction_21, reaction_22).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_29} = v_{21} - v_{22} \tag{202}$$

9.30 Species species_30

Name PEP

SBO:0000247 simple chemical

Initial concentration $5.79 \cdot 10^{-5}$ nmol · nl^{-1}

This species takes part in four reactions (as a reactant in reaction_23 and as a product in reaction_22 and as a modifier in reaction_22, reaction_23).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_30} = v_{22} - v_{23} \tag{203}$$

9.31 Species species_31

Name PYR

SBO:0000247 simple chemical

Initial concentration $0.00183\ \mathrm{nmol \cdot nl^{-1}}$

This species takes part in six reactions (as a reactant in reaction_24, reaction_28 and as a product in reaction_23 and as a modifier in reaction_23, reaction_24, reaction_28).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_31} = v_{23} - v_{24} - 0.08\, v_{28} \tag{204}$$

9.32 Species species_32

Name LAC

SBO:0000247 simple chemical

Initial concentration $0.0155\ \mathrm{nmol \cdot nl^{-1}}$

This species takes part in two reactions (as a product in reaction_24 and as a modifier in reaction_24), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_32} = 0 \tag{205}$$

9.33 Species species_33

Name CO2

SBO:0000247 simple chemical

Initial concentration $0.0214\ \mathrm{nmol \cdot nl^{-1}}$

This species takes part in two reactions (as a product in reaction_28 and as a modifier in reaction_28), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_33} = 0 \tag{206}$$

9.34 Species species_34

Name O2

SBO:0000247 simple chemical

Initial concentration $6.5 \cdot 10^{-5}\ \mathrm{nmol \cdot nl^{-1}}$

This species takes part in two reactions (as a reactant in reaction_28 and as a modifier in reaction_28), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_34} = 0 \tag{207}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000247 simple chemical: Simple, non-repetitive chemical entity

SBML2LaTeX 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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