SBML Model Report

Model name: "Koo2013 - Integrated shear stress induced NO production model"



May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following three authors: Nick Juty¹, Vijayalakshmi Chelliah² and Andrew Koo³ at August 19th 2013 at 1:38 p. m. and last time modified at May 22nd 2014 at 5:39 p. m. Table 1 provides an overview of the quantities of all components of this model.

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

Element	Quantity	Element	Quantity
compartment types	0	compartments	4
species types	0	species	79
events	0	constraints	0
reactions	74	function definitions	0
global parameters	47	unit definitions	10
rules	0	initial assignments	0

2 Unit Definitions

This is an overview of ten unit definitions.

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2.1 Unit time

Name time

Definition s

2.2 Unit substance

Name substance

Definition 10^{-9} mol

2.3 Unit area

Name area

 $\textbf{Definition}\ m^2$

2.4 Unit length

Name length

Definition m

2.5 Unit volume

Name volume

Definition 1

2.6 Unit sub_sec

Name sub_sec

Definition $10^{-9} \text{ mol} \cdot \text{s}^{-1}$

2.7 Unit inv_sec

Name inv_sec

Definition s^{-1}

2.8 Unit inv_sec_sub

Name inv_sec_sub

Definition $(10^{-9} \text{ mol})^{-1} \cdot \text{s}^{-1}$

2.9 Unit nM_inv_s

Name nM_inv_s

Definition $nmol \cdot s^{-1}$

2.10 Unit inv_nM_s

Name inv_nM_s

Definition $nmol^{-1} \cdot s^{-1}$

3 Compartments

This model contains four compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial	Size	Unit	Constant	Outside
			Dimensions				
default			3	1	litre		
c1	Cell		3	1	litre	$ \overline{\mathbf{A}} $	default
c2	ER		3	1	litre		c1
c3	nucleus		3	1	litre	$ \overline{\mathbf{Z}} $	c1

3.1 Compartment default

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

3.2 Compartment c1

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

Name Cell

3.3 Compartment c2

This is a three dimensional compartment with a constant size of one litre, which is surrounded by c1 (Cell).

Name ER

3.4 Compartment c3

This is a three dimensional compartment with a constant size of one litre, which is surrounded by c1 (Cell).

Name nucleus

4 Species

This model contains 79 species. Section 7 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
s1	Ca_ex	default	10^{-9}mol	\Box	
s2	Ca_s	c2	$10^{-9} \mathrm{mol}$		\Box
s3	Ca_c	c1	$10^{-9} \mathrm{mol}$		\Box
s4	Ca_B	c1	10^{-9} mol	\Box	
s 5	s5	default	$10^{-9} \mathrm{mol}$		\Box
s6	IP3	c1	$10^{-9} \mathrm{mol}$		\Box
s7	s7	c1	10^{-9} mol		
s8	s8	c1	10^{-9}mol		
s9	s9	c1	10^{-9}mol		
s10	s10	c1	10^{-9} mol	\Box	
s11	s11	c1	10^{-9}mol		
s12	TimeT	c1	10^{-9}mol		\Box
s13	s13	c1	$10^{-9} \mathrm{mol}$		
s14	PDK1	c1	10^{-9} mol		
s15	PP2A	c1	10^{-9} mol	\Box	
s16	AKT	c1	10^{-9} mol	\Box	
s17	PI3P	c1	10^{-9} mol		
s18	PTEN	c1	10^{-9} mol	\Box	
s19	PIP2	c1	10^{-9} mol		
s20	p-PI3K	c1	$10^{-9} \mathrm{mol}$		
s21	s3	c1	$10^{-9} \mathrm{mol}$		
s22	PI3K	c1	10^{-9} mol		\Box

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
s23	Time	c1	10^{-9}mol	В	
s24	PDK2	c1	10^{-9}mol		
s25	PDK1_cyto	c1	$10^{-9} \mathrm{mol}$		
s26	p-AKT:PI3P	c1	$10^{-9} \mathrm{mol}$		\Box
s27	pp-AKT:PI3P	c1	10^{-9}mol		\Box
s28	AKT:PI3P	c1	$10^{-9} \mathrm{mol}$		
s 35	s35	c1	$10^{-9} \mathrm{mol}$		
s37	s37	c1	$10^{-9} \mathrm{mol}$		\Box
s38	pre_time	c1	$10^{-9} \mathrm{mol}$		\Box
s39	Time	c1	10^{-9}mol		\Box
s42	AP-1	c3	$10^{-9} \mathrm{mol}$		
s43	pp-JNKK	c1	$10^{-9} \mathrm{mol}$		\Box
s44	pp-JNK	c1	$10^{-9} \mathrm{mol}$		\Box
s45	eNOS-CaM-Ca4	c1	$10^{-9} \mathrm{mol}$		\Box
s47	CaM-Ca4	c1	10^{-9}mol		\Box
s48	CaM-Ca2	c1	10^{-9} mol		\Box
s49	KLF2	c1	10^{-9}mol		\Box
s 50	eNOS-CaM-Ca2	c1	10^{-9}mol		\Box
s51	eNOS-Cav-1	c1	$10^{-9} \mathrm{mol}$		\Box
s52	Calmodulin	c1	10^{-9}mol		\Box
s57	Hsp90	c1	$10^{-9} \mathrm{mol}$		\Box
s58	Hsp90-eNOS-CaM-Ca4	c1	$10^{-9} \mathrm{mol}$		\Box
s60	Hsp90-p-eNOS-CaM-Ca4	c1	10^{-9}mol		\Box
s61	Hsp90-eNOS-CaM-Ca2	c1	10^{-9}mol		\Box
s62	Hsp90-p-eNOS-CaM-Ca2	c1	10^{-9}mol		\Box
s63	L-Arg	c1	$10^{-9} \mathrm{mol}$		
s64	NO	c1	10^{-9}mol		

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
s65	Hsp90-p-eNOS	c1	10^{-9}mol		
s66	Hsp90-eNOS	c1	10^{-9}mol		\Box
s91	Shc	c1	10^{-9}mol		
s92	p-Src	c1	10^{-9}mol		
s93	p-FAK	c1	10^{-9}mol		
s94	Src	c1	10^{-9}mol		\Box
s95	FAK	c1	10^{-9}mol	\Box	
s96	JNKK	c1	10^{-9}mol	\Box	
s97	MEKK1	c1	10^{-9}mol	\Box	
s98	p-Shc	c1	10^{-9}mol	\Box	
s99	JNK	c1	10^{-9}mol	\Box	
s100	p-JNKK	c1	10^{-9}mol	\Box	
s101	p-MEKK1	c1	10^{-9}mol		
s102	Ras:GTP	c1	10^{-9}mol		
s103	Ras:GDP	c1	10^{-9}mol		
s104	p-JNK	c1	$10^{-9} \mathrm{mol}$		
s105	KLF2	c1	10^{-9}mol		
s106	eNOS	c1	10^{-9}mol		
s107	aAP-1	c3	10^{-9}mol		
s108	eNOS	c3	$10^{-9} \mathrm{mol}$		
s110	p-FAK:Shc	c1	10^{-9} mol		
s111	Grb2:Sos	c1	$10^{-9} \mathrm{mol}$		
s112	p-FAK:p-Shc	c1	10^{-9}mol		
s113	p-FAK:p-Shc:Grb2:Sos	c1	10^{-9}mol		
s114	p-Shc:Grb2:Sos	c1	10^{-9}mol	\Box	\Box
s115	eNOS	с3	10^{-9}mol		\Box
s116	sa49_degraded	c1	$10^{-9} \mathrm{mol}$		

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
s117	s117	c1	10^{-9}mol		
s118	s118	c1	10^{-9}mol		\Box
s119	Shear Stress	default	$10^{-9} \mathrm{mol}$		

5 Parameters

This model contains 47 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
$R_{-}T$	$R_{-}T$		44000.000	dimensionless	Ø
k1	k1		0.001	$10^{-9} \text{ mol} \cdot \text{s}^{-1}$	$\overline{\mathbf{Z}}$
k2	k2		2.000	s^{-1}	$\overline{\mathbf{Z}}$
k3	k3		6.640	s^{-1}	
k4	k4		5000.000	$10^{-9} \text{ mol} \cdot \text{s}^{-1}$	
k5	k5		10^{-10}	$(10^{-9} \text{ mol})^{-1} \cdot \text{s}^{-1}$	
k6	k6		0.100	$(10^{-9} \text{ mol})^{-1} \cdot \text{s}^{-1}$	
k7	k7		300.000	s^{-1}	$\overline{\mathbf{Z}}$
K1	K1		0.000	10^{-9} mol	$\overline{\mathbf{Z}}$
K2	K2		200.000	10^{-9} mol	$\overline{\mathbf{Z}}$
КЗ	K3		150.000	10^{-9} mol	$\overline{\mathbf{Z}}$
K4	K4		80.000	10^{-9} mol	$\overline{\mathbf{Z}}$
K5	K5		321.000	10^{-9} mol	$ \overline{\mathcal{L}} $
K_{-} hi	K_hi		380.000	10^{-9} mol	\overline{Z}
k_CICR	k_CICR		1.000	dimensionless	
$K_{-}CICR$	K_CICR		0.000	10^{-9} mol	
$k_{-}CCE$	k_CCE		0.000	$(10^{-9} \text{ mol})^{-1} \cdot \text{s}^{-1}$	$ \overline{\mathcal{L}} $
$B_{-}T$	$B_{-}T$		120000.000	10^{-9} mol	
Vc_Vs	$Vc_{-}Vs$		3.500	dimensionless	
$\mathtt{dot}_\mathtt{Vp}$	$dot_{-}Vp$		1630.000	$10^{-9} \text{ mol} \cdot \text{s}^{-1}$	
dot_Vex	dot_Vex		18330.000	$10^{-9} \text{ mol} \cdot \text{s}^{-1}$	
$\mathtt{dot}_{\mathtt{-}}\mathtt{Vhi}$	dot_Vhi		4760.000	$10^{-9} \text{ mol} \cdot \text{s}^{-1}$	
$\mathtt{dot}_\mathtt{q}_\mathtt{inpass}$	dot_q_inpass		6000.000	$10^{-9} \text{ mol} \cdot \text{s}^{-1}$	
$\mathtt{dot}_\mathtt{q}_\mathtt{instim}$	dot_q_instim		2500.000	$10^{-9} \text{ mol} \cdot \text{s}^{-1}$	
Cao	Cao		100.000	10^{-9} mol	
$tau_{-}I$	tau_I		33.000	10^{-9} mol	
$tau_{-}II$	tau_II		0.005	10^{-9} mol	
half	half		0.500	dimensionless	
fracK	fracK		7071067.810	10^{-9} mol	
alp	alp		10.000	S	
gam	gam		0.100	S	
k8	k8		$7.5 \cdot 10^{-5}$	S	
k11	k11		0.004	$(10^{-9} \text{ mol})^{-1} \cdot \text{s}^{-1}$	
k12	k12		10.300	s^{-1}	$\overline{\mathbf{Z}}$
k13	k13		0.080	$(10^{-9} \text{ mol})^{-1} \cdot \text{s}^{-1}$	\mathbf{Z}
k14	k14		1152.000	s^{-1}	\mathbf{Z}

Id	Name	SBO	Value	Unit	Constant
k15	k15		0.015	$(10^{-9} \text{ mol})^{-1} \cdot \text{s}^{-1}$	
k16	k16		0.000	s^{-1}	$\overline{\mathbf{Z}}$
k17	k17		$1.5\cdot10^{-4}$	$(10^{-9} \text{ mol})^{-1} \cdot \text{s}^{-1}$	
k18	k18		1.500		$\overline{\mathbf{Z}}$
kp	kp		0.100		
Kmp	Kmp		5.000	10^{-9} mol	
Kmdp	Kmdp		20.000	10^{-9} mol	
Vdp	Vdp		4.000	$10^{-9} \text{ mol} \cdot \text{s}^{-1}$	
k90	k90		0.002	$(10^{-9} \text{ mol})^{-1} \cdot \text{s}^{-1}$	
kr90	kr90		1.500	s^{-1}	$\overline{\mathbf{Z}}$
kDD	kDD		$9.45 \cdot 10^{-5}$	s^{-1}	$ \overline{\mathbf{Z}} $

6 Reactions

This model contains 74 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

1 re3 re1 s4 $\frac{s3}{s+4}$ s3 2 re4 s5 $\frac{s1}{s+2}$ s1, s2 3 re5 s7 $\frac{s3}{s+12}$, s119, s12, s3 s6 4 re6 s6 $\frac{s6}{s}$ s8 5 re7 s2 $\frac{s6}{s+3}$, s6, s2 s3 6 re8 s3 $\frac{s3}{s}$ s9 7 re9 s3 $\frac{s3}{s+10}$ s10 8 re10 s11 \rightarrow s3 9 re11 s13 \rightarrow s12 10 re12 s3 $\frac{s3}{s}$ s9 11 re37 s51 $+$ s47 $\frac{s47}{s+7}$, s51 $+$ s45 12 re38 s48 $+$ s51 $\frac{s51}{s+3}$, s48, s50 $+$ s50 13 re41 s48 $\frac{s3}{s3}$, s3, s48, s47 $+$ s47 14 re42 s48 $\frac{s3}{s3}$, s45, s3, s50 $+$ s50 15 re50 s45 $\frac{s3}{s45}$, s3, s50 $+$ s50 16 re51 s45 $\frac{s3}{s45}$, s57 $\frac{s45}{s57}$, s58	N₀	Id	Name	Reaction Equation	SBO
3 re5 $s7 \frac{s3, s12, s119, s12, s3}{s6}$ s6 $\frac{s6}{5} s8$ 5 re7 $s2 \frac{s6, s3, s6, s2}{s3} s3$ s9 $s3 \frac{s3}{5} s9$ 8 re10 $s11 \longrightarrow s3$ 811 $\longrightarrow s3$ 9 re11 $s13 \longrightarrow s12$ 10 re12 $s3 \frac{s3}{5} s9$ 11 re37 $s51 + s47 \frac{s47, s51}{s51, s48, s50} s50$ 12 re38 $s48 + s51 \stackrel{\textstyle \smile}{\smile} \frac{s3, s3, s52, s48}{s48} s48$ 13 re41 $s47 = s47 = s45 = s45 = s45 = s47 = s45 =$	1	re3	re1	$s4 \xrightarrow{s3, s4} s3$	
4 re6 s6 $\frac{s6}{>}$ s8 5 re7 s2 $\frac{s6}{>}$ s3, s6, s2 s3 6 re8 s3 $\frac{s3}{>}$ s9 7 re9 s3 $\frac{s3}{>}$ s10 8 re10 s11 \rightarrow s3 9 re11 s13 \rightarrow s12 10 re12 s3 $\frac{s3}{>}$ s9 11 re37 s51 + s47 $\frac{s47}{>}$ s51 s48, s50 s50 12 re38 s48 + s51 $\frac{s51}{>}$ s48, s48 s48 s48 13 re41 s52 $\frac{s3}{>}$ s3, s3, s48, s47 s47 14 re42 s48 $\frac{s3}{>}$ s3, s3, s48, s37 s47 15 re50 s45 $\frac{s3}{>}$ s57 s50	2	re4		$s5 \xrightarrow{s1, s2, s1} s2$	
5 re7 s2 $\frac{s6, s3, s6, s2}{s3}$ s3 s3 s3 s9 7 re9 s3 $\frac{s3}{s3}$ s10 s11 \rightarrow s3 s12 s13 \rightarrow s12 s10 re11 s13 \rightarrow s12 s10 re12 s2	3	re5		$s7 \xrightarrow{s3, s12, s119, s12, s3} s6$	
6 re8 6 re8 7 re9 8 $3\frac{s3}{s} s9$ 8 re10 9 re11 10 re12 11 re37 12 re38 13 re41 14 re42 15 re50 8 $3\frac{s3}{s} s9$ 17 $3\frac{s3}{s} s9$ 18 so $3\frac{s3}{s} s9$ 19 so $3\frac{s3}{s} s9$ 10 $3\frac{s3}{s} s9$ 10 $3\frac{s3}{s} s9$ 11 re37 12 re38 13 $3\frac{s3}{s} s9$ 14 so $3\frac{s3}{s} s9$ 15 so $3\frac{s3}{s} s9$ 16 so $3\frac{s3}{s} s9$ 17 so $3\frac{s3}{s} s9$ 18 so $3\frac{s3}{s} s9$ 19 so $3\frac{s3}{s} s9$ 10 so $3\frac{s3}{s} s9$ 10 so $3\frac{s3}{s} s9$ 11 re37 12 re38 13 $3\frac{s3}{s} s9$ 14 so $3\frac{s3}{s} s9$ 15 so $3\frac{s3}{s} s9$ 16 so $3\frac{s3}{s} s9$ 17 so $3\frac{s3}{s} s9$ 18 so $3\frac{s3}{s} s9$ 19 so $3\frac{s3}{s} s9$ 10 re12 11 so $3\frac{s3}{s} s9$ 12 re38 13 $3\frac{s3}{s} s9$ 14 so $3\frac{s3}{s} s9$ 15 so $3\frac{s3}{s} s9$ 16 so $3\frac{s3}{s} s9$ 17 so $3\frac{s3}{s} s9$ 18 so $3\frac{s3}{s} s9$ 19 so $3\frac{s3}{s} s9$ 10 so $3\frac{s3}{s} s9$ 10 so $3\frac{s3}{s} s9$ 11 so $3\frac{s3}{s} s9$ 12 so $3\frac{s3}{s} s9$ 13 so $3\frac{s3}{s} s9$ 14 so $3\frac{s3}{s} s9$ 15 so $3\frac{s3}{s} s9$ 16 so $3\frac{s3}{s} s9$ 17 so $3\frac{s3}{s} s9$ 18 so $3\frac{s3}{s} s9$ 19 so $3\frac{s3}{s} s9$ 10 so $3\frac{s3}{s} s9$ 10 so $3\frac{s3}{s} s9$ 11 so $3\frac{s3}{s} s9$ 12 so $3\frac{s3}{s} s9$ 13 so $3\frac{s3}{s} s9$ 14 so $3\frac{s3}{s} s9$ 15 so $3\frac{s3}{s} s9$ 16 so $3\frac{s3}{s} s9$ 17 so $3\frac{s3}{s} s9$ 18 so $3\frac{s3}{s} s9$ 19 so $3\frac{s3}{s} s9$ 10 so $3\frac{s3}{s} s9$ 10 so $3\frac{s3}{s} s9$ 11 so $3\frac{s3}{s} s9$ 12 so $3\frac{s3}{s} s9$ 13 so $3\frac{s3}{s} s9$ 14 so $3\frac{s3}{s} s9$ 15 so $3\frac{s3}{s} s9$ 16 so $3\frac{s3}{s} s9$ 17 so $3\frac{s3}{s} s9$ 18 so $3\frac{s3}{s} s9$ 19 so $3\frac{s3}{s} s9$ 10 so $3\frac{s3}{s} s9$ 10 so $3\frac{s3}{s} s9$ 11 so $3\frac{s3}{s} s9$ 12 so $3\frac{s3}{s} s9$ 13 so $3\frac{s3}{s} s9$ 14 so $3\frac{s3}{s} s9$ 15 so $3\frac{s3}{s} s9$ 16 so $3\frac{s3}{s} s9$ 17 so $3\frac{s3}{s} s9$ 18 so $3\frac{s3}{s} s9$ 19 so $3\frac{s3}{s} s9$ 19 so $3\frac{s3}{s} s9$ 10 so $3\frac{s3}{s} s9$ 10 so $3\frac{s3}{s} s9$ 11 so $3\frac{s3}{s} s9$ 12 so $3\frac{s3}{s} s9$ 13 so $3\frac{s3}{s} s9$ 14 so $3\frac{s3}{s} s9$ 15 so $3\frac{s3}{s} s9$ 16 so $3\frac{s3}{s} s9$ 17 so $3\frac{s3}{s} s9$	4	re6		$s6 \xrightarrow{s6} s8$	
7 re9 8 re10 8 re10 9 re11 10 re12 11 re37 12 re38 13 re41 14 re42 15 re50 8 s $\frac{33}{5} \times 310$ 8 s $\frac{31}{5} \times 310$ 8 s $\frac{31}{5} \times 312$ 8 s $\frac{31}{5} \times $	5	re7		$s2 \xrightarrow{s6, s3, s6, s2} s3$	
8 re10 $s11 \longrightarrow s3$ 9 re11 $s13 \longrightarrow s12$ 10 re12 $s3 \xrightarrow{s3} s9$ 11 re37 $s51 + s47 \xrightarrow{s47, s51} s45$ 12 re38 $s48 + s51 \xrightarrow{s51, s48, s50} s50$ 13 re41 $s52 \xrightarrow{s3, s3, s52, s48} s48$ 14 re42 $s48 \xrightarrow{s3, s3, s48, s47} s47$ 15 re50 $s45 \xrightarrow{s3, s45, s3, s50} s50$	6	re8		$s3 \xrightarrow{s3} s9$	
9 re11 10 re12 11 re37 12 re38 13 re41 14 re42 15 re50 18 $\frac{s3}{s3} s9$ 19 $\frac{s3}{s3} s9$ 10 $\frac{s51 + s47}{s47} \frac{s47}{s45} s45$ 10 $\frac{s51}{s48} \frac{s50}{s52} s50$ 10 $\frac{s3}{s3} \frac{s3}{s52} \frac{s48}{s48} s48$ 11 $\frac{s3}{s3} \frac{s3}{s3} \frac{s52}{s45} \frac{s48}{s48} s48$ 12 $\frac{s3}{s3} \frac{s3}{s45} \frac{s48}{s3} \frac{s48}{s47} s47$ 15 re50 18 $\frac{s3}{s45} \frac{s3}{s57} s50$	7	re9		$s3 \xrightarrow{s3} s10$	
10 re12 $s3 \xrightarrow{s3} s9$ 11 re37 $s51 + s47 \xrightarrow{s47, s51} s45$ 12 re38 $s48 + s51 \xrightarrow{s51, s48, s50} s50$ 13 re41 $s52 \xrightarrow{s3, s3, s52, s48} s48$ 14 re42 $s48 \xrightarrow{s3, s3, s48, s47} s47$ 15 re50 $s45 \xrightarrow{s3, s45, s3, s50} s50$	8	re10		$s11 \longrightarrow s3$	
11 re37 12 re38 13 re41 14 re42 15 re50 $s51 + s47 \xrightarrow{s47, s51} s45$ $s48 + s51 \xrightarrow{s51, s48, s50} s50$ $s52 \xrightarrow{s3, s3, s52, s48} s48$ $s48 \xrightarrow{s3, s3, s48, s47} s47$ $s45 \xrightarrow{s3, s45, s3, s50} s50$	9	re11		$s13 \longrightarrow s12$	
12 re38 13 re41 14 re42 15 re50 $s48 + s51 \xrightarrow{s51, s48, s50} s50$ $s52 \xrightarrow{s3, s3, s52, s48} s48$ $s48 \xrightarrow{s3, s3, s48, s47} s47$ $s45 \xrightarrow{s3, s45, s3, s50} s50$	10	re12		$s3 \xrightarrow{s3} s9$	
13 re41 14 re42 15 re50 $s52 \xrightarrow{83, 83, 852, 848} s48$ $s48 \xrightarrow{83, 83, 848, 847} s47$ $s45 \xrightarrow{83, 845, 83, 850} s50$	11	re37		$s51 + s47 \xrightarrow{s47, s51} s45$	
14 re42 15 re50 $s48 \xrightarrow{s3, s3, s48, s47} s47$ $s45 \xrightarrow{s3, s45, s3, s50} s50$	12	re38		$s48 + s51 \xrightarrow{s51, s48, s50} s50$	
14 re42 $s48 \xrightarrow{s3, s3, s48, s47} s47$ 15 re50 $s45 \xrightarrow{s3, s45, s3, s50} s50$	13	re41		$s52 = \frac{s3, s3, s52, s48}{s48}$	
15 re50 $s45 \stackrel{\text{s3, s45, s3, s50}}{\underset{\text{s45, s57}}{}} s50$				·	
s45_s57	15			$s45 \stackrel{\text{s3, s45, s3, s50}}{\rightleftharpoons} s50$	
				$s45 + s57 \xrightarrow{s45, s57} s58$	

12	Nº	Id	Name	Reaction Equation S	ВВО
	17	re52		$s58 \xrightarrow{s3, s58, s3, s61} s61$	
	18	re53		$s61 \xrightarrow{s61} s50 + s57$	
	19	re54		$s60 \stackrel{\text{s3, s60, s3, s62}}{\longleftarrow} s62$	
	20	re55		$s58 \stackrel{\text{s27, s58, s27, s60}}{\longleftarrow} s60$	
	21	re56		$s61 \stackrel{\text{s27, s61, s27, s62}}{\longleftarrow} s62$	
	22	re57		$s22 \stackrel{\text{$23, $119, $23}}{\smile} s20$	
P	23	re58		$s19 \xrightarrow{s20, s19, s20} s17$	
rodu	24	re59		$s17 \xrightarrow{s18, s17, s18} s19$	
Produced by SBML218TEX	25	re60		$s17 + s16 = \frac{s17, s16, s28}{s28}$	
5 <i>y</i> S E	26	re61		$s28 \xrightarrow{s14, s28, s14} s26$	
SAINS	27	re62		$s26 \xrightarrow{s24, s26, s24} s27$	
ěTĘ>	28	re63		$s26 \xrightarrow{s15, s26, s15} s28$	
	29	re64		$s27 \xrightarrow{s15, s27, s15} s26$	
	30	re65		$s27 \xrightarrow{s15, s27, s15} s17 + s16$	
	31	re66		$s25 \xrightarrow{s17, s17, s25} s14$	
		re67		$s14 \xrightarrow{s14} s25$	
		re68		$s21 \longrightarrow s23$ s45 $s50$ $s61$ $s62$ $s58$ $s60$ $s65$ $s45$ $s58$ $s62$ $s65$	s60
	34	re69		s63 s45, s50, s61, s62, s58, s60, s65, s45, s58, s62, s65	\longrightarrow s64
	35	re70		$s65 \xrightarrow{s65} s66$	
	36	re71		$s66 \xrightarrow{s66} s51 + s57$	

N⁰	Id	Name	Reaction Equation	SBO
37	re72		$s62 \xrightarrow{s62, s65, s48} s65 + s48$	
38	re102		$s95 \stackrel{\underline{s39, s119, s39}}{\underbrace{\longrightarrow}} s93$	
39	re103		$s94 \xrightarrow{s39, s119, s39} s92$	
40	re104		$s91 + s93 \xrightarrow{s91, s93, s110} s110$	
41	re105		$s110 \stackrel{\text{s92, s110, s92, s112}}{\rightleftharpoons} s112$	
42	re106		$s112 + s111 \xrightarrow{s111, s112, s113} s113$	
43	re107		$s113 \xrightarrow{s113, s93, s114} s114 + s93$	
44	re108		$s98 \xrightarrow{s98} s91$	
45	re109		$s114 \xrightarrow{s114} s98 + s111$	
46	re110		$s115 \xrightarrow{s115} s106$	
47	re111		$s108 \xrightarrow{s107, s49, s107, s49} s115$	
48	re112		$s103 \xrightarrow{s114, s114, s103} s102$	
49	re113		$s102 \xrightarrow{s102} s103$	
50	re114		$s97 \xrightarrow{s102, s102, s97} s101$	
51	re115		$s101 \xrightarrow{s101} s97$	
52	re116		$s96 \xrightarrow{s101, s101, s96} s100$	
53	re117		$s100 \xrightarrow{s100} s96$ $s43 \xrightarrow{s99} s43$	
54	re118		$s99 \xrightarrow{s43, s99, s43} s104$	
55	re119		$s104 \xrightarrow{s104} s99$	
56	re120		$s106 \xrightarrow{s106} s35$	

14	Nº Id	Name	Reaction Equation SI	ВО
	57 re1	.21	$s37 \xrightarrow{s106, s106} s51$	
	58 re1	122	$s38 \longrightarrow s39$	
	59 re1	1.23	$s43 \xrightarrow{s43} s100$	
	60 re1	.24	$s100 \xrightarrow{s101, s100, s101} s43$	
	61 re1	.25	$s44 \xrightarrow{s44} s104$	
	62 re1	126	$s104 \xrightarrow{s43, s104, s43} s44$	
	63 re1	1.27	$s42 \xrightarrow{s44, s44, s42} s107$	
Pro	64 re1	1.28	$s107 \xrightarrow{s107} s42$	
duce	65 re1	.29	$s105 \xrightarrow{s39, s39} s49$	
ig p	66 re1	131	$s51 \xrightarrow{s51} s116$	
Produced by SBML214TEX	67 re1	.32	$s45 \xrightarrow{s45} s117 + s47$	
	68 re1	133	$s50 \xrightarrow{s50} s117 + s48$	
ATEX	69 re1	.34	$s66 \xrightarrow{s66} s57 + s118$	
	70 re1	.35	$s65 \xrightarrow{s65} s118 + s57$	
	71 re1	136	$s61 \xrightarrow{s61} s57 + s48$	
	72 re1	137	$s62 \xrightarrow{s62} s57 + s48$	
	73 re1	1.38	$s58 \xrightarrow{s58} s57 + s47$	
	74 re1	.39	$s60 \xrightarrow{s60} s57 + s47$	

6.1 Reaction re3

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

Name re1

Reaction equation

$$s4 \xrightarrow{s3, s4} s3 \tag{1}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
s4	Ca_B	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
	Ca_c	
84	Ca_B	

Product

Table 8: Properties of each product.

Id	Name	SBO
s3	Ca_c	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_1 = k6 \cdot s3 \cdot (B_T - s4) + k7 \cdot s4$$
 (2)

6.2 Reaction re4

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

Reaction equation

$$s5 \xrightarrow{s1, s2, s1} s2 \tag{3}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
s5	s5	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
s1	Ca_ex	
s2	Ca_s	
s1	Ca_ex	

Product

Table 11: Properties of each product.

Id	Name	SBO
s2	Ca_s	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9}$ mol

$$v_2 = k \text{-CCE} \cdot \left(\frac{\text{fracK} \cdot \text{Cao}}{\text{K3} + \text{Cao}} - \text{s2}\right) \cdot (\text{s1} - \text{s2})$$
 (4)

6.3 Reaction re5

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

Reaction equation

$$s7 \xrightarrow{s3, s12, s119, s12, s3} s6$$
 (5)

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
s7	s7	

Modifiers

Table 13: Properties of each modifier.

Id	Name	SBO
s3	Ca_c	
s12	TimeT	
s119	Shear Stress	
s12	TimeT	
s3	Ca_c	

Product

Table 14: Properties of each product.

Id	Name	SBO
s6	IP3	

Kinetic Law

Derived unit contains undeclared units

$$= \frac{0.5 \cdot k1 \cdot \left(R_T - half \cdot R_T \cdot \left(exp\left(\frac{s12}{tau_I}\right) + exp\left(\frac{s12}{tau_II}\right) + \frac{\left(exp\left(\frac{s12}{tau_I}\right) - exp\left(\frac{s12}{tau_II}\right)\right) \cdot (tau_I + tau_II)}{tau_I - tau_II}\right)\right) \cdot s3}{K1 + s3}$$

6.4 Reaction re6

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

Reaction equation

$$s6 \xrightarrow{s6} s8$$
 (7)

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
s6	IP3	

Modifier

Table 16: Properties of each modifier.

Id	Name	SBO
s6	IP3	

Product

Table 17: Properties of each product.

Id	Name	SBO
s8	s8	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = 0.5 \cdot k2 \cdot s6 \tag{8}$$

6.5 Reaction re7

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

Reaction equation

$$s2 \xrightarrow{s6, s3, s6, s2} s3$$
 (9)

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
s2	Ca_s	

Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
s6	IP3	
s3	Ca_c	
s6	IP3	
s2	Ca_s	

Product

Table 20: Properties of each product.

Id	Name	SBO
s3	Ca_c	

Kinetic Law

Derived unit contains undeclared units

$$v_{5} = 0.5 \cdot k3 \cdot \frac{\text{k_CICR} \cdot \text{s3}}{\text{K_CICR} + \text{s3}} \cdot \left(\frac{\text{s6}}{\text{K2} + \text{s6}}\right)^{3} \cdot \text{s2} - 0.5 \cdot k4 \cdot \left(\frac{\text{s3}}{\text{K3} + \text{s3}}\right)^{2} + 0.5 \cdot k5 \cdot \text{s2} \cdot \text{s2} \quad (10)$$

6.6 Reaction re8

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

Reaction equation

$$s3 \xrightarrow{s3} s9$$
 (11)

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
s3	Ca_c	

Table 22: Properties of each modifier.

Id	Name	SBO
s3	Ca_c	

Table 23: Properties of each product.

Id	Name	SBO
s 9	s9	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \frac{0.5 \cdot \text{dot_Vhi} \cdot \text{s3}^4}{\text{K.hi}^4 + \text{s3}^4}$$
 (12)

6.7 Reaction re9

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

Reaction equation

$$s3 \xrightarrow{s3} s10$$
 (13)

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
s3	Ca_c	

Table 25: Properties of each modifier.

Id	Name	SBO
s3	Ca_c	

Table 26: Properties of each product.

Id	Name	SBO
s10	s10	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \frac{0.5 \cdot \text{dot_Vex} \cdot \text{s3}}{\text{K5} + \text{s3}} \tag{14}$$

6.8 Reaction re10

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

Reaction equation

$$s11 \longrightarrow s3$$
 (15)

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
s11	s11	

Product

Table 28: Properties of each product.

Id	Name	SBO
s3	Ca_c	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = 0.5 \cdot \text{dot_q_inpass}$$
 (16)

6.9 Reaction re11

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

Reaction equation

$$s13 \longrightarrow s12$$
 (17)

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
s13	s13	

Product

Table 30: Properties of each product.

Id	Name	SBO
s12	TimeT	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{unisec} \cdot 0.5$$
 (18)

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
unisec			1.0	$10^{-9}~\text{mol}\cdot\text{s}^{-1}$	

6.10 Reaction re12

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

Reaction equation

$$s3 \xrightarrow{s3} s9$$
 (19)

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
s3	Ca_c	

Modifier

Table 33: Properties of each modifier.

Id	Name	SBO
s3	Ca_c	

Product

Table 34: Properties of each product.

Id	Name	SBO
s9	s9	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \frac{0.5 \cdot \text{dot} \cdot \text{Vp} \cdot \text{s}3^2}{\text{K}4^2 + \text{s}3^2}$$
 (20)

6.11 Reaction re37

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

Reaction equation

$$s51 + s47 \xrightarrow{s47, s51} s45$$
 (21)

Reactants

Table 35: Properties of each reactant.

Id	Name	SBO
s51	eNOS-Cav-1	
s47	CaM-Ca4	

Modifiers

Table 36: Properties of each modifier.

Id	Name	SBO
s47	CaM-Ca4	
s51	eNOS-Cav-1	

Product

Table 37: Properties of each product.

Id	Name	SBO
s45	eNOS-CaM-Ca4	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9}$ mol

$$v_{11} = k15 \cdot s47 \cdot s51 \tag{22}$$

6.12 Reaction re38

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

Reaction equation

$$s48 + s51 \xrightarrow{s51, s48, s50} s50$$
 (23)

Reactants

Table 38: Properties of each reactant.

Id	Name	SBO
s48	CaM-Ca2	
s51	eNOS-Cav-1	

Modifiers

Table 39: Properties of each modifier.

Id	Name	SBO
s51	eNOS-Cav-1	
s48	CaM-Ca2	
s50	eNOS-CaM-Ca2	

Product

Table 40: Properties of each product.

Id	Name	SBO
s50	eNOS-CaM-Ca2	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{12} = k17 \cdot s51 \cdot s48 - k18 \cdot s50 \tag{24}$$

6.13 Reaction re41

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

Reaction equation

$$s52 = \frac{s3, s3, s52, s48}{s48}$$
 s48 (25)

Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
s52	Calmodulin	

Table 42: Properties of each modifier.

Id	Name	SBO
s3	Ca_c	
s3	Ca_c	
s52	Calmodulin	
s48	CaM-Ca2	

Table 43: Properties of each product.

Id	Name	SBO
s48	CaM-Ca2	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{13} = k11 \cdot s3 \cdot s52 - k12 \cdot s48 \tag{26}$$

6.14 Reaction re42

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

Reaction equation

$$s48 \xrightarrow{s3, s3, s48, s47} s47$$
 (27)

Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
s48	CaM-Ca2	

Table 45: Properties of each modifier.

Id	Name	SBO
s3	Ca_c	
s3	Ca_c	
s48	CaM-Ca2	
s47	CaM-Ca4	

Table 46: Properties of each product.

Id	Name	SBO
s47	CaM-Ca4	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{14} = k13 \cdot s3 \cdot s48 - k14 \cdot s47 \tag{28}$$

6.15 Reaction re50

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

Reaction equation

$$s45 \rightleftharpoons s3, s45, s3, s50$$
 (29)

Reactant

Table 47: Properties of each reactant.

Id	Name	SBO
s45	eNOS-CaM-Ca4	

Table 48: Properties of each modifier.

Id	Name	SBO
s3	Ca_c	
s45	eNOS-CaM-Ca4	
s3	Ca_c	
s50	eNOS-CaM-Ca2	

Table 49: Properties of each product.

Id	Name	SBO
s50	eNOS-CaM-Ca2	

Kinetic Law

Derived unit 10^{-9} mol

$$v_{15} = \operatorname{gam} \cdot k14 \cdot s45 - k13 \cdot s3 \cdot s50 \tag{30}$$

6.16 Reaction re51

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

Reaction equation

$$s45 + s57 \xrightarrow{s45, s57} s58$$
 (31)

Reactants

Table 50: Properties of each reactant.

Id	Name	SBO
s45	eNOS-CaM-Ca4	
s 57	Hsp90	

Table 51: Properties of each modifier.

Id	Name	SBO
s45	eNOS-CaM-Ca4	
s57	Hsp90	

Table 52: Properties of each product.

Id	Name	SBO
s58	Hsp90-eNOS-CaM-Ca4	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{16} = k90 \cdot s45 \cdot s57 \tag{32}$$

6.17 Reaction re52

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

Reaction equation

$$s58 = \frac{s3, s58, s3, s61}{s58} s61$$
 (33)

Reactant

Table 53: Properties of each reactant.

Id	Name	SBO
s58	Hsp90-eNOS-CaM-Ca4	

Table 54: Properties of each modifier.

Id	Name	SBO
s3	Ca_c	
s58	Hsp90-eNOS-CaM-Ca4	

Id	Name	SBO
s3	Ca_c	
s61	Hsp90-eNOS-CaM-Ca2	

Table 55: Properties of each product.

Id	Name	SBO
s61	Hsp90-eNOS-CaM-Ca2	

Kinetic Law

Derived unit 10^{-9} mol

$$v_{17} = \operatorname{gam} \cdot k14 \cdot s58 - k13 \cdot s3 \cdot s61 \tag{34}$$

6.18 Reaction re53

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

Reaction equation

$$s61 \xrightarrow{s61} s50 + s57$$
 (35)

Reactant

Table 56: Properties of each reactant.

Id	Name	SBO
s61	Hsp90-eNOS-CaM-Ca2	

Modifier

Table 57: Properties of each modifier.

Id	Name	SBO
s61	Hsp90-eNOS-CaM-Ca2	

Table 58: Properties of each product.

Id	Name	SBO
s50	01100 00111 002	
ສ57	Hsp90	

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{18} = \text{kr}90 \cdot \text{s}61 \tag{36}$$

6.19 Reaction re54

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

Reaction equation

$$s60 \xrightarrow{\underline{s3, s60, s3, s62}} s62 \tag{37}$$

Reactant

Table 59: Properties of each reactant.

Id	Name	SBO
s60	Hsp90-p-eNOS-CaM-Ca4	

Modifiers

Table 60: Properties of each modifier.

	1	
Id	Name	SBO
s3	Ca_c	
s60	Hsp90-p-eNOS-CaM-Ca4	
s3	Ca_c	
s62	Hsp90-p-eNOS-CaM-Ca2	

Table 61: Properties of each product.

	Name	SBO
s62	Hsp90-p-eNOS-CaM-Ca2	

Derived unit 10^{-9} mol

$$v_{19} = \operatorname{gam} \cdot k14 \cdot s60 - k13 \cdot s3 \cdot s62 \tag{38}$$

6.20 Reaction re55

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

Reaction equation

$$s58 \xrightarrow{s27, s58, s27, s60} s60$$
 (39)

Reactant

Table 62: Properties of each reactant.

Id	Name	SBO
s58	Hsp90-eNOS-CaM-Ca4	

Modifiers

Table 63: Properties of each modifier.

Id	Name	SBO
s27	pp-AKT:PI3P	
s58	Hsp90-eNOS-CaM-Ca4	
s27	pp-AKT:PI3P	
s60	Hsp90-p-eNOS-CaM-Ca4	

Table 64: Properties of each product.

Id	Name	SBO
s60	Hsp90-p-eNOS-CaM-Ca4	

 $\textbf{Derived unit} \ \ s^{-1} \cdot 9.9999999999998 \cdot 10^{-10} \ mol$

$$v_{20} = \frac{kp \cdot s58 \cdot s27}{s58 + Kmp} - \frac{Vdp \cdot s60}{s60 + Kmdp}$$
 (40)

6.21 Reaction re56

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

Reaction equation

$$s61 \xrightarrow{\text{s27, s61, s27, s62}} s62 \tag{41}$$

Reactant

Table 65: Properties of each reactant.

1401	• oc. rropermes or emem rem	
Id	Name	SBO
s61	Hsp90-eNOS-CaM-Ca2	

Modifiers

Table 66: Properties of each modifier.

Id	Name	SBO
s27	pp-AKT:PI3P	
s61	Hsp90-eNOS-CaM-Ca2	
s27	pp-AKT:PI3P	
s62	Hsp90-p-eNOS-CaM-Ca2	

Table 67: Properties of each product.

Id	Name	SBO
s62	Hsp90-p-eNOS-CaM-Ca2	

 $\textbf{Derived unit} \ \ s^{-1} \cdot 9.9999999999998 \cdot 10^{-10} \ mol$

$$v_{21} = \frac{\text{kp} \cdot \text{s61} \cdot \text{s27}}{\text{s61} + \text{Kmp}} - \frac{\text{Vdp} \cdot \text{s62}}{\text{s62} + \text{Kmdp}}$$
 (42)

6.22 Reaction re57

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

Reaction equation

$$s22 = \frac{s23, s119, s23}{s20} s20 \tag{43}$$

Reactant

Table 68: Properties of each reactant.

Id	Name	SBO
s22	PI3K	

Modifiers

Table 69: Properties of each modifier.

Id	Name	SBO
s23 s119 s23	Time Shear Stress Time	

Table 70: Properties of each product.

Id	Name	SBO
s20	p-PI3K	

Derived unit contains undeclared units

$$v_{22} = \exp\left(\text{unity} - \left(\frac{\text{s23}}{\text{tf}}\right)^{1.8}\right) \cdot \text{normal} \cdot \left(\frac{\text{s23}}{\text{unimol}}\right)^{0.8} \cdot \left(\text{unity} - \left(\frac{\text{s23}}{\text{tf}}\right)^{1.8}\right)$$
(44)

Table 71: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
normal			0.907	$10^{-9} \text{mol} \cdot \text{s}^{-1}$	\checkmark
unity			1.000	dimensionless	\square
unimol			1.000	10^{-9}mol	\square
tf			15.000	10^{-9} mol	

6.23 Reaction re58

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

Reaction equation

$$s19 \xrightarrow{s20, s19, s20} s17$$
 (45)

Reactant

Table 72: Properties of each reactant.

Id	Name	SBO
s19	PIP2	

Table 73: Properties of each modifier.

Id	Name	SBO
s20	p-PI3K	
s19	PIP2	
s20	p-PI3K	

Table 74: Properties of each product.

Id	Name	SBO
s17	PI3P	

Kinetic Law

Derived unit $s^{-1} \cdot 9.999999999998 \cdot 10^{-10} \text{ mol}$

$$v_{23} = \frac{k58 \cdot s19 \cdot s20}{Km58 + s19} \tag{46}$$

Table 75: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k58			0.2	s^{-1}	
Km58			6170.0	10^{-9}mol	

6.24 Reaction re59

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

Reaction equation

$$s17 \xrightarrow{s18, s17, s18} s19$$
 (47)

Reactant

Table 76: Properties of each reactant.

Id	Name	SBO
s17	PI3P	

Id	Name	SBO

Modifiers

Table 77: Properties of each modifier.

Id	Name	SBO
s18	PTEN	
s17	PI3P	
s18	PTEN	

Product

Table 78: Properties of each product.

Id	Name	SBO
s19	PIP2	

Kinetic Law

Derived unit $s^{-1} \cdot 9.999999999998 \cdot 10^{-10} \text{ mol}$

$$v_{24} = \frac{k59 \cdot s17 \cdot s18}{Km59 + s17} \tag{48}$$

Table 79: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k59			7.5		
Km59			80.9	10^{-9} mol	

6.25 Reaction re60

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

Reaction equation

$$s17 + s16 \xrightarrow{\underline{s17, s16, s28}} s28 \tag{49}$$

Reactants

Table 80: Properties of each reactant.

Id	Name	SBO
s17	PI3P	
s16	AKT	

Modifiers

Table 81: Properties of each modifier.

Id	Name	SBO
s17	PI3P	
s16	AKT	
s28	AKT:PI3P	

Product

Table 82: Properties of each product.

Id	Name	SBO
s28	AKT:PI3P	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{25} = k60 \cdot s17 \cdot s16 - kr60 \cdot s28 \tag{50}$$

Table 83: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k60 kr60			0.045 0.089	$(10^{-9} \text{ mol})^{-1} \cdot \text{s}^{-1}$ s^{-1}	✓

6.26 Reaction re61

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

Reaction equation

$$s28 \xrightarrow{s14, s28, s14} s26$$
 (51)

Reactant

Table 84: Properties of each reactant.

Id	Name	SBO
s28	AKT:PI3P	

Modifiers

Table 85: Properties of each modifier.

Id	Name	SBO
s14	PDK1	
s28	AKT:PI3P	
s14	PDK1	

Product

Table 86: Properties of each product.

Id	Name	SBO
s26	p-AKT:PI3P	

Kinetic Law

 $\textbf{Derived unit} \ \ s^{-1} \cdot 9.999999999998 \cdot 10^{-10} \ mol$

$$v_{26} = \frac{\text{k61} \cdot \text{s28} \cdot \text{s14}}{\text{Km61} + \text{s28}} \tag{52}$$

Table 87: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k61			20.0		\overline{Z}
Km61			80000.0	10^{-9}mol	\square

6.27 Reaction re62

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

Reaction equation

$$s26 \xrightarrow{s24, s26, s24} s27$$
 (53)

Reactant

Table 88: Properties of each reactant.

Id	Name	SBO
s26	p-AKT:PI3P	

Modifiers

Table 89: Properties of each modifier.

Id	Name	SBO
s24	PDK2	
s26	p-AKT:PI3P	
s24	PDK2	

Product

Table 90: Properties of each product.

	1	<u> </u>
Id	Name	SBO
s27	pp-AKT:PI3P	

Kinetic Law

Derived unit $s^{-1} \cdot 9.999999999998 \cdot 10^{-10} \text{ mol}$

$$v_{27} = \frac{\text{k62} \cdot \text{s26} \cdot \text{s24}}{\text{Km62} + \text{s26}} \tag{54}$$

Table 91: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k62			20.0		\overline{Z}
Km62			80000.0	$10^{-9} { m mol}$	

6.28 Reaction re63

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

Reaction equation

$$s26 \xrightarrow{s15, s26, s15} s28$$
 (55)

Reactant

Table 92: Properties of each reactant.

Id	Name	SBO
s26	p-AKT:PI3P	

Modifiers

Table 93: Properties of each modifier.

Id	Name	SBO
s15	PP2A	
s26	p-AKT:PI3P	
s15	PP2A	

Product

Table 94: Properties of each product.

Id	Name	SBO
s28	AKT:PI3P	

Kinetic Law

Derived unit $s^{-1} \cdot 9.999999999998 \cdot 10^{-10} \text{ mol}$

$$v_{28} = \frac{\text{k63} \cdot \text{s26} \cdot \text{s15}}{\text{Km63} + \text{s26}} \tag{56}$$

Table 95: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k63			0.037	s^{-1}	$ \mathcal{L} $
Km63			8800.000	$10^{-9} \mathrm{mol}$	\checkmark

6.29 Reaction re64

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

Reaction equation

$$s27 \xrightarrow{s15, s27, s15} s26 \tag{57}$$

Reactant

Table 96: Properties of each reactant.

Id	Name	SBO
s27	pp-AKT:PI3P	

Modifiers

Table 97: Properties of each modifier.

Id	Name	SBO
s15	PP2A	
s27	pp-AKT:PI3P	
s15	PP2A	

Product

Table 98: Properties of each product.

Id	Name	SBO
s26	p-AKT:PI3P	

Kinetic Law

Derived unit $s^{-1} \cdot 9.9999999999998 \cdot 10^{-10} \text{ mol}$

$$v_{29} = \frac{\text{k64} \cdot \text{s27} \cdot \text{s15}}{\text{Km64} + \text{s27}} \tag{58}$$

Table 99: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k64 Km64			0.04 48000.00	s^{-1} 10^{-9} mol	✓ ✓

6.30 Reaction re65

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

Reaction equation

$$s27 \xrightarrow{s15, s27, s15} s17 + s16 \tag{59}$$

Reactant

Table 100: Properties of each reactant.

Id	Name	SBO
s27	pp-AKT:PI3P	

Modifiers

Table 101: Properties of each modifier.

Id	Name	SBO
s15	PP2A	
s27	pp-AKT:PI3P	
s15	PP2A	

Products

Table 102: Properties of each product.

Id	Name	SBO
s17	PI3P	
s16	AKT	

Kinetic Law

Derived unit $s^{-1} \cdot 9.999999999998 \cdot 10^{-10} \text{ mol}$

$$v_{30} = \frac{k65 \cdot s27 \cdot s15}{Km65 + s27} \tag{60}$$

Table 103: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k65			0.163		Ø
Km65			48000.000	10^{-9}mol	\mathbf{Z}

6.31 Reaction re66

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

Reaction equation

$$s25 \xrightarrow{s17, s17, s25} s14$$
 (61)

Reactant

Table 104: Properties of each reactant.

Id	Name	SBO
s25	PDK1_cyto	

Modifiers

Table 105: Properties of each modifier.

Id	Name	SBO
s17	PI3P	

Id	Name	SBO
s17	PI3P	
s25	PDK1_cyto	

Product

Table 106: Properties of each product.

Id	Name	SBO
s14	PDK1	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{31} = k66 \cdot s17 \cdot s25 \tag{62}$$

Table 107: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k66			$7 \cdot 10^{-4}$	$(10^{-9} \text{ mol})^{-1} \cdot \text{s}^{-1}$	$lue{}$

6.32 Reaction re67

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

Reaction equation

$$s14 \xrightarrow{s14} s25 \tag{63}$$

Reactant

Table 108: Properties of each reactant.

Id	Name	SBO
s14	PDK1	

Modifier

Table 109: Properties of each modifier.

Id	Name	SBO
s14	PDK1	

Product

Table 110: Properties of each product.

Id	Name	SBO
s25	PDK1_cyto	

Kinetic Law

Derived unit $10^{-9} \text{ mol} \cdot \text{s}^{-1}$

$$v_{32} = s14 \cdot k67 \tag{64}$$

Table 111: Properties of each parameter.

Id	Name	SBO V	/alue	Unit	Constant
k67		0	0.98	s^{-1}	

6.33 Reaction re68

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

Reaction equation

$$s21 \longrightarrow s23$$
 (65)

Reactant

Table 112: Properties of each reactant.

Id	Name	SBO
s21	s3	

Product

Table 113: Properties of each product.

Id	Name	SBO
s23	Time	

Kinetic Law

Derived unit $10^{-9} \text{ mol} \cdot \text{s}^{-1}$

$$v_{33} = \text{unitime}$$
 (66)

Table 114: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
unitime			1.0	$10^{-9}~\text{mol}\cdot\text{s}^{-1}$	

6.34 Reaction re69

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

Reaction equation

$$s63 \xrightarrow{s45, s50, s61, s62, s58, s60, s65, s45, s58, s62, s65, s60} s64$$
 (67)

Reactant

Table 115: Properties of each reactant.

Id	Name	SBO
s63	L-Arg	

Modifiers

Table 116: Properties of each modifier.

Id	Name	SBO
s45	eNOS-CaM-Ca4	
s50	eNOS-CaM-Ca2	
s61	Hsp90-eNOS-CaM-Ca2	

Id	Name	SBO
s62	Hsp90-p-eNOS-CaM-Ca2	
s58	Hsp90-eNOS-CaM-Ca4	
s60	Hsp90-p-eNOS-CaM-Ca4	
s65	Hsp90-p-eNOS	
s45	eNOS-CaM-Ca4	
s58	Hsp90-eNOS-CaM-Ca4	
s62	Hsp90-p-eNOS-CaM-Ca2	
s65	Hsp90-p-eNOS	
s60	Hsp90-p-eNOS-CaM-Ca4	

Product

Table 117: Properties of each product.

Id	Name	SBO
s64	NO	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{34} = K_{cam_no} \cdot (s45 + s58) + K_{p_no} \cdot (s62 + s65) + K_{pcam_no} \cdot s60$$
 (68)

Table 118: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K_cam_no			17.0	s^{-1}	\overline{Z}
K_p_no			5.0	s^{-1}	\mathbf{Z}
K_pcam_no			17.0	s^{-1}	

6.35 Reaction re70

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

Reaction equation

$$s65 \xrightarrow{s65} s66 \tag{69}$$

Table 119: Properties of each reactant.

Id	Name	SBO
s65	Hsp90-p-eNOS	

Modifier

Table 120: Properties of each modifier.

Id	Name	SBO
s65	Hsp90-p-eNOS	

Product

Table 121: Properties of each product.

Id	Name	SBO
s66	Hsp90-eNOS	

Kinetic Law

Derived unit $9.999999999998 \cdot 10^{-10} \ mol \cdot s^{-1}$

$$v_{35} = \frac{\text{Vdp} \cdot \text{s65}}{\text{s65} + \text{Kmdp}} \tag{70}$$

6.36 Reaction re71

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

Reaction equation

$$s66 \xrightarrow{s66} s51 + s57 \tag{71}$$

Table 122: Properties of each reactant.

Id	Name	SBO
s66	Hsp90-eNOS	

Modifier

Table 123: Properties of each modifier.

Id	Name	SBO
s66	Hsp90-eNOS	

Products

Table 124: Properties of each product.

Id	Name	SBO
s51	eNOS-Cav-1	
s57	Hsp90	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{36} = \text{kr}90 \cdot \text{s}66 \tag{72}$$

6.37 Reaction re72

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

Reaction equation

$$s62 \stackrel{\underline{s62, s65, s48}}{=\!\!\!\!=} s65 + s48$$
 (73)

Reactant

Table 125: Properties of each reactant.

Id	Name	SBO
s62	Hsp90-p-eNOS-CaM-Ca2	

Modifiers

Table 126: Properties of each modifier.

Id	Name	SBO
s65	Hsp90-p-eNOS-CaM-Ca2 Hsp90-p-eNOS CaM-Ca2	

Products

Table 127: Properties of each product.

Id	Name	SBO
s65	Hsp90-p-eNOS	
s48	CaM-Ca2	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{37} = k18 \cdot s62 - k17 \cdot s65 \cdot s48 \tag{74}$$

6.38 Reaction re102

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

Reaction equation

$$s95 \stackrel{\underline{s39, s119, s39}}{=\!=\!=\!=\!=} s93 \tag{75}$$

Reactant

Table 128: Properties of each reactant.

Id	Name	SBO
s95	FAK	

Modifiers

Table 129: Properties of each modifier.

Id	Name	SBO
s39	Time	
s119	Shear Stress	
s39	Time	

Product

Table 130: Properties of each product.

Id	Name	SBO
s93	p-FAK	

Kinetic Law

Derived unit contains undeclared units

$$v_{38} = \exp\left(\text{unity} - \left(\frac{\text{s39}}{\text{tf}}\right)^{0.35}\right) \cdot \text{normal} \cdot \left(\frac{\text{s39} + \text{tiny_num}}{\text{unimol}}\right)^{-0.65} \cdot \left(\text{unity} - \left(\frac{\text{s39}}{\text{tf}}\right)^{0.35}\right)$$
(76)

Table 131: Properties of each parameter.

		1	· · · · · · · · · · · · · · · · · · ·		
Id	Name	SBO	Value	Unit	Constant
normal				$nmol \cdot s^{-1}$	\square
tf			60.000	10^{-9}mol	
unity				dimensionless	
unimol				10^{-9}mol	
${\tt tiny_num}$			10^{-6}	10^{-9} mol	\square

6.39 Reaction re103

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

Reaction equation

$$s94 \xrightarrow{\underline{s39, s119, s39}} s92 \tag{77}$$

Reactant

Table 132: Properties of each reactant.

Id	Name	SBO
s94	Src	

Modifiers

Table 133: Properties of each modifier.

Id	Name	SBO
s39	Time	
s119	Shear Stress	
s39	Time	

Product

Table 134: Properties of each product.

Id	Name	SBO
s92	p-Src	

Kinetic Law

Derived unit contains undeclared units

$$v_{39} = \exp\left(\text{unity} - \left(\frac{\text{s39}}{\text{tf}}\right)^{1.3}\right) \cdot \text{normal} \cdot \left(\frac{\text{s39}}{\text{unimol}}\right)^{0.3} \cdot \left(\text{unity} - \left(\frac{\text{s39}}{\text{tf}}\right)^{1.3}\right)$$
 (78)

Table 135: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
normal				$nmol \cdot s^{-1}$	
tf			540.000	10^{-9}mol	
unity			1.000	dimensionless	
unimol			1.000	10^{-9} mol	\checkmark

6.40 Reaction re104

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

Reaction equation

$$s91 + s93 \xrightarrow{s91, s93, s110} s110 \tag{79}$$

Reactants

Table 136: Properties of each reactant.

Id	Name	SBO
s91	Shc	
s93	p-FAK	

Modifiers

Table 137: Properties of each modifier.

Id	Name	SBO
s91	Shc	
s93	p-FAK	
s110	p-FAK:Shc	

Product

Table 138: Properties of each product.

Id	Name	SBO
s110	p-FAK:Shc	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9}$ mol

$$v_{40} = k105 \cdot s91 \cdot s93 - k_{-}105 \cdot s110 \tag{80}$$

Table 139: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k105			0.1	$nmol^{-1} \cdot s^{-1}$	
$k_{-}105$			1.0	s^{-1}	

6.41 Reaction re105

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

Reaction equation

$$s110 \xrightarrow{s92, s110, s92, s112} s112$$
 (81)

Reactant

Table 140: Properties of each reactant.

Id	Name	SBO
s110	p-FAK:Shc	

Modifiers

Table 141: Properties of each modifier.

Id	Name	SBO
s92	p-Src	
s110	p-FAK:Shc	
s92	p-Src	
s112	p-FAK:p-Shc	

Product

Table 142: Properties of each product.

Id	Name	SBO
s112	p-FAK:p-Shc	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{41} = \text{kcat_src} \cdot \text{s}110 \cdot \text{s}92 - \text{k_6} \cdot \text{s}112$$
 (82)

Table 143: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcat_src k_6			8.33 5.00	$\begin{array}{c} nmol^{-1} \cdot s^{-1} \\ s^{-1} \end{array}$	✓

6.42 Reaction re106

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

Reaction equation

$$s112 + s111 \xrightarrow{\underline{s111, s112, s113}} s113$$
 (83)

Reactants

Table 144: Properties of each reactant.

Id	Name	SBO
s112	p-FAK:p-Shc	
s111	Grb2:Sos	

Modifiers

Table 145: Properties of each modifier.

Id	Name	SBO
s112	Grb2:Sos p-FAK:p-Shc p-FAK:p-Shc:Grb2:Sos	

Product

Table 146: Properties of each product.

	1 1	
Id	Name	SBO
s113	p-FAK:p-Shc:Grb2:Sos	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{42} = k107 \cdot s111 \cdot s112 - k_{-}107 \cdot s113$$
 (84)

Table 147: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k107				$nmol^{-1} \cdot s^{-1}$	
$k_{-}107$			546.0	s^{-1}	\square

6.43 Reaction re107

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

Reaction equation

$$s113 \stackrel{\underline{s113, s93, s114}}{=\!=\!=\!=\!=} s114 + s93$$
 (85)

Reactant

Table 148: Properties of each reactant.

Id	Name	SBO
s113	p-FAK:p-Shc:Grb2:Sos	

Modifiers

Table 149: Properties of each modifier.

Id	Name	SBO
s113	p-FAK:p-Shc:Grb2:Sos	
s93	p-FAK	
s114	p-Shc:Grb2:Sos	

Products

Table 150: Properties of each product.

Id	Name	SBO
s114	p-Shc:Grb2:Sos	
s93	p-FAK	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{43} = k108 \cdot s113 - k_{-}108 \cdot s93 \cdot s114 \tag{86}$$

Table 151: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k108			2040.0	s^{-1}	
$k_{-}108$			15700.0	$nmol^{-1} \cdot s^{-1}$	\checkmark

6.44 Reaction re108

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

Reaction equation

$$s98 \xrightarrow{s98} s91 \tag{87}$$

Reactant

Table 152: Properties of each reactant.

Id	Name	SBO
s98	p-Shc	

Modifier

Table 153: Properties of each modifier.

Id	Name	SBO
s98	p-Shc	

Product

Table 154: Properties of each product.

Kinetic Law

Derived unit $9.999999999998 \cdot 10^{-10} \text{ mol} \cdot \text{s}^{-1}$

$$v_{44} = \frac{V10 \cdot s98}{K10 + s98} \tag{88}$$

Table 155: Properties of each parameter.

Id	Name	SBO V	Value	Unit	Constant
V10 K10				$\begin{array}{c} \mathrm{nmol} \cdot \mathrm{s}^{-1} \\ 10^{-9} \ \mathrm{mol} \end{array}$	✓ ✓

6.45 Reaction re109

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

Reaction equation

$$s114 \xrightarrow{s114} s98 + s111 \tag{89}$$

Reactant

Table 156: Properties of each reactant.

Id	Name	SBO
s114	p-Shc:Grb2:Sos	

Modifier

Table 157: Properties of each modifier.

Id	Name	SBO
s114	p-Shc:Grb2:Sos	

Products

Table 158: Properties of each product.

Id	Name	SBO
s98	p-Shc	
s111	Grb2:Sos	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{45} = k9 \cdot s114 \tag{90}$$

Table 159: Properties of each parameter.

Id	Name	SBO Value	Unit	Constant
k9		40.8	s^{-1}	

6.46 Reaction re110

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

Reaction equation

$$s115 \xrightarrow{s115} s106$$
 (91)

Table 160: Properties of each reactant.

Id	Name	SBO
s115	eNOS	

Modifier

Table 161: Properties of each modifier.

Id	Name	SBO
s115	eNOS	

Product

Table 162: Properties of each product.

Id	Name	SBO
s106	eNOS	

Kinetic Law

Derived unit $10^{-9} \text{ mol} \cdot \text{s}^{-1}$

$$v_{46} = s115 \cdot kT \tag{92}$$

Table 163: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
kT		$0.001 s^{-1}$	lacksquare

6.47 Reaction re111

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

Reaction equation

$$s108 \xrightarrow{s107, s49, s107, s49} s115$$
 (93)

Table 164: Properties of each reactant.

Id	Name	SBO
s108	eNOS	

Modifiers

Table 165: Properties of each modifier.

Id	Name	SBO
s107	aAP-1	
s49	KLF2	
s107	aAP-1	
s49	KLF2	

Product

Table 166: Properties of each product.

Id	Name	SBO
s115	eNOS	

Kinetic Law

Derived unit $(10^{-9} \text{ mol})^2 \cdot \text{s}^{-1}$

$$v_{47} = ktr1 \cdot s107 + ktr1k2 \cdot s49 \tag{94}$$

Table 167: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ktr1			-	$nmol \cdot s^{-1}$	\overline{Z}
ktr1k2			$9 \cdot 10^{-6}$	$nmol \cdot s^{-1}$	
tr2			$3 \cdot 10^{-6}$	$nmol \cdot s^{-1}$	

6.48 Reaction re112

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

Reaction equation

$$s103 \xrightarrow{s114, s114, s103} s102 \tag{95}$$

Table 168: Properties of each reactant.

Id	Name	SBO
s103	Ras:GDP	

Modifiers

Table 169: Properties of each modifier.

Id	Name	SBO
s114	p-Shc:Grb2:Sos	
s114	p-Shc:Grb2:Sos	
s103	Ras:GDP	

Product

Table 170: Properties of each product.

Id	Name	SBO
s102	Ras:GTP	

Kinetic Law

Derived unit $s^{-1} \cdot 9.999999999998 \cdot 10^{-10} \text{ mol}$

$$v_{48} = \frac{k111 \cdot s114 \cdot s103}{s103 + K111} \tag{96}$$

Table 171: Properties of each parameter.

Id	Name	SBO Value	e Unit	Constant
k111		0.222	$2 s^{-1}$	\square
K111		0.181	10^{-9}mol	\square

6.49 Reaction re113

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

Reaction equation

$$s102 \xrightarrow{s102} s103$$
 (97)

Reactant

Table 172: Properties of each reactant.

Id	Name	SBO
s102	Ras:GTP	

Modifier

Table 173: Properties of each modifier.

Id	Name	SBO
s102	Ras:GTP	

Product

Table 174: Properties of each product.

Id	Name	SBO
s103	Ras:GDP	

Kinetic Law

 $\textbf{Derived unit} \ \ 9.9999999999998 \cdot 10^{-10} \ mol \cdot s^{-1}$

$$v_{49} = \frac{V12 \cdot s102}{K12 + s102} \tag{98}$$

Table 175: Properties of each parameter.

Id	Name	SBO Value	Unit	Constant
V12 K12			$\begin{array}{c} nmol \cdot s^{-1} \\ 10^{-9} \ mol \end{array}$	a

6.50 Reaction re114

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

Reaction equation

$$s97 \xrightarrow{s102, s102, s97} s101 \tag{99}$$

Reactant

Table 176: Properties of each reactant.

Id	Name	SBO
s97	MEKK1	

Modifiers

Table 177: Properties of each modifier.

Id	Name	SBO
s102	Ras:GTP	
s102	Ras:GTP	
s97	MEKK1	

Product

Table 178: Properties of each product.

Id	Name	SBO
s101	p-MEKK1	

Kinetic Law

Derived unit $s^{-1} \cdot 9.999999999998 \cdot 10^{-10} \text{ mol}$

$$v_{50} = \frac{k113 \cdot s102 \cdot s97}{K113 + s97} \tag{100}$$

Table 179: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k113			0.035		
K113			10.000	10^{-9}mol	\square

6.51 Reaction re115

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

Reaction equation

$$s101 \xrightarrow{s101} s97 \tag{101}$$

Reactant

Table 180: Properties of each reactant.

Id	Name	SBO
s101	p-MEKK1	

Modifier

Table 181: Properties of each modifier.

Id	Name	SBO
s101	p-MEKK1	

Product

Table 182: Properties of each product.

Id	Name	SBO
s97	MEKK1	

Kinetic Law

 $\textbf{Derived unit} \ \ 9.9999999999998 \cdot 10^{-10} \ mol \cdot s^{-1}$

$$v_{51} = \frac{V18 \cdot s101}{K18 + s101} \tag{102}$$

Table 183: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K18			8.000	10^{-9}mol	
V18			0.125	$nmol \cdot s^{-1}$	\checkmark

6.52 Reaction re116

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

Reaction equation

$$s96 \xrightarrow{s101, s101, s96} s100 \tag{103}$$

Reactant

Table 184: Properties of each reactant.

Id	Name	SBO
s96	JNKK	

Modifiers

Table 185: Properties of each modifier.

Id	Name	SBO
s101	p-MEKK1	
s101	p-MEKK1	
s96	JNKK	

Product

Table 186: Properties of each product.

Id	Name	SBO
s100	p-JNKK	

Kinetic Law

Derived unit $s^{-1} \cdot 9.999999999998 \cdot 10^{-10} \text{ mol}$

$$v_{52} = \frac{k19 \cdot s101 \cdot s96}{K19 + s96} \tag{104}$$

Table 187: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k19			0.005	s^{-1}	
K19			15.000	$10^{-9} \mathrm{mol}$	$ \overline{\mathbf{Z}} $

6.53 Reaction re117

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

Reaction equation

$$s100 \xrightarrow{s100} s96 \tag{105}$$

Reactant

Table 188: Properties of each reactant.

Id	Name	SBO
s100	p-JNKK	

Modifier

Table 189: Properties of each modifier.

Id	Name	SBO
s100	p-JNKK	

Product

Table 190: Properties of each product.

Id	Name	SBO
s96	JNKK	

Kinetic Law

Derived unit $9.999999999998 \cdot 10^{-10} \, \text{mol} \cdot \text{s}^{-1}$

$$v_{53} = \frac{\text{V20} \cdot \text{s}100}{\text{s}100 + \text{K20}} \tag{106}$$

Table 191: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K20			15.000	10^{-9}mol	\overline{Z}
V20			0.375	$nmol \cdot s^{-1}$	

6.54 Reaction re118

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

Reaction equation

$$s99 \xrightarrow{s43, s99, s43} s104$$
 (107)

Reactant

Table 192: Properties of each reactant.

Id	Name	SBO
s99	JNK	

Modifiers

Table 193: Properties of each modifier.

	_	
Id	Name	SBO
s43 s99	pp-JNKK JNK	
s43	pp-JNKK	

Product

Table 194: Properties of each product.

Id	Name	SBO
s104	p-JNK	

Kinetic Law

 $\textbf{Derived unit} \ \ s^{-1} \cdot 9.999999999998 \cdot 10^{-10} \ mol$

$$v_{54} = \frac{k21 \cdot s99 \cdot s43}{s99 + K21} \tag{108}$$

Table 195: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k21			0.002		
K21			30.000	10^{-9}mol	$ \mathcal{L}$

6.55 Reaction re119

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

Reaction equation

$$s104 \xrightarrow{s104} s99$$
 (109)

Reactant

Table 196: Properties of each reactant.

Id	Name	SBO
s104	p-JNK	

Modifier

Table 197: Properties of each modifier.

Id	Name	SBO
s104	p-JNK	

Product

Table 198: Properties of each product.

Id	Name	SBO
s99	JNK	

Kinetic Law

 $\textbf{Derived unit} \ \ 9.9999999999998 \cdot 10^{-10} \ mol \cdot s^{-1}$

$$v_{55} = \frac{\text{V22} \cdot \text{s}104}{\text{s}104 + \text{K22}} \tag{110}$$

Table 199: Properties of each parameter.

Id	Name	SBO Value	Unit	Constant
K22			10^{-9} mol	
V22		0.05	$nmol \cdot s^{-1}$	

6.56 Reaction re120

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

Reaction equation

$$s106 \xrightarrow{s106} s35$$
 (111)

Reactant

Table 200: Properties of each reactant.

Id	Name	SBO
s106	eNOS	

Modifier

Table 201: Properties of each modifier.

Id	Name	SBO
s106	eNOS	

Product

Table 202: Properties of each product.

Id	Name	SBO
s35	s35	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{56} = kD \cdot s106 \tag{112}$$

Table 203: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kD			$2.8\cdot10^{-5}$	s^{-1}	

6.57 Reaction re121

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

Reaction equation

$$s37 \xrightarrow{s106, s106} s51$$
 (113)

Reactant

Table 204: Properties of each reactant.

Id	Name	SBO
s37	s37	

Modifiers

Table 205: Properties of each modifier.

Id	Name	SBO
s106	eNOS	
s106	eNOS	

Table 206: Properties of each product.

Id	Name	SBO
s51	eNOS-Cav-1	

Kinetic Law

Derived unit $9.999999999998 \cdot 10^{-10} \ mol \cdot s^{-1}$

$$v_{57} = \frac{kP \cdot s106}{s106 + K30} \tag{114}$$

Table 207: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kP K30				$\begin{array}{c} nmol \cdot s^{-1} \\ 10^{-9} mol \end{array}$	✓

6.58 Reaction re122

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

Reaction equation

$$s38 \longrightarrow s39$$
 (115)

Reactant

Table 208: Properties of each reactant.

Id	Name	SBO
s38	pre_time	

Table 209: Properties of each product.

Id	Name	SBO
s39	Time	

Kinetic Law

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

$$v_{58} = \text{unitime}$$
 (116)

Table 210: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
unitime			1.0	$nmol \cdot s^{-1}$	

6.59 Reaction re123

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

Reaction equation

$$s43 \xrightarrow{s43} s100 \tag{117}$$

Reactant

Table 211: Properties of each reactant.

Id	Name	SBO
s43	pp-JNKK	

Modifier

Table 212: Properties of each modifier.

Id	Name	SBO
s43	pp-JNKK	

Table 213: Properties of each product.

Id	Name	SBO
s100	p-JNKK	

Kinetic Law

Derived unit $9.999999999998 \cdot 10^{-10} \text{ mol} \cdot \text{s}^{-1}$

$$v_{59} = \frac{\text{V37} \cdot \text{s43}}{\text{s43} + \text{K37}} \tag{118}$$

Table 214: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V37				$nmol \cdot s^{-1}$	Ø
K37			15.000	10^{-9}mol	\mathbf{Z}

6.60 Reaction re124

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

Reaction equation

$$s100 \xrightarrow{s101, s100, s101} s43$$
 (119)

Reactant

Table 215: Properties of each reactant.

Id	Name	SBO
s100	p-JNKK	

Modifiers

Table 216: Properties of each modifier.

Id	Name	SBO
s101	p-MEKK1	
s100	p-JNKK	
s101	p-MEKK1	

Table 217: Properties of each product.

Id	Name	SBO
s43	pp-JNKK	

Kinetic Law

Derived unit $s^{-1} \cdot 9.999999999998 \cdot 10^{-10} \text{ mol}$

$$v_{60} = \frac{k38 \cdot s100 \cdot s101}{K38 + s100} \tag{120}$$

Table 218: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k38			0.005	s^{-1}	$ \overline{\checkmark} $
K38			15.000	10^{-9}mol	

6.61 Reaction re125

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

Reaction equation

$$s44 \xrightarrow{s44} s104 \tag{121}$$

Reactant

Table 219: Properties of each reactant.

Id	Name	SBO
s44	pp-JNK	

Id	Name	SBO

Modifier

Table 220: Properties of each modifier.

Id	Name	SBO
s44	pp-JNK	

Product

Table 221: Properties of each product.

Id	Name	SBO
s104	p-JNK	

Kinetic Law

Derived unit $9.999999999998 \cdot 10^{-10} \ mol \cdot s^{-1}$

$$v_{61} = \frac{\text{V39} \cdot \text{s44}}{\text{K39} + \text{s44}} \tag{122}$$

Table 222: Properties of each parameter.

Id	Name	SBO Va	llue Unit	Constant
V39		0	$0.05 \text{nmol} \cdot \text{s}^{-1}$	\blacksquare
K39		15	10^{-9} mol	\square

6.62 Reaction re126

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

Reaction equation

$$s104 \xrightarrow{s43, s104, s43} s44$$
 (123)

Reactant

Table 223: Properties of each reactant.

Id	Name	SBO
s104	p-JNK	

Modifiers

Table 224: Properties of each modifier.

Id	Name	SBO
s43	pp-JNKK	
s104	p-JNK	
s43	pp-JNKK	

Product

Table 225: Properties of each product.

Id	Name	SBO
s44	pp-JNK	

Kinetic Law

 $\textbf{Derived unit} \ \ s^{-1} \cdot 9.999999999998 \cdot 10^{-10} \ mol$

$$v_{62} = \frac{k40 \cdot s104 \cdot s43}{K40 + s104} \tag{124}$$

Table 226: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k40			0.002	s^{-1}	\overline{Z}
K40			30.000	10^{-9}mol	

6.63 Reaction re127

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

Reaction equation

$$s42 \xrightarrow{s44, s44, s42} s107$$
 (125)

Reactant

Table 227: Properties of each reactant.

Id	Name	SBO
s42	AP-1	

Modifiers

Table 228: Properties of each modifier.

Id	Name	SBO
s44	pp-JNK	
s44	pp-JNK	
s42	AP-1	

Product

Table 229: Properties of each product.

Id	Name	SBO
s107	aAP-1	

Kinetic Law

Derived unit $9.999999999998 \cdot 10^{-10} \, \text{mol} \cdot \text{s}^{-1}$

$$v_{63} = \frac{\text{s44} \cdot \text{s42} \cdot \text{k43}}{\text{K43} + \text{s42}} \tag{126}$$

Table 230: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K43			$25.000 \\ 4 \cdot 10^{-5}$	10^{-9} mol 10^{-9} mol 	

6.64 Reaction re128

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

Reaction equation

$$s107 \xrightarrow{s107} s42$$
 (127)

Reactant

Table 231: Properties of each reactant.

Id	Name	SBO
s107	aAP-1	

Modifier

Table 232: Properties of each modifier.

Id	Name	SBO
s107	aAP-1	

Product

Table 233: Properties of each product.

Id	Name	SBO
s42	AP-1	

Kinetic Law

Derived unit $9.999999999998 \cdot 10^{-10} \, mol \cdot s^{-1}$

$$v_{64} = \frac{\text{V44} \cdot \text{s107}}{\text{s107} + \text{K44}} \tag{128}$$

Table 234: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K44			5.000	10^{-9}mol	
V44			0.002	$nmol \cdot s^{-1}$	\square

6.65 Reaction re129

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

Reaction equation

$$s105 \xrightarrow{s39, s39} s49 \tag{129}$$

Reactant

Table 235: Properties of each reactant.

Id	Name	SBO
s105	KLF2	

Modifiers

Table 236: Properties of each modifier.

Id	Name	SBO
s39	Time	
s39	Time	

Product

Table 237: Properties of each product.

Id	Name	SBO
s49	KLF2	

Kinetic Law

Derived unit contains undeclared units

$$v_{65} = \frac{\frac{\exp\left(\tan\left(\det \left(\text{delay} - \frac{\$39}{\text{tc}}\right)\right)}{1 + 2 \cdot \exp\left(\tan\left(\det \left(\text{delay} - \frac{\$39}{\text{tc}}\right)\right) + \exp\left(2 \cdot \tan\left(\det \left(\text{delay} - \frac{\$39}{\text{tc}}\right)\right)\right)}}{\text{uc}} \cdot 29.256$$
(130)

Table 238: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
tau				dimensionless	
tc			3600.00	10^{-9}mol	\square
uc			3600.00	dimensionless	\square
delay			5.00	dimensionless	\square
unity			20.00	$nmol \cdot s^{-1}$	\square

6.66 Reaction re131

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

Reaction equation

$$s51 \xrightarrow{s51} s116 \tag{131}$$

Reactant

Table 239: Properties of each reactant.

Id	Name	SBO
s51	eNOS-Cav-1	

Modifier

Table 240: Properties of each modifier.

Id	Name	SBO
s51	eNOS-Cav-1	

Product

Table 241: Properties of each product.

Id	Name	SBO
s116	sa49_degraded	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{66} = \text{kDD} \cdot \text{s51} \tag{132}$$

6.67 Reaction re132

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

Reaction equation

$$s45 \xrightarrow{s45} s117 + s47$$
 (133)

Reactant

Table 242: Properties of each reactant.

Id	Name	SBO
s45	eNOS-CaM-Ca4	

Modifier

Table 243: Properties of each modifier.

Id	Name	SBO
s45	eNOS-CaM-Ca4	

Products

Table 244: Properties of each product.

Id	Name	SBO
s117	s117	
s47	CaM-Ca4	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{67} = kDD \cdot s45 \tag{134}$$

6.68 Reaction re133

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

Reaction equation

$$s50 \xrightarrow{s50} s117 + s48$$
 (135)

Reactant

Table 245: Properties of each reactant.

Id	Name	SBO
s50	eNOS-CaM-Ca2	

Modifier

Table 246: Properties of each modifier.

Id	Name	SBO
s50	eNOS-CaM-Ca2	

Products

Table 247: Properties of each product.

Id	Name	SBO
s117	s117 CaM-Ca2	
540	Calvi-Ca2	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{68} = kDD \cdot s50 \tag{136}$$

6.69 Reaction re134

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

Reaction equation

$$s66 \xrightarrow{s66} s57 + s118$$
 (137)

Reactant

Table 248: Properties of each reactant.

Id	Name	SBO
s66	Hsp90-eNOS	

Modifier

Table 249: Properties of each modifier.

Id	Name	SBO
s66	Hsp90-eNOS	

Products

Table 250: Properties of each product.

Id	Name	SBO
s57	Hsp90	
s118	s118	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9}$ mol

$$v_{69} = kDD \cdot s66 \tag{138}$$

6.70 Reaction re135

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

Reaction equation

$$s65 \xrightarrow{s65} s118 + s57 \tag{139}$$

Reactant

Table 251: Properties of each reactant.

Id	Name	SBO
s65	Hsp90-p-eNOS	

Modifier

Table 252: Properties of each modifier.

Id	Name	SBO
s65	Hsp90-p-eNOS	

Products

Table 253: Properties of each product.

Id	Name	SBO
s118	s118	
s57	Hsp90	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{70} = kDD \cdot s65 \tag{140}$$

6.71 Reaction re136

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

Reaction equation

$$s61 \xrightarrow{s61} s57 + s48$$
 (141)

Reactant

Table 254: Properties of each reactant.

Id	Name	SBO
s61	Hsp90-eNOS-CaM-Ca2	

Modifier

Table 255: Properties of each modifier.

-		Name	SBO
	s61	Hsp90-eNOS-CaM-Ca2	

Table 256: Properties of each product.

Id	Name	SBO
s57	Hsp90	
s48	CaM-Ca2	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{71} = kDD \cdot s61 \tag{142}$$

6.72 Reaction re137

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

Reaction equation

$$s62 \xrightarrow{s62} s57 + s48$$
 (143)

Reactant

Table 257: Properties of each reactant.

Tuble 2571 Troporties of each reactant.		
Id	Name	SBO
s62	Hsp90-p-eNOS-CaM-Ca2	

Modifier

Table 258: Properties of each modifier.

Id	Name	SBO
s62	Hsp90-p-eNOS-CaM-Ca2	

Table 259: Properties of each product.

Id	Name	SBO
s57	Hsp90	
s48	CaM-Ca2	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{72} = kDD \cdot s62 \tag{144}$$

6.73 Reaction re138

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

Reaction equation

$$s58 \xrightarrow{s58} s57 + s47$$
 (145)

Reactant

Table 260: Properties of each reactant.

Id	Name	SBO
s58	Hsp90-eNOS-CaM-Ca4	

Modifier

Table 261: Properties of each modifier.

Id	Name	SBO
s58	Hsp90-eNOS-CaM-Ca4	

Products

Table 262: Properties of each product.

Id	Name	SBO
s57	Hsp90	
s47	CaM-Ca4	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{73} = kDD \cdot s58 \tag{146}$$

6.74 Reaction re139

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

Reaction equation

$$s60 \xrightarrow{s60} s57 + s47$$
 (147)

Reactant

Table 263: Properties of each reactant.

Id	Name	SBO
s60	Hsp90-p-eNOS-CaM-Ca4	

Modifier

Table 264: Properties of each modifier.

Table 20 11 Troperties of each infoamer.			
Id	Name	SBO	
s60	Hsp90-p-eNOS-CaM-Ca4		

Products

Table 265: Properties of each product.

Id	Name	SBO
s57 s47	Hsp90 CaM-Ca4	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-9} \text{ mol}$

$$v_{74} = kDD \cdot s60 \tag{148}$$

7 Derived Rate Equations

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

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

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

7.1 Species s1

Name Ca_ex

Initial amount 1500000

Charge 0

This species takes part in two reactions (as a modifier in re4, re4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}1 = 0\tag{149}$$

7.2 Species s2

Name Ca_s

Initial amount 2830000

Charge 0

This species takes part in four reactions (as a reactant in re7 and as a product in re4 and as a modifier in re4, re7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}2 = v_2 - v_5 \tag{150}$$

7.3 Species s3

Name Ca_c

Initial amount 117.2

Charge 0

This species takes part in 23 reactions (as a reactant in re8, re9, re12 and as a product in re3, re7, re10 and as a modifier in re3, re5, re5, re7, re8, re9, re12, re41, re41, re42, re42, re50, re50, re52, re52, re54, re54).

$$\frac{\mathrm{d}}{\mathrm{d}t}s3 = v_1 + v_5 + v_8 - v_6 - v_7 - v_{10} \tag{151}$$

7.4 Species s4

Name Ca_B

SBO:0000297 protein complex

Initial amount 3870

Charge 0

This species takes part in two reactions (as a reactant in re3 and as a modifier in re3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}4 = -v_1\tag{152}$$

7.5 Species s5

Name s5

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in one reaction (as a reactant in re4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}5 = -v_2\tag{153}$$

7.6 Species s6

Name IP3

Initial amount 0

Charge 0

This species takes part in five reactions (as a reactant in re6 and as a product in re5 and as a modifier in re6, re7, re7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}6 = v_3 - v_4 \tag{154}$$

7.7 Species s7

Name s7

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in one reaction (as a reactant in re5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}7 = -v_3\tag{155}$$

7.8 Species s8

Name s8

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in one reaction (as a product in re6).

$$\frac{\mathrm{d}}{\mathrm{d}t}s8 = v_4 \tag{156}$$

7.9 Species s9

Name s9

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in two reactions (as a product in re8, re12).

$$\frac{d}{dt}s9 = v_6 + v_{10} \tag{157}$$

7.10 Species s10

Name s10

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in one reaction (as a product in re9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}10 = v_7 \tag{158}$$

7.11 Species s11

Name s11

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in one reaction (as a reactant in re10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}11 = -v_8\tag{159}$$

7.12 Species s12

Name TimeT

SBO:0000331 half-life

Initial amount 0

Charge 0

This species takes part in three reactions (as a product in re11 and as a modifier in re5, re5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}12 = v_9 \tag{160}$$

7.13 Species s13

Name s13

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in one reaction (as a reactant in re11).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}13 = -v_9\tag{161}$$

7.14 Species s14

Name PDK1

Initial amount 0.246

This species takes part in five reactions (as a reactant in re67 and as a product in re66 and as a modifier in re61, re61, re67).

$$\frac{d}{dt}s14 = v_{31} - v_{32} \tag{162}$$

7.15 Species s15

Name PP2A

Initial amount 150

Charge 0

This species takes part in six reactions (as a modifier in re63, re64, re64, re65, re65).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}15 = 0\tag{163}$$

7.16 Species s16

Name AKT

Initial amount 167.616

Charge 0

This species takes part in three reactions (as a reactant in re60 and as a product in re65 and as a modifier in re60).

$$\frac{d}{dt}s16 = v_{30} - v_{25} \tag{164}$$

7.17 Species s17

Name PI3P

Initial amount 0.345

Charge 0

This species takes part in eight reactions (as a reactant in re59, re60 and as a product in re58, re65 and as a modifier in re59, re60, re66, re66).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{s}17 = v_{23} + v_{30} - v_{24} - v_{25} \tag{165}$$

7.18 Species s18

Name PTEN

Initial amount 0.1

This species takes part in two reactions (as a modifier in re59, re59).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}18 = 0\tag{166}$$

7.19 Species s19

Name PIP2

Initial amount 6967.271

Charge 0

This species takes part in three reactions (as a reactant in re58 and as a product in re59 and as a modifier in re58).

$$\frac{\mathrm{d}}{\mathrm{d}t}s19 = v_{24} - v_{23} \tag{167}$$

7.20 Species s20

Name p-PI3K

Initial amount 0.03

Charge 0

This species takes part in three reactions (as a product in re57 and as a modifier in re58, re58).

$$\frac{d}{dt}s20 = v_{22} {168}$$

7.21 Species s21

Name s3

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in one reaction (as a reactant in re68).

$$\frac{d}{dt}s21 = -v_{33} {169}$$

7.22 Species s22

Name PI3K

Initial amount 99.97

Charge 0

This species takes part in one reaction (as a reactant in re57).

$$\frac{d}{dt}s22 = -v_{22} \tag{170}$$

7.23 Species s23

Name Time

Initial amount 0

 $\textbf{Charge} \ \ 0$

This species takes part in three reactions (as a product in re68 and as a modifier in re57, re57).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}23 = v_{33} \tag{171}$$

7.24 Species s24

Name PDK2

Initial amount 3

Charge 0

This species takes part in two reactions (as a modifier in re62, re62).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}24 = 0\tag{172}$$

7.25 Species s25

Name PDK1_cyto

Initial amount 999.754

Charge 0

This species takes part in three reactions (as a reactant in re66 and as a product in re67 and as a modifier in re66).

$$\frac{\mathrm{d}}{\mathrm{d}t}s25 = v_{32} - v_{31} \tag{173}$$

7.26 Species s26

Name p-AKT:PI3P

Initial amount 1.457

This species takes part in six reactions (as a reactant in re62, re63 and as a product in re61, re64 and as a modifier in re62, re63).

$$\frac{\mathrm{d}}{\mathrm{d}t}s26 = v_{26} + v_{29} - v_{27} - v_{28} \tag{174}$$

7.27 Species s27

Name pp-AKT:PI3P

Initial amount 1.723

Charge 0

This species takes part in nine reactions (as a reactant in re64, re65 and as a product in re62 and as a modifier in re55, re55, re56, re56, re64, re65).

$$\frac{\mathrm{d}}{\mathrm{d}t}s27 = v_{27} - v_{29} - v_{30} \tag{175}$$

7.28 Species s28

Name AKT:PI3P

Initial amount 29.203

Charge 0

This species takes part in five reactions (as a reactant in re61 and as a product in re60, re63 and as a modifier in re60, re61).

$$\frac{\mathrm{d}}{\mathrm{d}t}s28 = v_{25} + v_{28} - v_{26} \tag{176}$$

7.29 Species s35

Name s35

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in one reaction (as a product in re120).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}35 = v_{56} \tag{177}$$

7.30 Species s37

Name s37

SBO:0000291 empty set

Initial amount 10000

Charge 0

This species takes part in one reaction (as a reactant in re121).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}37 = -v_{57}\tag{178}$$

7.31 Species s38

Name pre_time

SBO:0000347 duration

Initial amount 0

Charge 0

This species takes part in one reaction (as a reactant in re122).

$$\frac{\mathrm{d}}{\mathrm{d}t}s38 = -v_{58} \tag{179}$$

7.32 Species s39

Name Time

Initial amount 0

Charge 0

This species takes part in seven reactions (as a product in re122 and as a modifier in re102, re102, re103, re103, re129, re129).

$$\frac{\mathrm{d}}{\mathrm{d}t}s39 = v_{58} \tag{180}$$

7.33 Species s42

Name AP-1

Initial amount 50

Charge 0

This species takes part in three reactions (as a reactant in re127 and as a product in re128 and as a modifier in re127).

$$\frac{d}{dt}s42 = v_{64} - v_{63} \tag{181}$$

7.34 Species s43

Name pp-JNKK

Initial amount 0.0060

This species takes part in seven reactions (as a reactant in re123 and as a product in re124 and as a modifier in re118, re118, re123, re126, re126).

$$\frac{d}{dt}s43 = v_{60} - v_{59} \tag{182}$$

7.35 Species s44

Name pp-JNK

Initial amount 0

Charge 0

This species takes part in five reactions (as a reactant in re125 and as a product in re126 and as a modifier in re125, re127, re127).

$$\frac{d}{dt}s44 = v_{62} - v_{61} \tag{183}$$

7.36 Species s45

Name eNOS-CaM-Ca4

Initial amount 0.0415

Charge 0

This species takes part in nine reactions (as a reactant in re50, re51, re132 and as a product in re37 and as a modifier in re50, re51, re69, re69, re132).

$$\frac{\mathrm{d}}{\mathrm{d}t}s45 = v_{11} - |v_{15}| - v_{16} - v_{67} \tag{184}$$

7.37 Species s47

Name CaM-Ca4

Initial amount 2.827

Charge 0

This species takes part in seven reactions (as a reactant in re37 and as a product in re42, re132, re138, re139 and as a modifier in re37, re42).

$$\frac{\mathrm{d}}{\mathrm{d}t}s47 = v_{14} + v_{67} + v_{73} + v_{74} - v_{11} \tag{185}$$

7.38 Species s48

Name CaM-Ca2

Initial amount 347.52

Charge 0

This species takes part in eleven reactions (as a reactant in re38, re42 and as a product in re41, re72, re133, re136, re137 and as a modifier in re38, re41, re42, re72).

$$\frac{\mathrm{d}}{\mathrm{d}t}s48 = v_{13} + v_{37} + v_{68} + v_{71} + v_{72} - v_{12} - v_{14} \tag{186}$$

7.39 Species s49

Name KLF2

Initial amount 10

Charge 0

This species takes part in three reactions (as a product in re129 and as a modifier in re111, re111).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}49 = v_{65} \tag{187}$$

7.40 Species s50

Name eNOS-CaM-Ca2

Initial amount 2.12

Charge 0

This species takes part in eight reactions (as a reactant in re133 and as a product in re38, re50, re53 and as a modifier in re38, re50, re69, re133).

$$\frac{\mathrm{d}}{\mathrm{d}t}s50 = v_{12} + |v_{15}| + v_{18} - v_{68} \tag{188}$$

7.41 Species s51

Name eNOS-Cav-1

Initial amount 34.98

This species takes part in eight reactions (as a reactant in re37, re38, re131 and as a product in re71, re121 and as a modifier in re37, re38, re131).

$$\frac{\mathrm{d}}{\mathrm{d}t}s51 = v_{36} + v_{57} - v_{11} - v_{12} - v_{66} \tag{189}$$

7.42 Species s52

Name Calmodulin

Initial amount 7635.36

Charge 0

This species takes part in two reactions (as a reactant in re41 and as a modifier in re41).

$$\frac{d}{dt}s52 = -v_{13} \tag{190}$$

7.43 Species s57

Name Hsp90

Initial amount 199987

Charge 0

This species takes part in ten reactions (as a reactant in re51 and as a product in re53, re71, re134, re135, re136, re137, re138, re139 and as a modifier in re51).

$$\frac{\mathrm{d}}{\mathrm{d}t}s57 = v_{18} + v_{36} + v_{69} + v_{70} + v_{71} + v_{72} + v_{73} + v_{74} - v_{16}$$
(191)

7.44 Species s58

Name Hsp90-eNOS-CaM-Ca4

Initial amount 1.037

Charge 0

This species takes part in nine reactions (as a reactant in re52, re55, re138 and as a product in re51 and as a modifier in re52, re55, re69, re69, re138).

$$\frac{\mathrm{d}}{\mathrm{d}t}s58 = v_{16} - |v_{17}| - v_{20} - v_{73} \tag{192}$$

7.45 Species s60

Name Hsp90-p-eNOS-CaM-Ca4

Initial amount 0.0089

Charge 0

This species takes part in eight reactions (as a reactant in re54, re139 and as a product in re55 and as a modifier in re54, re55, re69, re69, re139).

$$\frac{\mathrm{d}}{\mathrm{d}t}s60 = v_{20} - |v_{19}| - v_{74} \tag{193}$$

7.46 Species s61

Name Hsp90-eNOS-CaM-Ca2

Initial amount 10.98

Charge 0

This species takes part in nine reactions (as a reactant in re53, re56, re136 and as a product in re52 and as a modifier in re52, re53, re56, re69, re136).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}61 = v_{17} - v_{18} - v_{21} - v_{71} \tag{194}$$

7.47 Species s62

Name Hsp90-p-eNOS-CaM-Ca2

Initial amount 0.106

Charge 0

This species takes part in ten reactions (as a reactant in re72, re137 and as a product in re54, re56 and as a modifier in re54, re56, re69, re69, re72, re137).

$$\frac{\mathrm{d}}{\mathrm{d}t}s62 = v_{19} + v_{21} - v_{37} - v_{72} \tag{195}$$

7.48 Species s63

Name L-Arg

SBO:0000291 empty set

Initial amount 500000

Charge 0

This species takes part in one reaction (as a reactant in re69).

$$\frac{d}{dt}s63 = -v_{34} \tag{196}$$

7.49 Species s64

Name NO

Initial amount 0

Charge 0

This species takes part in one reaction (as a product in re69).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}64 = v_{34} \tag{197}$$

7.50 Species s65

Name Hsp90-p-eNOS

Initial amount 0.643

Charge 0

This species takes part in eight reactions (as a reactant in re70, re135 and as a product in re72 and as a modifier in re69, re69, re70, re72, re135).

$$\frac{\mathrm{d}}{\mathrm{d}t}s65 = v_{37} - v_{35} - v_{70} \tag{198}$$

7.51 Species s66

Name Hsp90-eNOS

Initial amount 0.083

Charge 0

This species takes part in five reactions (as a reactant in re71, re134 and as a product in re70 and as a modifier in re71, re134).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{s}66 = v_{35} - v_{36} - v_{69} \tag{199}$$

7.52 Species s91

Name Shc

Initial amount 819.25

Charge 0

This species takes part in three reactions (as a reactant in re104 and as a product in re108 and as a modifier in re104).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}91 = v_{44} - v_{40} \tag{200}$$

7.53 Species s92

Name p-Src

Initial amount 18

Charge 0

This species takes part in three reactions (as a product in re103 and as a modifier in re105, re105).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}92 = v_{39} \tag{201}$$

7.54 Species s93

Name p-FAK

Initial amount 0.605

Charge 0

This species takes part in five reactions (as a reactant in re104 and as a product in re102, re107 and as a modifier in re104, re107).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}93 = v_{38} + v_{43} - v_{40} \tag{202}$$

7.55 Species s94

Name Src

Initial amount 72

Charge 0

This species takes part in one reaction (as a reactant in re103).

$$\frac{d}{dt}s94 = -v_{39} \tag{203}$$

7.56 Species s95

Name FAK

Initial amount 57

Charge 0

This species takes part in one reaction (as a reactant in re102).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}95 = -v_{38} \tag{204}$$

7.57 Species s96

Name JNKK

Initial amount 299.706

Charge 0

This species takes part in three reactions (as a reactant in re116 and as a product in re117 and as a modifier in re116).

$$\frac{d}{dt}s96 = v_{53} - v_{52} \tag{205}$$

7.58 Species s97

Name MEKK1

Initial amount 98.514

Charge 0

This species takes part in three reactions (as a reactant in re114 and as a product in re115 and as a modifier in re114).

$$\frac{d}{dt}s97 = v_{51} - v_{50} \tag{206}$$

7.59 Species s98

Name p-Shc

Initial amount 157.162

Charge 0

This species takes part in three reactions (as a reactant in re108 and as a product in re109 and as a modifier in re108).

$$\frac{d}{dt}s98 = v_{45} - v_{44} \tag{207}$$

7.60 Species s99

Name JNK

Initial amount 299.997

Charge 0

This species takes part in three reactions (as a reactant in re118 and as a product in re119 and as a modifier in re118).

$$\frac{d}{dt}s99 = v_{55} - v_{54} \tag{208}$$

7.61 Species s100

Name p-JNKK

Initial amount 0.288

Charge 0

This species takes part in six reactions (as a reactant in re117, re124 and as a product in re116, re123 and as a modifier in re117, re124).

$$\frac{\mathrm{d}}{\mathrm{d}t}s100 = v_{52} + v_{59} - v_{53} - v_{60} \tag{209}$$

7.62 Species s101

Name p-MEKK1

Initial amount 1.486

Charge 0

This species takes part in seven reactions (as a reactant in re115 and as a product in re114 and as a modifier in re115, re116, re116, re124, re124).

$$\frac{\mathrm{d}}{\mathrm{d}t}s101 = v_{50} - v_{51} \tag{210}$$

7.63 Species s102

Name Ras:GTP

Initial amount 0.616

Charge 0

This species takes part in five reactions (as a reactant in re113 and as a product in re112 and as a modifier in re113, re114, re114).

$$\frac{\mathrm{d}}{\mathrm{d}t} s102 = v_{48} - v_{49} \tag{211}$$

7.64 Species s103

Name Ras:GDP

Initial amount 119.384

Charge 0

This species takes part in three reactions (as a reactant in re112 and as a product in re113 and as a modifier in re112).

$$\frac{\mathrm{d}}{\mathrm{d}t}s103 = v_{49} - v_{48} \tag{212}$$

7.65 Species s104

Name p-JNK

Initial amount 0.0030

Charge 0

This species takes part in six reactions (as a reactant in re119, re126 and as a product in re118, re125 and as a modifier in re119, re126).

$$\frac{\mathrm{d}}{\mathrm{d}t}s104 = v_{54} + v_{61} - v_{55} - v_{62} \tag{213}$$

7.66 Species s105

Name KLF2

SBO:0000278 messenger RNA

Initial amount 0

Charge 0

This species takes part in one reaction (as a reactant in re129).

$$\frac{d}{dt}s105 = -v_{65} \tag{214}$$

7.67 Species s106

Name eNOS

SBO:0000278 messenger RNA

Initial amount 3.214

Charge 0

This species takes part in five reactions (as a reactant in re120 and as a product in re110 and as a modifier in re120, re121, re121).

$$\frac{\mathrm{d}}{\mathrm{d}t}s106 = v_{46} - v_{56} \tag{215}$$

7.68 Species s107

Name aAP-1

Initial amount 0

Charge 0

This species takes part in five reactions (as a reactant in re128 and as a product in re127 and as a modifier in re111, re111, re128).

$$\frac{d}{dt}s107 = v_{63} - v_{64} \tag{216}$$

7.69 Species s108

Name eNOS

SBO:0000243 gene

Initial amount 0

Charge 0

This species takes part in one reaction (as a reactant in re111).

$$\frac{d}{dt}s108 = -v_{47} \tag{217}$$

7.70 Species s110

Name p-FAK:Shc

Initial amount 0.857

Charge 0

This species takes part in four reactions (as a reactant in re105 and as a product in re104 and as a modifier in re104, re105).

$$\frac{\mathrm{d}}{\mathrm{d}t}s110 = v_{40} - v_{41} \tag{218}$$

7.71 Species s111

Name Grb2:Sos

Initial amount 3.23

Charge 0

This species takes part in three reactions (as a reactant in re106 and as a product in re109 and as a modifier in re106).

$$\frac{\mathrm{d}}{\mathrm{d}t}s111 = v_{45} - v_{42} \tag{219}$$

7.72 Species s112

Name p-FAK:p-Shc

Initial amount 15.962

Charge 0

This species takes part in four reactions (as a reactant in re106 and as a product in re105 and as a modifier in re105, re106).

$$\frac{\mathrm{d}}{\mathrm{d}t}s112 = v_{41} - v_{42} \tag{220}$$

7.73 Species s113

Name p-FAK:p-Shc:Grb2:Sos

Initial amount 5.577

Charge 0

This species takes part in four reactions (as a reactant in re107 and as a product in re106 and as a modifier in re106, re107).

$$\frac{\mathrm{d}}{\mathrm{d}t}s113 = v_{42} - v_{43} \tag{221}$$

7.74 Species s114

Name p-Shc:Grb2:Sos

Initial amount 1.193

Charge 0

This species takes part in six reactions (as a reactant in re109 and as a product in re107 and as a modifier in re107, re109, re112, re112).

$$\frac{\mathrm{d}}{\mathrm{d}t}s114 = v_{43} - v_{45} \tag{222}$$

7.75 Species s115

Name eNOS

SBO:0000278 messenger RNA

Initial amount 0.09

Charge 0

This species takes part in three reactions (as a reactant in re110 and as a product in re111 and as a modifier in re110).

$$\frac{d}{dt}s115 = |v_{47}| - v_{46} \tag{223}$$

7.76 Species s116

Name sa49_degraded

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in one reaction (as a product in re131).

$$\frac{d}{dt}s116 = v_{66} \tag{224}$$

7.77 Species s117

Name s117

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in two reactions (as a product in re132, re133).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}117 = v_{67} + v_{68} \tag{225}$$

7.78 Species s118

Name s118

SBO:0000291 empty set

Initial amount 0

Charge 0

This species takes part in two reactions (as a product in re134, re135).

$$\frac{d}{dt}s118 = v_{69} + v_{70} \tag{226}$$

7.79 Species s119

Name Shear Stress

Initial amount 0

This species takes part in four reactions (as a modifier in re5, re57, re102, re103).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}119 = 0\tag{227}$$

A Glossary of Systems Biology Ontology Terms

- **SBO:0000243 gene:** A locatable region of genomic sequence, corresponding to a unit of inheritance, which is associated with regulatory regions, transcribed regions and/or other functional sequence regions. Sequence Ontology SO:000070
- **SBO:0000278 messenger RNA:** A messenger RNA is a ribonucleic acid synthesized during the transcription of a gene, and that carries the information to encode one or several proteins
- **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.
- **SBO:0000297 protein complex:** Macromolecular complex containing one or more polypeptide chains possibly associated with simple chemicals. CHEBI:3608
- **SBO:0000331 half-life:** Time interval over which a quantified entity is reduced to half its original value

SBO:0000347 duration: Amount of time during which an event persists

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