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SBML Model Report

Model name: “Yugi2014 - Insulin induced signalling (PFKL phosphorylation) - model 2”



September 9, 2014

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following three authors: Vijayalakshmi Chelliah¹, Katsuyuki Yugi² and Audald Lloret i Villas³ at August 14th 2014 at 12:59 a. m. and last time modified at September eighth 2014 at 2:32 p. m. Table 1 provides an overview of the quantities of all components of this model.

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

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	37
events	7	constraints	0
reactions	30	function definitions	0
global parameters	22	unit definitions	5
rules	1	initial assignments	0

Model Notes

Yugi2014 - Insulin induced signalling (PFKLphosphorylation) - model 2

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Insulin induces phosphorylation and activation of liver-type phosphofructokinase 1, which thereby controls a key reaction in glycolysis. This mechanism is revealed using the mathematical model. In this model, the PFKL phosphorylation time courses are calculation from the signalling pathway model developed by Kubata et al. (2012) ([MODEL1204060000](#) - Kubota2012_InsulinAction_AKTpathway).

Author's Note: Katsuyuki Yugi thank Akira Funahashi (Keio University, Japan) for his kind advice in converting the model from MATLAB to SBML.

This model is described in the article:[Reconstruction of insulin signal flow from phosphoproteome and metabolome data](#). Yugi K, Kubota H, Toyoshima Y, Noguchi R, Kawata K, Komori Y, Uda S, Kunida K, Tomizawa Y, Funato Y, Miki H, Matsumoto M, Nakayama KI, Kashikura K, Endo K, Ikeda K, Soga T, Kuroda S. Cell Rep 2014 Aug; 8(4): 1171-1183

Abstract:

Cellular homeostasis is regulated by signals through multiple molecular networks that include protein phosphorylation and metabolites. However, where and when the signal flows through a network and regulates homeostasis has not been explored. We have developed a reconstruction method for the signal flow based on time-course phosphoproteome and metabolome data, using multiple databases, and have applied it to acute action of insulin, an important hormone for metabolic homeostasis. An insulin signal flows through a network, through signaling pathways that involve 13 protein kinases, 26 phosphorylated metabolic enzymes, and 35 allosteric effectors, resulting in quantitative changes in 44 metabolites. Analysis of the network reveals that insulin induces phosphorylation and activation of liver-type phosphofructokinase 1, thereby controlling a key reaction in glycolysis. We thus provide a versatile method of reconstruction of signal flow through the network using phosphoproteome and metabolome data.

This model is hosted on [BioModels Database](#) and identified by: [BIOMD0000000541](#).

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

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2 Unit Definitions

This is an overview of five unit definitions.

2.1 Unit substance

Name substance

Definition mol

2.2 Unit volume

Name volume

Definition l

2.3 Unit area

Name area

Definition m²

2.4 Unit length

Name length

Definition m

2.5 Unit time

Name time

Definition s

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
default			3	1	litre	<input checked="" type="checkbox"/>	

3.1 Compartment default

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

4 Species

This model contains 37 species. The boundary condition of seven 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
s1	PFKL	default	mol	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
s2	FBPase	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
s3	F6P	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
s4	F1,6BP	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
s5	PEP	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
s6	Isocitrate	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
s7	2-oxoglutarate	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
s8	Malate	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
s9	F2,6BP	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
s10	Citrate	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
s11	sa4_degraded	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s12	ALDO	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
s13	pPFKL	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
s14	sa8_degraded	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s15	sa7_degraded	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s16	sa5_degraded	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s17	sa6_degraded	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s18	sa9_degraded	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s21	sa3_degraded	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s19	sa10_degraded	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s23	IR_complex	default	mol	<input type="checkbox"/>	<input type="checkbox"/>

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
s24	pro_IR_complex	default	mol	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
s25	p1IR_complex	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
s26	p2IR_complex	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
s27	p1p2IRcomplex	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
s28	AKT	default	mol	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
s29	pAKT	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
s30	mTOR	default	mol	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
s31	pmTOR	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
s32	S6K	default	mol	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
s33	pS6K	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
s34	X	default	mol	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
s35	pX	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
s36	sa28_degraded	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s37	sa27_degraded	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s38	sa26_degraded	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s22	F6P_proxy	default	mol	<input type="checkbox"/>	<input checked="" type="checkbox"/>

5 Parameters

This model contains 22 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K_FBPase_cit	K_FBPase_cit		0.021	dimensionless	✓
K_FBPase-f16bp	K_FBPase_f16bp		0.104	dimensionless	✓
K_FBPase-f26bp	K_FBPase_f26bp		17.517	dimensionless	✓
K_PFKL_PHOS-S775	K_PFKL_PHOS-S775		6.284	dimensionless	✓
K_PFKL_akg	K_PFKL_akg		24661.012	dimensionless	✓
K_PFKL_cit	K_PFKL_cit		41.304	dimensionless	✓
K_PFKL_f26bp	K_PFKL_f26bp		1.282	dimensionless	✓
K_PFKL_f6p	K_PFKL_f6p		0.014	dimensionless	✓
K_PFKL_icit	K_PFKL_icit		1784.508	dimensionless	✓
K_PFKL_mal	K_PFKL_mal		9.545	dimensionless	✓
K_PFKL_pep	K_PFKL_pep		0.634	dimensionless	✓
Vf_FBPase	Vf_FBPase		9.933	dimensionless	✓
Vf_PFKL	Vf_PFKL		695063.719	dimensionless	✓
k_ALDO	k_ALDO		0.008	dimensionless	✓
k_mal	k_mal		1.006	mol	☐
k_akg	k_akg		−3.544	mol	☐
k_pep	k_pep		43.992	mol	☐
k_icit	k_icit		−0.038	mol	☐
k_f26bp	k_f26bp		−0.083	mol	☐
k_cit	k_cit		−0.352	mol	☐
k_f6p	k_f6p		−0.930	dimensionless	☐
insulin	insulin		1.000	dimensionless	✓

6 Rule

This is an overview of one rule.

6.1 Rule s22

Rule s22 is an assignment rule for species s22:

$$[s22] = s3 \quad (1)$$

Derived unit mol

7 Events

This is an overview of seven events. Each event is initiated whenever its trigger condition switches from `false` to `true`. A delay function postpones the effects of an event to a later time point. At the time of execution, an event can assign values to species, parameters or compartments if these are not set to constant.

7.1 Event `ev2min`

Name `ev2min`

Trigger condition

$$t > 2 \quad (2)$$

Assignments

$$k_{\text{akg}} = -1.357466063 \quad (3)$$

$$k_{\text{cit}} = 0.351935646 \quad (4)$$

$$k_{\text{f6p}} = 1.357466063 \quad (5)$$

$$k_{\text{icit}} = -0.038210156 \quad (6)$$

$$k_{\text{f26bp}} = 0.028924455 \quad (7)$$

$$k_{\text{mal}} = -1.508295626 \quad (8)$$

$$k_{\text{pep}} = 7.54147813 \quad (9)$$

7.2 Event `ev5min`

Name `ev5min`

Trigger condition

$$t > 5 \quad (10)$$

Assignments

$$k_{\text{akg}} = 0 \quad (11)$$

$$k_{\text{cit}} = -0.211161388 \quad (12)$$

$$k_{\text{f6p}} = 0.271493213 \quad (13)$$

$$k_{\text{icit}} = -0.038210156 \quad (14)$$

$$k_{\text{f26bp}} = 0.119075279 \quad (15)$$

$$k_{\text{mal}} = -0.904977376 \quad (16)$$

$$k_{\text{pep}} = -6.334841629 \quad (17)$$

7.3 Event `ev10min`

Name `ev10min`

Trigger condition

$$t > 10 \quad (18)$$

Assignments

$$k_{\text{akg}} = 0.36199095 \quad (19)$$

$$k_{\text{cit}} = 1.085972851 \quad (20)$$

$$k_{\text{f6p}} = -1.055806938 \quad (21)$$

$$k_{\text{icit}} = -0.038210156 \quad (22)$$

$$k_{\text{f26bp}} = -0.050207413 \quad (23)$$

$$k_{\text{mal}} = 3.921568627 \quad (24)$$

$$k_{\text{pep}} = 9.049773756 \quad (25)$$

7.4 Event `ev15min`

Name `ev15min`

Trigger condition

$$t > 15 \quad (26)$$

Assignments

$$k_{\text{akg}} = 1.085972851 \quad (27)$$

$$k_{\text{cit}} = 0.452488688 \quad (28)$$

$$k_{\text{f6p}} = -0.12066365 \quad (29)$$

$$k_{\text{icit}} = -0.018099548 \quad (30)$$

$$k_{\text{f26bp}} = 0.100115778 \quad (31)$$

$$k_{\text{mal}} = 1.809954751 \quad (32)$$

$$k_{\text{pep}} = -4.826546003 \quad (33)$$

7.5 Event `ev20min`

Name `ev20min`

Trigger condition

$$t > 20 \quad (34)$$

Assignments

$$k_{\text{akg}} = 0.226244344 \quad (35)$$

$$k_{\text{cit}} = 0.377073906 \quad (36)$$

$$k_{\text{f6p}} = -0.165912519 \quad (37)$$

$$k_{\text{icit}} = 0.031674208 \quad (38)$$

$$k_{\text{f26bp}} = -0.032601514 \quad (39)$$

$$k_{\text{mal}} = 1.206636501 \quad (40)$$

$$k_{\text{pep}} = -3.619909502 \quad (41)$$

7.6 Event `ev30min`

Name `ev30min`

Trigger condition

$$t > 30 \quad (42)$$

Assignments

$$k_{\text{akg}} = 0.369532428 \quad (43)$$

$$k_{\text{cit}} = 0.306686777 \quad (44)$$

$$k_{\text{f6p}} = 0.070387129 \quad (45)$$

$$k_{\text{icit}} = 0.031674208 \quad (46)$$

$$k_{\text{f26bp}} = -0.003055632 \quad (47)$$

$$k_{\text{mal}} = 0.502765209 \quad (48)$$

$$k_{\text{pep}} = -0.301659125 \quad (49)$$

7.7 Event `ev45min`

Name `ev45min`

Trigger condition

$$t > 45 \quad (50)$$

Assignments

$$k_{\text{akg}} = 0.369532428 \quad (51)$$

$$k_{\text{cit}} = 0.306686777 \quad (52)$$

$$k_{\text{f6p}} = 0.070387129 \quad (53)$$

$$k_{\text{icit}} = 0.031674208 \quad (54)$$

$$k_{\text{f26bp}} = -0.003055632 \quad (55)$$

$$k_{\text{mal}} = 0.502765209 \quad (56)$$

$$k_{\text{pep}} = -0.301659125 \quad (57)$$

8 Reactions

This model contains 30 reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 5: Overview of all reactions

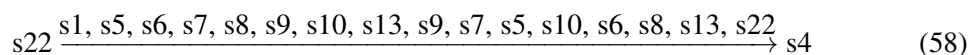
Nº	Id	Name	Reaction Equation	SBO
1	re30		$s_{22} \xrightarrow{s_1, s_5, s_6, s_7, s_8, s_9, s_{10}, s_{13}, s_9, s_7, s_5, s_{10}, s_6, s_8, s_{13}, s_{22}} s_4$	
2	re31		$s_4 \xrightarrow{s_2, s_9, s_{10}, s_9, s_{10}, s_4} s_{22}$	
3	re32		$s_4 \xrightarrow{s_{12}, s_4} s_{11}$	
4	re33		$s_8 \longrightarrow s_{14}$	
5	re34		$s_7 \longrightarrow s_{15}$	
6	re35		$s_5 \longrightarrow s_{16}$	
7	re36		$s_6 \longrightarrow s_{17}$	
8	re37		$s_9 \longrightarrow s_{18}$	
9	re38		$s_{10} \longrightarrow s_{19}$	
10	re39		$s_3 \longrightarrow s_{21}$	
11	re40		$s_{24} \xrightarrow{s_{24}, s_{23}} s_{23}$	
12	re41		$s_{23} \xrightleftharpoons{s_{23}, s_{25}} s_{25}$	
13	re42		$s_{23} \xrightarrow{s_{31}, s_{23}, s_{31}} s_{26}$	
14	re43		$s_{26} \xrightleftharpoons{s_{26}, s_{27}} s_{27}$	
15	re44		$s_{25} \xrightarrow{s_{31}, s_{25}, s_{31}} s_{27}$	
16	re45		$s_{27} \xrightarrow{s_{27}} s_{25}$	
17	re46		$s_{26} \xrightarrow{s_{26}} s_{23}$	
18	re47		$s_{27} \xrightarrow{s_{27}} s_{36}$	

Nº	Id	Name	Reaction Equation	SBO
19	re48		$s_{28} \xrightarrow{s_{25}, s_{28}, s_{29}, s_{25}} s_{29}$	
20	re49		$s_{29} \xrightarrow{s_{29}} s_{28}$	
21	re50		$s_{26} \xrightarrow{s_{26}} s_{37}$	
22	re51		$s_{25} \xrightarrow{s_{25}} s_{38}$	
23	re52		$s_{30} \xrightarrow{s_{29}, s_{30}, s_{31}, s_{29}} s_{31}$	
24	re53		$s_{31} \xrightarrow{s_{31}} s_{30}$	
25	re54		$s_{32} \xrightarrow{s_{31}, s_{32}, s_{33}, s_{31}} s_{33}$	
26	re55		$s_{33} \xrightarrow{s_{35}, s_{33}, s_{35}} s_{32}$	
27	re56		$s_{34} \xrightarrow{s_{31}, s_{34}, s_{35}, s_{31}} s_{35}$	
28	re57		$s_{35} \xrightarrow{s_{35}} s_{34}$	
29	re58		$s_1 \xrightarrow{s_{33}, s_1, s_{13}, s_{33}} s_{13}$	
30	re59		$s_{13} \xrightarrow{s_{13}} s_1$	

8.1 Reaction re30

This is an irreversible reaction of one reactant forming one product influenced by 16 modifiers.

Reaction equation



Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
s22	F6P_proxy	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
s1	PFKL	
s5	PEP	
s6	Isocitrate	
s7	2-oxoglutarate	
s8	Malate	
s9	F2,6BP	
s10	Citrate	
s13	pPFKL	
s9	F2,6BP	
s7	2-oxoglutarate	
s5	PEP	
s10	Citrate	
s6	Isocitrate	
s8	Malate	
s13	pPFKL	
s22	F6P_proxy	

Product

Table 8: Properties of each product.

Id	Name	SBO
s4	F1,6BP	

Kinetic Law

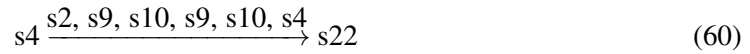
Derived unit mol³

$$v_1 = \frac{s_9}{K_PFKL_f26bp + s_9} \cdot \frac{K_PFKL_akg}{K_PFKL_akg + s_7} \cdot \frac{K_PFKL_pep}{K_PFKL_pep + s_5} \cdot \frac{K_PFKL_cit}{K_PFKL_cit + s_{10}} \cdot \frac{K_PFKL_icit}{K_PFKL_icit + s_6} \cdot \frac{K_PFKL_mal}{K_PFKL_mal + s_8} \cdot \frac{s_{13}}{Vf_PFKL \cdot s_{22}} \cdot \frac{K_PFKL_PHOS_S775 + s_{13}}{K_PFKL_f6p + s_{22}} \quad (59)$$

8.2 Reaction re31

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

Reaction equation



Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
s4	F1,6BP	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
s2	FBPase	
s9	F2,6BP	
s10	Citrate	
s9	F2,6BP	
s10	Citrate	

Id	Name	SBO
s4	F1,6BP	

Product

Table 11: Properties of each product.

Id	Name	SBO
s22	F6P_proxy	

Kinetic Law

Derived unit mol²

$$v_2 = \frac{K_FBPase_f26bp}{K_FBPase_f26bp + s9} \cdot \frac{s10}{K_FBPase_cit + s10} \cdot \frac{Vf_FBPase \cdot s4}{K_FBPase_f16bp + s4} \quad (61)$$

8.3 Reaction re32

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

Reaction equation



Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
s4	F1,6BP	

Modifiers

Table 13: Properties of each modifier.

Id	Name	SBO
s12	ALDO	
s4	F1,6BP	

Product

Table 14: Properties of each product.

Id	Name	SBO
s11	sa4_degraded	

Kinetic Law

Derived unit mol

$$v_3 = k_ALDO \cdot s4 \quad (63)$$

8.4 Reaction re33

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

Reaction equation



Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
s8	Malate	

Product

Table 16: Properties of each product.

Id	Name	SBO
s14	sa8_degraded	

Kinetic Law

Derived unit mol

$$v_4 = k_mal \quad (65)$$

8.5 Reaction re34

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

Reaction equation



Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
s7	2-oxoglutarate	

Product

Table 18: Properties of each product.

Id	Name	SBO
s15	sa7_degraded	

Kinetic Law

Derived unit mol

$$v_5 = k_{\text{akg}} \quad (67)$$

8.6 Reaction re35

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

Reaction equation



Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
s5	PEP	

Product

Table 20: Properties of each product.

Id	Name	SBO
s16	sa5_degraded	

Kinetic Law

Derived unit mol

$$v_6 = k_pep \quad (69)$$

8.7 Reaction re36

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

Reaction equation



Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
s6	Isocitrate	

Product

Table 22: Properties of each product.

Id	Name	SBO
s17	sa6_degraded	

Kinetic Law

Derived unit mol

$$v_7 = k_icit \quad (71)$$

8.8 Reaction re37

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

Reaction equation



Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
s9	F2,6BP	

Product

Table 24: Properties of each product.

Id	Name	SBO
s18	sa9_degraded	

Kinetic Law

Derived unit mol

$$v_8 = k_{f26bp} \quad (73)$$

8.9 Reaction re38

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

Reaction equation



Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
s10	Citrate	

Product

Table 26: Properties of each product.

Id	Name	SBO
s19	sa10_degraded	

Kinetic Law

Derived unit mol

$$v_9 = k_{\text{cit}} \quad (75)$$

8.10 Reaction re39

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

Reaction equation



Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
s3	F6P	

Product

Table 28: Properties of each product.

Id	Name	SBO
s21	sa3_degraded	

Kinetic Law

Derived unit dimensionless

$$v_{10} = k_{\text{f6p}} \quad (77)$$

8.11 Reaction re40

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

Reaction equation



Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
s24	pro_IR_complex	

Modifiers

Table 30: Properties of each modifier.

Id	Name	SBO
s24	pro_IR_complex	
s23	IR_complex	

Product

Table 31: Properties of each product.

Id	Name	SBO
s23	IR_complex	

Kinetic Law

Derived unit mol

$$v_{11} = k1 \cdot (s24 - s23) \quad (79)$$

Table 32: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.048	dimensionless	<input checked="" type="checkbox"/>

8.12 Reaction re41

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

Reaction equation



Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
s23	IR_complex	

Modifiers

Table 34: Properties of each modifier.

Id	Name	SBO
s23	IR_complex	
s25	p1IR_complex	

Product

Table 35: Properties of each product.

Id	Name	SBO
s25	p1IR_complex	

Kinetic Law

Derived unit mol

$$v_{12} = k1 \cdot \text{insulin} \cdot s23 - k2 \cdot s25 \quad (81)$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		7.782	dimensionless	✓
k2	k2		1.611	dimensionless	✓

8.13 Reaction re42

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

Reaction equation



Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
s23	IR_complex	

Modifiers

Table 38: Properties of each modifier.

Id	Name	SBO
s31	pmTOR	
s23	IR_complex	
s31	pmTOR	

Product

Table 39: Properties of each product.

Id	Name	SBO
s26	p2IR_complex	

Kinetic Law

Derived unit mol²

$$v_{13} = k1 \cdot s23 \cdot s31 \quad (83)$$

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		9.933	dimensionless	<input checked="" type="checkbox"/>

8.14 Reaction re43

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

Reaction equation



Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
s26	p2IR_complex	

Modifiers

Table 42: Properties of each modifier.

Id	Name	SBO
s26	p2IR_complex	
s27	p1p2IRcomplex	

Product

Table 43: Properties of each product.

Id	Name	SBO
s27	p1p2IRcomplex	

Kinetic Law

Derived unit mol

$$v_{14} = k1 \cdot \text{insulin} \cdot s26 - k2 \cdot s27 \quad (85)$$

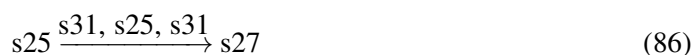
Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.363	dimensionless	✓
k2	k2		0.408	dimensionless	✓

8.15 Reaction re44

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

Reaction equation



Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
s25	p1IR_complex	

Modifiers

Table 46: Properties of each modifier.

Id	Name	SBO
s31	pmTOR	
s25	p1IR_complex	
s31	pmTOR	

Product

Table 47: Properties of each product.

Id	Name	SBO
s27	p1p2IRcomplex	

Kinetic Law

Derived unit mol²

$$v_{15} = k1 \cdot s25 \cdot s31 \quad (87)$$

Table 48: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$3.88248960751442 \cdot 10^{-5}$	dimensionless	<input checked="" type="checkbox"/>

8.16 Reaction re45

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

Reaction equation



Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
s27	p1p2IRcomplex	

Modifier

Table 50: Properties of each modifier.

Id	Name	SBO
s27	p1p2IRcomplex	

Product

Table 51: Properties of each product.

Id	Name	SBO
s25	p1IR_complex	

Kinetic Law

Derived unit mol

$$v_{16} = k1 \cdot s27 \quad (89)$$

Table 52: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.284	dimensionless	<input checked="" type="checkbox"/>

8.17 Reaction re46

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

Reaction equation



Reactant

Table 53: Properties of each reactant.

Id	Name	SBO
s26	p2IR_complex	

Modifier

Table 54: Properties of each modifier.

Id	Name	SBO
s26	p2IR_complex	

Product

Table 55: Properties of each product.

Id	Name	SBO
s23	IR_complex	

Kinetic Law

Derived unit mol

$$v_{17} = k1 \cdot \text{s26} \quad (91)$$

Table 56: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$1.00000000282413 \cdot 10^{-5}$	dimensionless	<input checked="" type="checkbox"/>

8.18 Reaction re47

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

Reaction equation



Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
s27	p1p2IRcomplex	

Modifier

Table 58: Properties of each modifier.

Id	Name	SBO
s27	p1p2IRcomplex	

Product

Table 59: Properties of each product.

Id	Name	SBO
s36	sa28_degraded	

Kinetic Law

Derived unit mol

$$v_{18} = k1 \cdot s27 \quad (93)$$

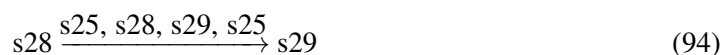
Table 60: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.095	dimensionless	<input checked="" type="checkbox"/>

8.19 Reaction re48

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

Reaction equation



Reactant

Table 61: Properties of each reactant.

Id	Name	SBO
s28	AKT	

Modifiers

Table 62: Properties of each modifier.

Id	Name	SBO
s25	p1IR_complex	
s28	AKT	
s29	pAKT	
s25	p1IR_complex	

Product

Table 63: Properties of each product.

Id	Name	SBO
s29	pAKT	

Kinetic Law

Derived unit mol²

$$v_{19} = k1 \cdot (s28 - s29) \cdot s25 \quad (95)$$

Table 64: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.009	dimensionless	<input checked="" type="checkbox"/>

8.20 Reaction re49

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

Reaction equation



Reactant

Table 65: Properties of each reactant.

Id	Name	SBO
s29	pAKT	

Modifier

Table 66: Properties of each modifier.

Id	Name	SBO
s29	pAKT	

Product

Table 67: Properties of each product.

Id	Name	SBO
s28	AKT	

Kinetic Law

Derived unit mol

$$v_{20} = k1 \cdot s29 \quad (97)$$

Table 68: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		7.706	dimensionless	<input checked="" type="checkbox"/>

8.21 Reaction re50

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

Reaction equation



Reactant

Table 69: Properties of each reactant.

Id	Name	SBO
s26	p2IR_complex	

Modifier

Table 70: Properties of each modifier.

Id	Name	SBO
s26	p2IR_complex	

Product

Table 71: Properties of each product.

Id	Name	SBO
s37	sa27_degraded	

Kinetic Law

Derived unit mol

$$v_{21} = k1 \cdot s26 \quad (99)$$

Table 72: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$1.00277786609339 \cdot 10^{-5}$	dimensionless	<input checked="" type="checkbox"/>

8.22 Reaction re51

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

Reaction equation



Reactant

Table 73: Properties of each reactant.

Id	Name	SBO
s25	p1IR_complex	

Modifier

Table 74: Properties of each modifier.

Id	Name	SBO
s25	p1IR_complex	

Product

Table 75: Properties of each product.

Id	Name	SBO
s38	sa26_degraded	

Kinetic Law

Derived unit mol^2

$$v_{22} = k1 \cdot s25 \quad (101)$$

Table 76: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.008	mol	<input checked="" type="checkbox"/>

8.23 Reaction re52

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

Reaction equation



Reactant

Table 77: Properties of each reactant.

Id	Name	SBO
s30	mTOR	

Modifiers

Table 78: Properties of each modifier.

Id	Name	SBO
s29	pAKT	
s30	mTOR	
s31	pmTOR	
s29	pAKT	

Product

Table 79: Properties of each product.

Id	Name	SBO
s31	pmTOR	

Kinetic Law

Derived unit mol²

$$v_{23} = k1 \cdot (s30 - s31) \cdot s29 \quad (103)$$

Table 80: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.420	dimensionless	<input checked="" type="checkbox"/>

8.24 Reaction re53

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

Reaction equation



Reactant

Table 81: Properties of each reactant.

Id	Name	SBO
s31	pmTOR	

Modifier

Table 82: Properties of each modifier.

Id	Name	SBO
s31	pmTOR	

Product

Table 83: Properties of each product.

Id	Name	SBO
s30	mTOR	

Kinetic Law

Derived unit mol

$$v_{24} = k1 \cdot s31 \quad (105)$$

Table 84: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.124	dimensionless	<input checked="" type="checkbox"/>

8.25 Reaction re54

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

Reaction equation



Reactant

Table 85: Properties of each reactant.

Id	Name	SBO
s32	S6K	

Modifiers

Table 86: Properties of each modifier.

Id	Name	SBO
s31	pmTOR	
s32	S6K	
s33	pS6K	
s31	pmTOR	

Product

Table 87: Properties of each product.

Id	Name	SBO
s33	pS6K	

Kinetic Law

Derived unit mol²

$$v_{25} = k1 \cdot (s32 - s33) \cdot s31 \quad (107)$$

Table 88: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.008	dimensionless	<input checked="" type="checkbox"/>

8.26 Reaction re55

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

Reaction equation



Reactant

Table 89: Properties of each reactant.

Id	Name	SBO
s33	pS6K	

Modifiers

Table 90: Properties of each modifier.

Id	Name	SBO
s35	pX	
s33	pS6K	
s35	pX	

Product

Table 91: Properties of each product.

Id	Name	SBO
s32	S6K	

Kinetic Law

Derived unit mol²

$$v_{26} = k1 \cdot s33 \cdot s35 \quad (109)$$

Table 92: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		1.955	dimensionless	<input checked="" type="checkbox"/>

8.27 Reaction re56

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

Reaction equation



Reactant

Table 93: Properties of each reactant.

Id	Name	SBO
s34	X	

Modifiers

Table 94: Properties of each modifier.

Id	Name	SBO
s31	pmTOR	
s34	X	
s35	pX	
s31	pmTOR	

Product

Table 95: Properties of each product.

Id	Name	SBO
s35	pX	

Kinetic Law**Derived unit** mol²

$$v_{27} = k1 \cdot (s34 - s35) \cdot s31 \quad (111)$$

Table 96: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.001	dimensionless	<input checked="" type="checkbox"/>

8.28 Reaction re57

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

Reaction equation**Reactant**

Table 97: Properties of each reactant.

Id	Name	SBO
s35	pX	

Modifier

Table 98: Properties of each modifier.

Id	Name	SBO
s35	pX	

Product

Table 99: Properties of each product.

Id	Name	SBO
s34	X	

Kinetic Law

Derived unit mol²

$$v_{28} = k1 \cdot s35 \quad (113)$$

Table 100: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.001	mol	<input checked="" type="checkbox"/>

8.29 Reaction re58

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

Reaction equation



Reactant

Table 101: Properties of each reactant.

Id	Name	SBO
s1	PFKL	

Modifiers

Table 102: Properties of each modifier.

Id	Name	SBO
s33	pS6K	
s1	PFKL	
s13	pPFKL	
s33	pS6K	

Product

Table 103: Properties of each product.

Id	Name	SBO
s13	pPFKL	

Kinetic Law

Derived unit mol²

$$v_{29} = k1 \cdot (s1 - s13) \cdot s33 \quad (115)$$

Table 104: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		26.832	dimensionless	<input checked="" type="checkbox"/>

8.30 Reaction re59

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

Reaction equation



Reactant

Table 105: Properties of each reactant.

Id	Name	SBO
s13	pPFKL	

Modifier

Table 106: Properties of each modifier.

Id	Name	SBO
s13	pPFKL	

Product

Table 107: Properties of each product.

Id	Name	SBO
s1	PFKL	

Kinetic Law

Derived unit mol

$$v_{30} = k1 \cdot s13 \quad (117)$$

Table 108: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.017	dimensionless	<input checked="" type="checkbox"/>

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 s1

Name PFKL

Initial amount 1.235570941

Charge 0

This species takes part in four reactions (as a reactant in [re58](#) and as a product in [re59](#) and as a modifier in [re30](#), [re58](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}s1 = 0 \quad (118)$$

9.2 Species s2

Name FB Pase

Initial amount 1 mol

Charge 0

This species takes part in one reaction (as a modifier in [re31](#)).

$$\frac{d}{dt}s_2 = 0 \quad (119)$$

9.3 Species s3

Name F6P

Initial amount 14.0774258421 mol

Charge 0

This species takes part in one reaction (as a reactant in [re39](#)).

$$\frac{d}{dt}s_3 = -v_{10} \quad (120)$$

9.4 Species s4

Name F1,6BP

Initial amount 104.07239819 mol

Charge 0

This species takes part in five reactions (as a reactant in [re31](#), [re32](#) and as a product in [re30](#) and as a modifier in [re31](#), [re32](#)).

$$\frac{d}{dt}s_4 = v_1 - v_2 - v_3 \quad (121)$$

9.5 Species s5

Name PEP

Initial amount 108.094519859 mol

Charge 0

This species takes part in three reactions (as a reactant in [re35](#) and as a modifier in [re30](#), [re30](#)).

$$\frac{d}{dt}s_5 = -v_6 \quad (122)$$

9.6 Species s_6

Name Isocitrate

Initial amount 1.79487179487 mol

Charge 0

This species takes part in three reactions (as a reactant in [re36](#) and as a modifier in [re30](#), [re30](#)).

$$\frac{d}{dt}s_6 = -v_7 \quad (123)$$

9.7 Species s_7

Name 2-oxoglutarate

Initial amount 25.1885369533 mol

Charge 0

This species takes part in three reactions (as a reactant in [re34](#) and as a modifier in [re30](#), [re30](#)).

$$\frac{d}{dt}s_7 = -v_5 \quad (124)$$

9.8 Species s_8

Name Malate

Initial amount 68.8788335846 mol

Charge 0

This species takes part in three reactions (as a reactant in [re33](#) and as a modifier in [re30](#), [re30](#)).

$$\frac{d}{dt}s_8 = -v_4 \quad (125)$$

9.9 Species s_9

Name F2,6BP

Initial amount 1 mol

Charge 0

This species takes part in five reactions (as a reactant in [re37](#) and as a modifier in [re30](#), [re30](#), [re31](#), [re31](#)).

$$\frac{d}{dt}s_9 = -v_8 \quad (126)$$

9.10 Species s10

Name Citrate

Initial amount 17.7476118652 mol

Charge 0

This species takes part in five reactions (as a reactant in [re38](#) and as a modifier in [re30](#), [re30](#), [re31](#), [re31](#)).

$$\frac{d}{dt}s_{10} = -v_9 \quad (127)$$

9.11 Species s11

Name sa4_degraded

SBO:0000291 empty set

Initial amount 0 mol

This species takes part in one reaction (as a product in [re32](#)).

$$\frac{d}{dt}s_{11} = v_3 \quad (128)$$

9.12 Species s12

Name ALDO

Initial amount 1 mol

Charge 0

This species takes part in one reaction (as a modifier in [re32](#)).

$$\frac{d}{dt}s_{12} = 0 \quad (129)$$

9.13 Species s13

Name pPFKL

Initial amount 0.759332005

Charge 0

This species takes part in six reactions (as a reactant in [re59](#) and as a product in [re58](#) and as a modifier in [re30](#), [re30](#), [re58](#), [re59](#)).

$$\frac{d}{dt}s_{13} = v_{29} - v_{30} \quad (130)$$

9.14 Species s14

Name sa8_degraded

SBO:0000291 empty set

Initial amount 0 mol

This species takes part in one reaction (as a product in [re33](#)).

$$\frac{d}{dt}s14 = v_4 \quad (131)$$

9.15 Species s15

Name sa7_degraded

SBO:0000291 empty set

Initial amount 0 mol

This species takes part in one reaction (as a product in [re34](#)).

$$\frac{d}{dt}s15 = v_5 \quad (132)$$

9.16 Species s16

Name sa5_degraded

SBO:0000291 empty set

Initial amount 0 mol

This species takes part in one reaction (as a product in [re35](#)).

$$\frac{d}{dt}s16 = v_6 \quad (133)$$

9.17 Species s17

Name sa6_degraded

SBO:0000291 empty set

Initial amount 0 mol

This species takes part in one reaction (as a product in [re36](#)).

$$\frac{d}{dt}s17 = v_7 \quad (134)$$

9.18 Species s18

Name sa9_degraded

SBO:0000291 empty set

Initial amount 0 mol

This species takes part in one reaction (as a product in [re37](#)).

$$\frac{d}{dt}s18 = v_8 \quad (135)$$

9.19 Species s21

Name sa3_degraded

SBO:0000291 empty set

Initial amount 0 mol

This species takes part in one reaction (as a product in [re39](#)).

$$\frac{d}{dt}s21 = v_{10} \quad (136)$$

9.20 Species s19

Name sa10_degraded

SBO:0000291 empty set

Initial amount 0 mol

This species takes part in one reaction (as a product in [re38](#)).

$$\frac{d}{dt}s19 = v_9 \quad (137)$$

9.21 Species s23

Name IR_complex

Initial amount 37.81914621 mol

Charge 0

This species takes part in seven reactions (as a reactant in [re41](#), [re42](#) and as a product in [re40](#), [re46](#) and as a modifier in [re40](#), [re41](#), [re42](#)).

$$\frac{d}{dt}s23 = v_{11} + v_{17} - v_{12} - v_{13} \quad (138)$$

9.22 Species s24

Name pro_IR_complex

Initial amount 46.2222520609226 mol

Charge 0

This species takes part in two reactions (as a reactant in [re40](#) and as a modifier in [re40](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}s_{24} = 0 \quad (139)$$

9.23 Species s25

Name p1IR_complex

Initial amount 2.507671281 mol

Charge 0

This species takes part in nine reactions (as a reactant in [re44](#), [re51](#) and as a product in [re41](#), [re45](#) and as a modifier in [re41](#), [re44](#), [re48](#), [re51](#)).

$$\frac{d}{dt}s_{25} = v_{12} + v_{16} - v_{15} - v_{22} \quad (140)$$

9.24 Species s26

Name p2IR_complex

Initial amount 852.608418 mol

Charge 0

This species takes part in seven reactions (as a reactant in [re43](#), [re46](#), [re50](#) and as a product in [re42](#) and as a modifier in [re43](#), [re46](#), [re50](#)).

$$\frac{d}{dt}s_{26} = v_{13} - v_{14} - v_{17} - v_{21} \quad (141)$$

9.25 Species s27

Name p1p2IRcomplex

Initial amount 3.930695895 mol

Charge 0

This species takes part in seven reactions (as a reactant in [re45](#), [re47](#) and as a product in [re43](#), [re44](#) and as a modifier in [re43](#), [re45](#), [re47](#)).

$$\frac{d}{dt}s_{27} = v_{14} + v_{15} - v_{16} - v_{18} \quad (142)$$

9.26 Species [s28](#)

Name AKT

Initial amount 4.33812187331668 mol

Charge 0

This species takes part in three reactions (as a reactant in [re48](#) and as a product in [re49](#) and as a modifier in [re48](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}s_{28} = 0 \quad (143)$$

9.27 Species [s29](#)

Name pAKT

Initial amount 0.012942682 mol

Charge 0

This species takes part in six reactions (as a reactant in [re49](#) and as a product in [re48](#) and as a modifier in [re48](#), [re49](#), [re52](#), [re52](#)).

$$\frac{d}{dt}s_{29} = v_{19} - v_{20} \quad (144)$$

9.28 Species [s30](#)

Name mTOR

Initial amount 0.0959163701057347 mol

Charge 0

This species takes part in three reactions (as a reactant in [re52](#) and as a product in [re53](#) and as a modifier in [re52](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}s_{30} = 0 \quad (145)$$

9.29 Species s31

Name pmTOR

Initial amount 0.004015031 mol

Charge 0

This species takes part in twelve reactions (as a reactant in [re53](#) and as a product in [re52](#) and as a modifier in [re42](#), [re42](#), [re44](#), [re44](#), [re52](#), [re53](#), [re54](#), [re54](#), [re56](#), [re56](#)).

$$\frac{d}{dt}s_{31} = v_{23} - v_{24} \quad (146)$$

9.30 Species s32

Name S6K

Initial amount 2.7769943784158 mol

Charge 0

This species takes part in three reactions (as a reactant in [re54](#) and as a product in [re55](#) and as a modifier in [re54](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}s_{32} = 0 \quad (147)$$

9.31 Species s33

Name pS6K

Initial amount $9.88831 \cdot 10^{-4}$ mol

Charge 0

This species takes part in six reactions (as a reactant in [re55](#) and as a product in [re54](#) and as a modifier in [re54](#), [re55](#), [re58](#), [re58](#)).

$$\frac{d}{dt}s_{33} = v_{25} - v_{26} \quad (148)$$

9.32 Species s34

Name X

Initial amount 14.9913345914433 mol

Charge 0

This species takes part in three reactions (as a reactant in [re56](#) and as a product in [re57](#) and as a modifier in [re56](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}s_{34} = 0 \quad (149)$$

9.33 Species [s35](#)

Name pX

Initial amount 0.043352951 mol

Charge 0

This species takes part in six reactions (as a reactant in [re57](#) and as a product in [re56](#) and as a modifier in [re55](#), [re55](#), [re56](#), [re57](#)).

$$\frac{d}{dt}s_{35} = v_{27} - v_{28} \quad (150)$$

9.34 Species [s36](#)

Name sa28_degraded

SBO:0000291 empty set

Initial amount 0 mol

This species takes part in one reaction (as a product in [re47](#)).

$$\frac{d}{dt}s_{36} = v_{18} \quad (151)$$

9.35 Species [s37](#)

Name sa27_degraded

SBO:0000291 empty set

Initial amount 0 mol

This species takes part in one reaction (as a product in [re50](#)).

$$\frac{d}{dt}s_{37} = v_{21} \quad (152)$$

9.36 Species s38

Name sa26_degraded

SBO:0000291 empty set

Initial amount 0 mol

This species takes part in one reaction (as a product in [re51](#)).

$$\frac{d}{dt}s38 = v_{22} \quad (153)$$

9.37 Species s22

Name F6P_proxy

Initial amount 14.0774258421

Charge 0

Involved in rule [s22](#)

This species takes part in three reactions (as a reactant in [re30](#) and as a product in [re31](#) and as a modifier in [re30](#)). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

A Glossary of Systems Biology Ontology Terms

SBO:0000291 empty set: Entity defined by the absence of any actual object. An empty set is often used to represent the source of a creation process or the result of a degradation process.

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