SBML Model Report

Model name: "Leloup2003_CircClock_LD"



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Enuo He¹ at October 17th 2006 at 3:43 p.m. and last time modified at July eleventh 2012 at 6:31 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	16
events	0	constraints	0
reactions	48	function definitions	5
global parameters	2	unit definitions	2
rules	2	initial assignments	0

Model Notes

This model is described in the paper *Toward a detailed computational model for the mammalian circadian clock*. In this model only interlocked negative and positive regulation of Per, Cry, Bmal gene are involved. Some initial values were not provided, therefore they were chosen to fit the curves from the paper.

Figure2C is re-produced by odeSolver.

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

2 Unit Definitions

This is an overview of five unit definitions of which three are predefined by SBML and not mentioned in the model.

2.1 Unit time

Definition 3600 s

2.2 Unit substance

Definition nmol

2.3 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition 1

2.4 Unit area

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

Definition m²

2.5 Unit length

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

Definition m

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
cell	cell		3	1	litre		

3.1 Compartment cell

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

Name cell

4 Species

This model contains 16 species. 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 Condi-
					tion
species_0	Mb	cell	$nmol \cdot l^{-1}$		
species_1	Bc	cell	$nmol \cdot l^{-1}$		\Box
species_2	Вср	cell	$nmol \cdot l^{-1}$	\Box	\Box
species_3	Bn	cell	$nmol \cdot l^{-1}$	\Box	\Box
species_4	Cc	cell	$nmol \cdot l^{-1}$		\Box
species_5	Mc	cell	$nmol \cdot l^{-1}$		\Box
species_6	Сср	cell	$\mathrm{nmol}\cdot\mathrm{l}^{-1}$		
species_7	Mp	cell	$\mathrm{nmol}\cdot\mathrm{l}^{-1}$		\Box
species_8	Pc	cell	$\mathrm{nmol}\cdot\mathrm{l}^{-1}$		\Box
species_9	Pcp	cell	$nmol \cdot l^{-1}$		\Box
species_10	PCc	cell	$nmol \cdot l^{-1}$		\Box
species_11	PCcp	cell	$nmol \cdot l^{-1}$		\Box
species_12	PCn	cell	$\mathrm{nmol}\cdot\mathrm{l}^{-1}$		
species_13	Bnp	cell	$\mathrm{nmol}\cdot\mathrm{l}^{-1}$	\Box	
species_14	PCnp	cell	$\mathrm{nmol}\cdot\mathrm{l}^{-1}$	\Box	\Box
species_15	In	cell	$\mathrm{nmol}\cdot\mathrm{l}^{-1}$	\Box	

5 Parameters

This model contains two global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
parameter- _0000081	LD	0.0	
parameter- _0000082	vsp	0.0	

6 Function definitions

This is an overview of five function definitions.

6.1 Function definition function_3

Name Activation of gene

Arguments Vs, B, n, K

Mathematical Expression

$$\frac{Vs \cdot B^n}{K^n + B^n} \tag{1}$$

6.2 Function definition function_2

Name Michaelis-Menten(irreversible)

Arguments V, substrate, Km

Mathematical Expression

$$\frac{V \cdot substrate}{Km + substrate}$$
 (2)

6.3 Function definition function_1

Name mRNA translated into protein

Arguments k, mRNA

Mathematical Expression

$$k \cdot mRNA$$
 (3)

6.4 Function definition function_0

Name Inhibition of gene

Arguments vsb, K, m, Bn

Mathematical Expression

$$\frac{vsb \cdot K^m}{K^m + Bn^m} \tag{4}$$

6.5 Function definition functionDefinition_0000005

Name ceiling

Argument length

Mathematical Expression

$$\left\lceil \frac{\sin\left(\frac{\pi \cdot \text{time}}{\text{length}} + 0.0010\right)}{2} \right\rceil$$
(5)

7 Rules

This is an overview of two rules.

7.1 Rule parameter_0000081

Rule parameter_0000081 is an assignment rule for parameter parameter_0000081:

$$parameter_0000081 = functionDefinition_0000005 (12)$$
 (6)

Derived unit dimensionless

7.2 Rule parameter_0000082

Rule parameter_0000082 is an assignment rule for parameter parameter_0000082:

parameter_0000082 =
$$1.5 + (1.8 - 1.5) \cdot \text{parameter} = 0000081$$
 (7)

8 Reactions

This model contains 48 reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 5: Overview of all reactions

Nº	Id	Name	Reaction Equation	SBO
1	reaction_0	Mb synthesized	$\emptyset \xrightarrow{\text{species}_3} \text{species}_0$	
2	reaction_1	Mb translated into protein	$\emptyset \xrightarrow{\text{species}_0} \text{species}_1$	
3	reaction_2	Mb nonspecific degradation	species_0 $\longrightarrow \emptyset$	
		, ,	•	
4	reaction_3	Bc phosphorylation	$species_1 \longrightarrow species_2$	
5	${\tt reaction_4}$	Bc transfered from cytosolic to nuclear	species_1 ====================================	
6	reaction_5	Mc translated into protein	$\emptyset \xrightarrow{\text{species}_5} \text{species}_4$	
7	$reaction_6$	Mc nonspecific degradation	species_5 $\longrightarrow \emptyset$	
8	$reaction_{-}7$	Cc phosphorylation	species_4 → species_6	
9	reaction_8	Ccp specific degradation	species_6 $\longrightarrow \emptyset$	
10	reaction_9	Mp synthesis	$\emptyset \xrightarrow{\text{species}_3} \text{species}_7$	
11	reaction_10	Mp translated into protein	$\emptyset \xrightarrow{\text{species}_7} \text{species}_8$	
12	$reaction_11$	Pcp specific degradation	species_9 $\longrightarrow \emptyset$	
13	$reaction_12$	Pc phosphorylation	species_8 → species_9	
14	$reaction_13$	Cc and Pc produce complex Per_Cry	$species_4 + species_8 \Longrightarrow species_10$	
15	${\tt reaction_14}$	PCc phosphorylation	$species_10 \longrightarrow species_11$	
16	$reaction_15$	PCcp specific degradation	species_ $11 \longrightarrow \emptyset$	
17	${\tt reaction_16}$	PCc transfered into nuclear	species_10 ⇒ species_12	
18	$reaction_17$	PCnp nonspecific degradation	species_ $14 \longrightarrow \emptyset$	
19	reaction_18	Bcp nonspecific degradation	species_2 $\longrightarrow \emptyset$	
20	$reaction_19$	Bnp nonspecific degradation	species_ $13 \longrightarrow \emptyset$	
			-	

No	Id	Name	Reaction Equation	SBO
21	reaction 20	Mc synthesis	$\emptyset \xrightarrow{\text{species}_3} \text{species}_5$	
22	reaction_21	PCn phosphorylation	species_12 \longrightarrow species_14	
23	reaction_22	Mp nonspecific degradation	species_7 $\longrightarrow \emptyset$	
24	reaction_23	Per_Cry and Clock_Bmal form inactive com-	$species_12 + species_3 \Longrightarrow species_15$	
		plex	T. C.	
25	reaction_24	Mb specific degradation	species_ $0 \longrightarrow \emptyset$	
26	reaction_25	Mc specific degradation	species_5 $\longrightarrow \emptyset$	
27	reaction_26	Mp specific degradation	species_7 $\longrightarrow \emptyset$	
28	reaction_27	Pc nonspecific degradation	species_8 $\longrightarrow \emptyset$	
29	reaction_28	Cc nonspecific degradation	species_4 $\longrightarrow \emptyset$	
30	reaction_29	Pcp nonspecific degradation	species_9 $\longrightarrow \emptyset$	
31	reaction_30	Ccp nonspecific degradation	species_6 $\longrightarrow \emptyset$	
32	reaction_31	PCcp nonspecific degradation	species_ $11 \longrightarrow \emptyset$	
33	reaction_32	PCc nonspecific degradation	species_ $10 \longrightarrow \emptyset$	
34	reaction_33	PCnp specific degradation	species_ $14 \longrightarrow \emptyset$	
35	reaction_34	Bc nonspecific degradation	$species_1 \longrightarrow \emptyset$	
36	reaction_35	Bcp specific degradation	species_2 $\longrightarrow \emptyset$	
37	reaction_36	Bn phosphorylation	species_3 → species_13	
38	reaction_37	Bnp specific degradation	species_ $13 \longrightarrow \emptyset$	
39	reaction_38	In nonspecific degration	species_ $15 \longrightarrow \emptyset$	
40	reaction_39	In specific degradation	species_ $15 \longrightarrow \emptyset$	
41	$reaction_40$	Bn nonspecific degradation	species_3 $\longrightarrow \emptyset$	
42	${\tt reaction_41}$	Bcp dephosphorylation	$species_2 \longrightarrow species_1$	
43	${\tt reaction_42}$	Bnp dephosphorylation	species_13 → species_3	
44	$reaction_43$	Ccp dephosphorylation	species_6 → species_4	
45	$reaction_44$	Pcp dephosphorylation	species_9 → species_8	
46	$reaction_45$	PCnp dephosphorylation	species_14 → species_12	
47	$reaction_46$	PCn nonspecific degradation	species_ $12 \longrightarrow \emptyset$	

N₀	Id	Name	Reaction Equation	SBO
48	reaction_47	PCcp dephosphorylation	species_11 → species_10	

8.1 Reaction reaction_0

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

Name Mb synthesized

Reaction equation

$$\emptyset \xrightarrow{\text{species} .3} \text{species}.0 \tag{8}$$

Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
species_3	Bn	

Product

Table 7: Properties of each product.

Id	Name	SBO
species_0	Mb	

Kinetic Law

$$v_1 = \text{vol}(\text{cell}) \cdot \text{function}_0(\text{vsb}, \text{K}, \text{m}, [\text{species}_3])$$
 (9)

$$function_0 (vsb, K, m, Bn) = \frac{vsb \cdot K^m}{K^m + Bn^m}$$
 (10)

$$function_0\left(vsb,K,m,Bn\right) = \frac{vsb\cdot K^m}{K^m + Bn^m} \tag{11}$$

Table 8: Properties of each parameter.

	14010 0	rangerines of each parameter.	
Id	Name	SBO Value Unit	Constant
vsb		1.0	
K	Kib	2.2	$ \overline{\checkmark} $
m		2.0	

8.2 Reaction reaction_1

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

Name Mb translated into protein

Reaction equation

$$\emptyset \xrightarrow{\text{species}_0} \text{species}_1 \tag{12}$$

Modifier

Table 9: Properties of each modifier.

Id	Name	SBO
species_0	Mb	

Product

Table 10: Properties of each product.

Id	Name	SBO
species_1	Вс	

Kinetic Law

$$v_2 = \text{vol}(\text{cell}) \cdot \text{function}_1(k, [\text{species}_0])$$
 (13)

$$function_{-1}(k, mRNA) = k \cdot mRNA \tag{14}$$

$$function_{-}1(k, mRNA) = k \cdot mRNA \tag{15}$$

Table 11: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k	ksb	0.12	

8.3 Reaction reaction_2

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

Name Mb nonspecific degradation

Reaction equation

$$species_{-}0 \longrightarrow \emptyset$$
 (16)

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
species_0	Mb	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{species_0}]$$
 (17)

Table 13: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	kdmb	0.01	

8.4 Reaction reaction_3

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

Name Bc phosphorylation

Reaction equation

$$species_1 \longrightarrow species_2 \tag{18}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
species_1	Вс	

Product

Table 15: Properties of each product.

Id	Name	SBO
species_2	Вср	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{vol}(\text{cell}) \cdot \text{function}_2(V, [\text{species}_1], Km)$$
 (19)

$$function_2\left(V, substrate, Km\right) = \frac{V \cdot substrate}{Km + substrate} \tag{20}$$

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (21)

Table 16: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	V1b	0.5	
Km	Kp	0.1	

8.5 Reaction reaction_4

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

Name Bc transfered from cytosolic to nuclear

Reaction equation

$$species_1 \Longrightarrow species_3$$
 (22)

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
species_1	Вс	

Product

Table 18: Properties of each product.

Id	Name	SBO
species_3	Bn	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{species}_1] - \text{k2} \cdot [\text{species}_3])$$
 (23)

Table 19: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k5	0.4	
k2	k6	0.2	\checkmark

8.6 Reaction reaction_5

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

Name Mc translated into protein

Reaction equation

$$\emptyset \xrightarrow{\text{species.5}} \text{species.4} \tag{24}$$

Modifier

Table 20: Properties of each modifier.

Id	Name	SBO
species_5	Mc	

Product

Table 21: Properties of each product.

Id	Name	SBO
species_4	Cc	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{vol}(\text{cell}) \cdot \text{function}_1(k, [\text{species}_5])$$
 (25)

$$function_{-1}(k, mRNA) = k \cdot mRNA \tag{26}$$

function_1
$$(k, mRNA) = k \cdot mRNA$$
 (27)

Table 22: Properties of each parameter.

10	Name	SBO Value Unit	Constant
K	ksc	1.0	<u> </u>

8.7 Reaction reaction_6

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

Name Mc nonspecific degradation

Reaction equation

species_5
$$\longrightarrow \emptyset$$
 (28)

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
species_5	Mc	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{species}_5]$$
 (29)

Table 24: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	kdmc	0.01	\square

8.8 Reaction reaction_7

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

Name Cc phosphorylation

Reaction equation

$$species_4 \longrightarrow species_6$$
 (30)

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
species_4	Сс	

Product

Table 26: Properties of each product.

Id	Name	SBO
species_6	Ccp	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{vol}(\text{cell}) \cdot \text{function}_2(V, [\text{species}_4], \text{Km})$$
 (31)

$$function_{2}(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (32)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (33)

Table 27: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	V1c	0.6	$ \overline{\mathscr{A}} $
Km	Kp	0.1	

8.9 Reaction reaction_8

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

Name Ccp specific degradation

Reaction equation

$$species_6 \longrightarrow \emptyset \tag{34}$$

Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
species_6	Ccp	

Kinetic Law

$$v_9 = \text{vol}(\text{cell}) \cdot \text{function.} 2(V, [\text{species.} 6], \text{Km})$$
 (35)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (36)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
(37)

Table 29: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	vdcc	0.7	
Km	Kd	0.3	

8.10 Reaction reaction_9

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

Name Mp synthesis

Reaction equation

$$\emptyset \xrightarrow{\text{species}_3} \text{species}_7 \tag{38}$$

Modifier

Table 30: Properties of each modifier.

Id	Name	SBO
species_3	Bn	

Product

Table 31: Properties of each product.

Id	Name	SBO
species_7	Mp	

Kinetic Law

$$v_{10} = \text{vol}(\text{cell}) \cdot \text{function}_3(\text{parameter}_0000082, [\text{species}_3], n, K)$$
 (39)

$$function_3\left(Vs,B,n,K\right) = \frac{Vs \cdot B^n}{K^n + B^n} \tag{40}$$

$$\text{function_3}\left(Vs,B,n,K\right) = \frac{Vs \cdot B^n}{K^n + B^n} \tag{41} \label{eq:41}$$

Table 32: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
n		4.0	\overline{Z}
K	Kap	0.7	

8.11 Reaction reaction_10

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

Name Mp translated into protein

Reaction equation

$$\emptyset \xrightarrow{\text{species}_7} \text{species}_8 \tag{42}$$

Modifier

Table 33: Properties of each modifier.

Id	Name	SBO
species_7	Mp	

Product

Table 34: Properties of each product.

Id	Name	SBO
species_8	Pc	

Kinetic Law

$$v_{11} = \text{vol}(\text{cell}) \cdot \text{function}_1(k, [\text{species}_7])$$
 (43)

$$function_{-1}(k, mRNA) = k \cdot mRNA \tag{44}$$

$$function_{-1}(k, mRNA) = k \cdot mRNA \tag{45}$$

Table 35: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k	ksp	0.6	

8.12 Reaction reaction_11

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

Name Pcp specific degradation

Reaction equation

$$species_{9} \longrightarrow \emptyset$$
 (46)

Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
species_9	Pcp	

Kinetic Law

$$v_{12} = \text{vol}(\text{cell}) \cdot \text{function}_2(V, [\text{species}_9], \text{Km})$$
 (47)

$$function_{-}2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (48)

$$function_2\left(V, substrate, Km\right) = \frac{V \cdot substrate}{Km + substrate} \tag{49}$$

Table 37: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	vdpc	0.7	
Km	Kd	0.3	\checkmark

8.13 Reaction reaction_12

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

Name Pc phosphorylation

Reaction equation

$$species_8 \longrightarrow species_9$$
 (50)

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
species_8	Pc	

Product

Table 39: Properties of each product.

Id	Name	SBO
species_9	Pcp	

Kinetic Law

$$v_{13} = \text{vol}(\text{cell}) \cdot \text{function}_2(V, [\text{species}_8], \text{Km})$$
 (51)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (52)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (53)

Table 40: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	V1p	0.4	
Km	Kp	0.1	

8.14 Reaction reaction_13

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

Name Cc and Pc produce complex Per_Cry

Reaction equation

$$species_4 + species_8 \Longrightarrow species_{10}$$
 (54)

Reactants

Table 41: Properties of each reactant.

Id	Name	SBO
species_4 species_8	Cc Pc	

Product

Table 42: Properties of each product.

Id	Name	SBO
species_10	PCc	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{species_4}] \cdot [\text{species_8}] - \text{k2} \cdot [\text{species_10}])$$
 (55)

Table 43: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k3	0.4	\square
k2	k4	0.2	\square

8.15 Reaction reaction_14

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

Name PCc phosphorylation

Reaction equation

$$species_10 \longrightarrow species_11$$
 (56)

Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
species_10	PCc	

Product

Table 45: Properties of each product.

Id	Name	SBO
species_11	PCcp	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{vol}(\text{cell}) \cdot \text{function}_2(V, [\text{species}_10], \text{Km})$$
 (57)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (58)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (59)

Table 46: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	V1pc	0.4	\overline{Z}
Km	Kp	0.1	\checkmark

8.16 Reaction reaction_15

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

Name PCcp specific degradation

Reaction equation

$$species_{-}11 \longrightarrow \emptyset \tag{60}$$

Reactant

Table 47: Properties of each reactant.

Id	Name	SBO
species_11	PCcp	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \text{vol}(\text{cell}) \cdot \text{function} 2(V, [\text{species}_11], \text{Km})$$
 (61)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (62)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (63)

Table 48: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	vdpcc	0.7	\overline{Z}
Km	Kd	0.3	$\overline{\checkmark}$

8.17 Reaction reaction_16

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

Name PCc transfered into nuclear

Reaction equation

$$species_10 \Longrightarrow species_12$$
 (64)

Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
species_10	PCc	

Product

Table 50: Properties of each product.

Id	Name	SBO
species_12	PCn	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{species}_10] - \text{k2} \cdot [\text{species}_12])$$
(65)

Table 51: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.4	\overline{Z}
k2	k2	0.2	\square

8.18 Reaction reaction_17

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

Name PCnp nonspecific degradation

Reaction equation

$$species_1 4 \longrightarrow \emptyset$$
 (66)

Reactant

Table 52: Properties of each reactant.

Id	Name	SBO
species_14	PCnp	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{species}_14]$$
 (67)

Table 53: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	kdn	0.01	

8.19 Reaction reaction_18

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

Name Bcp nonspecific degradation

Reaction equation

$$species_2 \longrightarrow \emptyset \tag{68}$$

Reactant

Table 54: Properties of each reactant.

Id	Name	SBO
species_2	Вср	

Kinetic Law

$$v_{19} = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{species.2}]$$
 (69)

Table 55: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	kdn	0.01	

8.20 Reaction reaction_19

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

Name Bnp nonspecific degradation

Reaction equation

$$species_{-}13 \longrightarrow \emptyset \tag{70}$$

Reactant

Table 56: Properties of each reactant.

Id	Name	SBO
species_13	Bnp	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{species}_{-}13] \tag{71}$$

Table 57: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	kdn	0.01	

8.21 Reaction reaction_20

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

Name Mc synthesis

Reaction equation

$$\emptyset \xrightarrow{\text{species}_3} \text{species}_5 \tag{72}$$

Modifier

Table 58: Properties of each modifier.

Id	Name	SBO
species_3	Bn	

Product

Table 59: Properties of each product.

Id	Name	SBO
species_5	Mc	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \text{vol}(\text{cell}) \cdot \text{function}_3(\text{Vs},[\text{species}_3], n, K)$$
 (73)

$$function_3\left(Vs,B,n,K\right) = \frac{Vs \cdot B^n}{K^n + B^n} \tag{74} \label{eq:74}$$

$$\text{function_3}\left(Vs,B,n,K\right) = \frac{Vs \cdot B^n}{K^n + B^n} \tag{75} \label{eq:75}$$

Table 60: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
Vs	VSC	1.1	\square
n		4.0	
K	Kac	0.6	\square

8.22 Reaction reaction_21

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

Name PCn phosphorylation

Reaction equation

$$species_12 \longrightarrow species_14$$
 (76)

Reactant

Table 61: Properties of each reactant.

Id	Name	SBO
species_12	PCn	

Product

Table 62: Properties of each product.

Id	Name	SBO
species_14	PCnp	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \text{vol}(\text{cell}) \cdot \text{function} 2(V, [\text{species}_12], Km)$$
 (77)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (78)

$$function_2\left(V, substrate, Km\right) = \frac{V \cdot substrate}{Km + substrate} \tag{79}$$

Table 63: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	V3pc	0.4	
Km	Kp	0.1	$\overline{\checkmark}$

8.23 Reaction reaction_22

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

Name Mp nonspecific degradation

Reaction equation

species_7
$$\longrightarrow \emptyset$$
 (80)

Reactant

Table 64: Properties of each reactant.

Id	Name	SBO
species_7	Mp	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{species}_{-7}]$$
 (81)

Table 65: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	kdmp	0.01	

8.24 Reaction reaction_23

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

Name Per_Cry and Clock_Bmal form inactive complex

Reaction equation

$$species_12 + species_3 \Longrightarrow species_15$$
 (82)

Reactants

Table 66: Properties of each reactant.

Id	Name	SBO
species_12 species_3	PCn Bn	

Product

Table 67: Properties of each product.

Id	Name	SBO
species_15	In	

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{species}_12] \cdot [\text{species}_3] - \text{k2} \cdot [\text{species}_15])$$
 (83)

Table 68: Properties of each parameter.

		* *	
Id	Name	SBO Value Unit	Constant
k1	k7	0.5	
k2	k8	0.1	

8.25 Reaction reaction_24

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

Name Mb specific degradation

Reaction equation

$$species_0 \longrightarrow \emptyset$$
 (84)

Reactant

Table 69: Properties of each reactant.

Id	Name	SBO
species_0	Mb	

Kinetic Law

$$v_{25} = \text{vol}(\text{cell}) \cdot \text{function}_2(V, [\text{species}_0], Km)$$
 (85)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (86)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
(87)

Table 70: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	vmb	0.8	
Km	Kmb	0.4	

8.26 Reaction reaction_25

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

Name Mc specific degradation

Reaction equation

$$species_5 \longrightarrow \emptyset$$
 (88)

Reactant

Table 71: Properties of each reactant.

Id	Name	SBO
species_5	Mc	

Kinetic Law

$$v_{26} = \text{vol}(\text{cell}) \cdot \text{function}_2(V, [\text{species}_5], Km)$$
 (89)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
(90)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (91)

Table 72: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	vmc	1.0	\checkmark
Km	Kmc	0.4	\checkmark

8.27 Reaction reaction_26

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

Name Mp specific degradation

Reaction equation

$$species_{-}7 \longrightarrow \emptyset \tag{92}$$

Reactant

Table 73: Properties of each reactant.

Id	Name	SBO
species_7	Mp	

Kinetic Law

$$v_{27} = \text{vol}(\text{cell}) \cdot \text{function}_2(V, [\text{species}_7], Km)$$
 (93)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
(94)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
(95)

Table 74: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	vmp	1.10	
Km	Kmp	0.31	\checkmark

8.28 Reaction reaction_27

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

Name Pc nonspecific degradation

Reaction equation

species_
$$8 \longrightarrow \emptyset$$
 (96)

Reactant

Table 75: Properties of each reactant.

Id	Name	SBO
species_8	Pc	

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{species_8}] \tag{97}$$

Table 76: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	kdn	0.01	

8.29 Reaction reaction_28

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

Name Cc nonspecific degradation

Reaction equation

$$species_4 \longrightarrow \emptyset \tag{98}$$

Reactant

Table 77: Properties of each reactant.

Id	Name	SBO
species_4	Cc	

Kinetic Law

Derived unit contains undeclared units

$$v_{29} = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{species_4}] \tag{99}$$

Table 78: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	kdnc	0.12	\checkmark

8.30 Reaction reaction_29

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

Name Pcp nonspecific degradation

Reaction equation

$$species_9 \longrightarrow \emptyset \tag{100}$$

Reactant

Table 79: Properties of each reactant.

Id	Name	SBO
species_9	Pcp	

Kinetic Law

$$v_{30} = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{species_9}] \tag{101}$$

Table 80: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	kdn	0.01	

8.31 Reaction reaction_30

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

Name Ccp nonspecific degradation

Reaction equation

$$species_{-}6 \longrightarrow \emptyset$$
 (102)

Reactant

Table 81: Properties of each reactant.

Id	Name	SBO
species_6	Ccp	

Kinetic Law

Derived unit contains undeclared units

$$v_{31} = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{species_6}] \tag{103}$$

Table 82: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	kdn	0.01	

8.32 Reaction reaction_31

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

Name PCcp nonspecific degradation

$$species_{-}11 \longrightarrow \emptyset \tag{104}$$

Table 83: Properties of each reactant.

Id	Name	SBO
species_11	PCcp	

Kinetic Law

Derived unit contains undeclared units

$$v_{32} = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{species_11}] \tag{105}$$

Table 84: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	kdn	0.01	

8.33 Reaction reaction_32

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

Name PCc nonspecific degradation

Reaction equation

$$species_{-}10 \longrightarrow \emptyset \tag{106}$$

Reactant

Table 85: Properties of each reactant.

Id	Name	SBO
species_10	PCc	

Kinetic Law

Derived unit contains undeclared units

$$v_{33} = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{species}_10] \tag{107}$$

Table 86: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	kdn	0.01	

8.34 Reaction reaction_33

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

Name PCnp specific degradation

Reaction equation

species_
$$14 \longrightarrow \emptyset$$
 (108)

Reactant

Table 87: Properties of each reactant.

Id	Name	SBO
species_14	PCnp	

Kinetic Law

Derived unit contains undeclared units

$$v_{34} = \text{vol}(\text{cell}) \cdot \text{function}_2(V, [\text{species}_14], Km)$$
 (109)

$$function_{-}2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (110)

$$function_2\left(V, substrate, Km\right) = \frac{V \cdot substrate}{Km + substrate} \tag{111}$$

Table 88: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	vdpcn	0.7	
Km	Kd	0.3	

8.35 Reaction reaction_34

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

Name Bc nonspecific degradation

Reaction equation

$$species_{-}1 \longrightarrow \emptyset$$
 (112)

Reactant

Table 89: Properties of each reactant.

Id	Name	SBO
species_1	Вс	

Kinetic Law

Derived unit contains undeclared units

$$v_{35} = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{species_1}]$$
 (113)

Table 90: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	kdn	0.01	

8.36 Reaction reaction_35

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

Name Bcp specific degradation

Reaction equation

species_2
$$\longrightarrow \emptyset$$
 (114)

Table 91: Properties of each reactant.

Id	Name	SBO
species_2	Bcp	

Kinetic Law

Derived unit contains undeclared units

$$v_{36} = \text{vol}(\text{cell}) \cdot \text{function}_2(V, [\text{species}_2], \text{Km})$$
 (115)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (116)

$$function_2\left(V, substrate, Km\right) = \frac{V \cdot substrate}{Km + substrate} \tag{117}$$

Table 92: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	vdbc	0.5	Ø
Km	Kd	0.3	\square

8.37 Reaction reaction_36

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

Name Bn phosphorylation

Reaction equation

$$species_3 \longrightarrow species_13$$
 (118)

Table 93: Properties of each reactant.

Id	Name	SBO
species_3	Bn	

Product

Table 94: Properties of each product.

Id	Name	SBO
species_13	Bnp	

Kinetic Law

Derived unit contains undeclared units

$$v_{37} = \text{vol}(\text{cell}) \cdot \text{function}_2(V, [\text{species}_3], \text{Km})$$
 (119)

$$function_2\left(V, substrate, Km\right) = \frac{V \cdot substrate}{Km + substrate} \tag{120}$$

$$function_2\left(V, substrate, Km\right) = \frac{V \cdot substrate}{Km + substrate} \tag{121}$$

Table 95: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
Λ	V3b	0.5	
Km	Kp	0.1	\checkmark

8.38 Reaction reaction_37

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

Name Bnp specific degradation

Reaction equation

$$species_{-}13 \longrightarrow \emptyset \tag{122}$$

Table 96: Properties of each reactant.

Id	Name	SBO
species_13	Bnp	

Kinetic Law

Derived unit contains undeclared units

$$v_{38} = \text{vol}(\text{cell}) \cdot \text{function}_2(V, [\text{species}_13], Km)$$
 (123)

$$function_2\left(V, substrate, Km\right) = \frac{V \cdot substrate}{Km + substrate} \tag{124} \label{eq:124}$$

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (125)

Table 97: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	vdbn	0.6	\square
Km	Kd	0.3	

8.39 Reaction reaction_38

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

Name In nonspecific degration

Reaction equation

$$species_15 \longrightarrow \emptyset \tag{126}$$

Reactant

Table 98: Properties of each reactant.

Id	Name	SBO
species_15	In	

Kinetic Law

Derived unit contains undeclared units

$$v_{39} = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{species}_15] \tag{127}$$

Table 99: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	kdn	0.01	

8.40 Reaction reaction_39

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

Name In specific degradation

Reaction equation

$$species_{-}15 \longrightarrow \emptyset \tag{128}$$

Reactant

Table 100: Properties of each reactant.

Id	Name	SBO
species_15	In	

Kinetic Law

Derived unit contains undeclared units

$$v_{40} = \text{vol}(\text{cell}) \cdot \text{function}_2(V, [\text{species}_15], \text{Km})$$
 (129)

$$function_{-}2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (130)

$$function_2\left(V, substrate, Km\right) = \frac{V \cdot substrate}{Km + substrate} \tag{131}$$

Table 101: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	vdin	0.8	$ \overline{\mathscr{A}} $
Km	Kd	0.3	\square

8.41 Reaction reaction_40

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

Name Bn nonspecific degradation

Reaction equation

species_3
$$\longrightarrow \emptyset$$
 (132)

Reactant

Table 102: Properties of each reactant.

Id	Name	SBO
species_3	Bn	

Kinetic Law

Derived unit contains undeclared units

$$v_{41} = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{species}_3]$$
 (133)

Table 103: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	kdn	0.01	$ \checkmark $

8.42 Reaction reaction_41

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

Name Bcp dephosphorylation

Reaction equation

$$species_2 \longrightarrow species_1 \tag{134}$$

Table 104: Properties of each reactant.

Id	Name	SBO
species_2	Bcp	

Product

Table 105: Properties of each product.

Id	Name	SBO
species_1	Bc	

Kinetic Law

Derived unit contains undeclared units

$$v_{42} = \text{vol}(\text{cell}) \cdot \text{function}_2(V, [\text{species}_2], Km)$$
 (135)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (136)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (137)

Table 106: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	V2b	0.1	
Km	Kdp	0.1	

8.43 Reaction reaction_42

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

Name Bnp dephosphorylation

$$species_13 \longrightarrow species_3$$
 (138)

Table 107: Properties of each reactant.

Id	Name	SBO
species_13	Bnp	

Product

Table 108: Properties of each product.

Id	Name	SBO
species_3	Bn	

Kinetic Law

Derived unit contains undeclared units

$$v_{43} = \text{vol}(\text{cell}) \cdot \text{function}_2(V, [\text{species}_13], Km)$$
 (139)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (140)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (141)

Table 109: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
Λ	V4b	0.2	\overline{Z}
Km	Kdp	0.1	$\overline{\mathbf{Z}}$

8.44 Reaction reaction_43

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

Name Ccp dephosphorylation

$$species_6 \longrightarrow species_4$$
 (142)

Table 110: Properties of each reactant.

Id	Name	SBO
species_6	Ccp	

Product

Table 111: Properties of each product.

Id	Name	SBO
species_4	Cc	

Kinetic Law

Derived unit contains undeclared units

$$v_{44} = \text{vol}(\text{cell}) \cdot \text{function}_2(V, [\text{species}_6], \text{Km})$$
 (143)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (144)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (145)

Table 112: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	V2c	0.1	
Km	Kdp	0.1	\checkmark

8.45 Reaction reaction_44

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

Name Pcp dephosphorylation

$$species_9 \longrightarrow species_8$$
 (146)

Table 113: Properties of each reactant.

Id	Name	SBO
species_9	Pcp	

Product

Table 114: Properties of each product.

Id	Name	SBO
species_8	Pc	

Kinetic Law

Derived unit contains undeclared units

$$v_{45} = \text{vol}(\text{cell}) \cdot \text{function} 2(V, [\text{species}_9], \text{Km})$$
 (147)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (148)

$$function_2\left(V, substrate, Km\right) = \frac{V \cdot substrate}{Km + substrate} \tag{149}$$

Table 115: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	V2p	0.3	\overline{Z}
Km	Kdp	0.1	$ \overline{\checkmark} $

8.46 Reaction reaction_45

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

Name PCnp dephosphorylation

$$species_{-}14 \longrightarrow species_{-}12 \tag{150}$$

Table 116: Properties of each reactant.

Id	Name	SBO
species_14	PCnp	

Product

Table 117: Properties of each product.

Id	Name	SBO
species_12	PCn	

Kinetic Law

Derived unit contains undeclared units

$$v_{46} = \text{vol}(\text{cell}) \cdot \text{function}_2(V, [\text{species}_14], \text{Km})$$
 (151)

$$function_{-}2\left(V, substrate, Km\right) = \frac{V \cdot substrate}{Km + substrate} \tag{152}$$

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (153)

Table 118: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
Λ	V4pc	0.1	$\overline{\checkmark}$
Km	Kdp	0.1	$\overline{\mathbf{Z}}$

8.47 Reaction reaction_46

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

Name PCn nonspecific degradation

$$species_{-}12 \longrightarrow \emptyset \tag{154}$$

Table 119: Properties of each reactant.

Id	Name	SBO
species_12	PCn	

Kinetic Law

Derived unit contains undeclared units

$$v_{47} = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{species}_12] \tag{155}$$

Table 120: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	kdn	0.01	

8.48 Reaction reaction_47

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

Name PCcp dephosphorylation

Reaction equation

$$species_11 \longrightarrow species_10$$
 (156)

Reactant

Table 121: Properties of each reactant.

Id	Name	SBO
species_11	PCcp	

Product

Table 122: Properties of each product.

Id	Name	SBO
species 10	PCc	

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_{48} = \text{vol}(\text{cell}) \cdot \text{function}_2(V, [\text{species}_11], Km)$$
 (157)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (158)

$$function_2(V, substrate, Km) = \frac{V \cdot substrate}{Km + substrate}$$
 (159)

Table 123: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	V2pc	0.1	
Km	Kdp	0.1	

9 Derived Rate Equations

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

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

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

9.1 Species species_0

Name Mb

Notes The initial concentration of Mb got from the curve in the paper at time=0

Initial concentration 9.5 nmol·l⁻¹

This species takes part in four reactions (as a reactant in reaction_2, reaction_24 and as a product in reaction_0 and as a modifier in reaction_1).

$$\frac{d}{dt} \text{species}_{0} = |v_{1}| - |v_{3}| - |v_{25}| \tag{160}$$

9.2 Species species_1

Name Bc

Notes In order to get the similar shape of the plot,we assigned 2nM as initial concentration for Bc

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

This species takes part in five reactions (as a reactant in reaction_3, reaction_4, reaction_34 and as a product in reaction_1, reaction_41).

$$\frac{d}{dt} \text{species}_{1} = |v_{2}| + |v_{42}| - |v_{4}| - |v_{5}| - |v_{35}|$$
(161)

9.3 Species species_2

Name Bcp

Initial concentration $0 \text{ nmol} \cdot 1^{-1}$

This species takes part in four reactions (as a reactant in reaction_18, reaction_35, reaction_41 and as a product in reaction_3).

$$\frac{d}{dt} \text{species}_2 = |v_4| - |v_{19}| - |v_{36}| - |v_{42}| \tag{162}$$

9.4 Species species_3

Name Bn

Initial concentration $1.9 \text{ nmol} \cdot l^{-1}$

This species takes part in eight reactions (as a reactant in reaction_23, reaction_36, reaction_40 and as a product in reaction_4, reaction_42 and as a modifier in reaction_0, reaction_9, reaction_20).

$$\frac{d}{dt} \text{species}_{3} = |v_{5}| + |v_{43}| - |v_{24}| - |v_{37}| - |v_{41}|$$
(163)

9.5 Species species_4

Name Cc

Initial concentration $0 \text{ nmol} \cdot 1^{-1}$

This species takes part in five reactions (as a reactant in reaction_7, reaction_13, reaction_28 and as a product in reaction_5, reaction_43).

$$\frac{d}{dt} \text{species}_{4} = |v_{6}| + |v_{44}| - |v_{8}| - |v_{14}| - |v_{29}|$$
(164)

9.6 Species species_5

Name Mc

Notes Initial concentration for Mc got from the value of the curve at time=0 in the paper.

Initial concentration $1.7 \text{ nmol} \cdot l^{-1}$

This species takes part in four reactions (as a reactant in reaction_6, reaction_25 and as a product in reaction_20 and as a modifier in reaction_5).

$$\frac{d}{dt} \text{species} = v_{21} - v_7 - v_{26} \tag{165}$$

9.7 Species species_6

Name Ccp

Initial concentration $0 \text{ nmol} \cdot l^{-1}$

This species takes part in four reactions (as a reactant in reaction_8, reaction_30, reaction_43 and as a product in reaction_7).

$$\frac{d}{dt} \text{species}_{6} = |v_{8}| - |v_{9}| - |v_{31}| - |v_{44}| \tag{166}$$

9.8 Species species_7

Name Mp

Notes Initial concentration for Mp got from the value of curve at time=0 in the paper.

Initial concentration $2.5 \text{ nmol} \cdot 1^{-1}$

This species takes part in four reactions (as a reactant in reaction_22, reaction_26 and as a product in reaction_9 and as a modifier in reaction_10).

$$\frac{d}{dt} \text{species}_{7} = |v_{10}| - |v_{23}| - |v_{27}| \tag{167}$$

9.9 Species species_8

Name Pc

Initial concentration $0 \text{ nmol} \cdot l^{-1}$

This species takes part in five reactions (as a reactant in reaction_12, reaction_13, reaction_27 and as a product in reaction_10, reaction_44).

$$\frac{d}{dt} \text{species}_{8} = |v_{11}| + |v_{45}| - |v_{13}| - |v_{14}| - |v_{28}|$$
(168)

9.10 Species species_9

Name Pcp

Initial concentration $0 \text{ nmol} \cdot l^{-1}$

This species takes part in four reactions (as a reactant in reaction_11, reaction_29, reaction_44 and as a product in reaction_12).

$$\frac{d}{dt} \text{species}_{9} = |v_{13}| - |v_{12}| - |v_{30}| - |v_{45}| \tag{169}$$

9.11 Species species_10

Name PCc

Initial concentration $0 \text{ nmol} \cdot l^{-1}$

This species takes part in five reactions (as a reactant in reaction_14, reaction_16, reaction_32 and as a product in reaction_13, reaction_47).

$$\frac{d}{dt} \text{species}_{10} = |v_{14}| + |v_{48}| - |v_{15}| - |v_{17}| - |v_{33}|$$
(170)

9.12 Species species_11

Name PCcp

Initial concentration $0 \text{ nmol} \cdot 1^{-1}$

This species takes part in four reactions (as a reactant in reaction_15, reaction_31, reaction_47 and as a product in reaction_14).

$$\frac{d}{dt} \text{species}_{-}11 = |v_{15}| - |v_{16}| - |v_{32}| - |v_{48}| \tag{171}$$

9.13 Species species_12

Name PCn

Initial concentration 1 nmol·l⁻¹

This species takes part in five reactions (as a reactant in reaction_21, reaction_23, reaction_46 and as a product in reaction_16, reaction_45).

$$\frac{d}{dt} \text{species}_{12} = |v_{17}| + |v_{46}| - |v_{22}| - |v_{24}| - |v_{47}|$$
(172)

9.14 Species species_13

Name Bnp

Initial concentration $0 \text{ nmol} \cdot l^{-1}$

This species takes part in four reactions (as a reactant in reaction_19, reaction_37, reaction_42 and as a product in reaction_36).

$$\frac{d}{dt} \text{species}_{13} = |v_{37}| - |v_{20}| - |v_{38}| - |v_{43}| \tag{173}$$

9.15 Species species_14

Name PCnp

Initial concentration $0 \text{ nmol} \cdot l^{-1}$

This species takes part in four reactions (as a reactant in reaction_17, reaction_33, reaction_45 and as a product in reaction_21).

$$\frac{d}{dt} \text{species}_{14} = |v_{22}| - |v_{18}| - |v_{34}| - |v_{46}| \tag{174}$$

9.16 Species species_15

Name In

Initial concentration $0 \text{ nmol} \cdot l^{-1}$

This species takes part in three reactions (as a reactant in reaction_38, reaction_39 and as a product in reaction_23).

$$\frac{d}{dt} \text{species}_{15} = |v_{24}| - |v_{39}| - |v_{40}| \tag{175}$$

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