# **SBML Model Report**

# Model name: "Bray1993\_chemotaxis"



May 6, 2016

# 1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following four authors: Nicolas Le Novre<sup>1</sup>, Lukas Endler<sup>2</sup>, Vijayalakshmi Chelliah<sup>3</sup> and Dennis Bray<sup>4</sup> at November third 2008 at 11:29 a. m. and last time modified at March eighth 2012 at 11:12 a. 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	29
events	2	constraints	0
reactions	35	function definitions	6
global parameters	7	unit definitions	0
rules	2	initial assignments	0

#### **Model Notes**

This version of the model is very close to the version described in the paper with one exception: the binding of aspartate to the various receptor complexes, as well as the formation of the different complexes are modeled using chemical kinetics (mass action law), rather than instant

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equilibrium. The qualitative behaviour of the model is unchanged. Note that in order to quantitatively replicate the figure 8b, and in particular to have a basal bias of 0.7, we have to change the rate constant of the aspartate-triggered dephosphorylation of CheY from 59000 to 70000. The peaks have then slightly different values.

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

# 2.1 Unit substance

**Notes** Mole is the predefined SBML unit for substance.

**Definition** mol

#### 2.2 Unit volume

**Notes** Litre is the predefined SBML unit for volume.

**Definition** 1

#### 2.3 Unit area

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

**Definition** m<sup>2</sup>

#### 2.4 Unit length

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

**Definition** m

#### 2.5 Unit time

**Notes** Second is the predefined SBML unit for time.

**Definition** s

# 3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
cell	cell	0000290	3	$1.41 \cdot 10^{-15}$	1	<b>√</b>	

# 3.1 Compartment cell

This is a three dimensional compartment with a constant size of  $1.41 \cdot 10^{-15}$  litre.

Name cell

SBO:0000290 physical compartment

# 4 Species

This model contains 29 species. The boundary condition of three of these species is set to true so that these species' amount cannot be changed by any reaction. Section 10 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
asp	asp	cell	$\text{mol} \cdot l^{-1}$		
ni	ni	cell	$\text{mol} \cdot l^{-1}$		$\square$
T	T	cell	$\text{mol} \cdot l^{-1}$		
Tasp	Tasp	cell	$\text{mol} \cdot l^{-1}$		
Tni	Tni	cell	$\text{mol} \cdot l^{-1}$		
W	W	cell	$\text{mol} \cdot l^{-1}$		
TW	TW	cell	$\text{mol} \cdot l^{-1}$	$\Box$	
${\tt Tasp\_W}$	$Tasp_W$	cell	$\text{mol} \cdot l^{-1}$	$\Box$	$\Box$
$\mathtt{Tni}_{-}\mathtt{W}$	$\mathrm{Tni}_{-}\mathrm{W}$	cell	$\text{mol} \cdot l^{-1}$	$\Box$	$\Box$
TA	TA	cell	$\text{mol} \cdot l^{-1}$	$\Box$	$\Box$
Tasp_A	Tasp_A	cell	$\text{mol} \cdot l^{-1}$		
$\mathtt{Tni}_{-}\mathtt{A}$	Tni_A	cell	$\text{mol} \cdot l^{-1}$		
WA	WA	cell	$\text{mol} \cdot l^{-1}$		
TWA	TWA	cell	$\text{mol} \cdot l^{-1}$	$\Box$	
${\tt Tasp\_WA}$	Tasp_WA	cell	$\text{mol} \cdot l^{-1}$	$\Box$	$\Box$
${\tt Tni\_WA}$	$Tni_{-}WA$	cell	$\text{mol} \cdot l^{-1}$	$\Box$	
A	A	cell	$\text{mol} \cdot l^{-1}$	$\Box$	
Ap	Ap	cell	$\text{mol} \cdot l^{-1}$	$\Box$	
В	В	cell	$\text{mol} \cdot l^{-1}$	$\Box$	$\Box$
Вр	Вр	cell	$\text{mol} \cdot l^{-1}$	$\Box$	$\Box$
Z	Z	cell	$\text{mol} \cdot l^{-1}$		

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
Y	Y	cell	$\text{mol} \cdot l^{-1}$		
Yp	Yp	cell	$\text{mol} \cdot l^{-1}$		
M	M	cell	$\operatorname{mol} \cdot 1^{-1}$		
MYp	MYp	cell	$\operatorname{mol} \cdot 1^{-1}$		
MYpYp	MYpYp	cell	$\operatorname{mol} \cdot 1^{-1}$		
MYpYpYp	MYpYpYp	cell	$\operatorname{mol} \cdot 1^{-1}$		
MYpYpYpYp	MYpYpYpYp	cell	$\operatorname{mol} \cdot 1^{-1}$		
${ t species\_1}$	ATP	cell	$\text{mol} \cdot l^{-1}$		

## **5 Parameters**

This model contains seven global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
alpha	alpha		0.140		
kappa	kappa		$2.25 \cdot 10^{-7}$		$\mathbf{Z}$
ka	ka		0.100		$\mathbf{Z}$
Bias	Bias		0.701		
$parameter_1$	asp_pulse		$10^{-7}$		$\mathbf{Z}$
$parameter_2$	autoPhospho		0.997		
${\tt parameter\_3}$	KmATP		$3 \cdot 10^{-4}$		

# 6 Function definitions

This is an overview of six function definitions.

#### **6.1 Function definition** function\_4\_motor\_r1

Name function\_4\_motor\_r1

Arguments [M], [MYp], [Yp], vol (cell), ka, kappa

**Mathematical Expression** 

$$\frac{ka \cdot \left([M] \cdot [Yp] - \frac{kappa}{4} \cdot [MYp]\right)}{vol\left(cell\right)} \tag{1}$$

#### **6.2 Function definition** function\_4\_motor\_r2

Name function\_4\_motor\_r2

Arguments [MYp], [MYpYp], [Yp], alpha, vol (cell), ka, kappa

# **Mathematical Expression**

$$\frac{ka \cdot \left( [MYp] \cdot [Yp] - \frac{2 \cdot alpha \cdot kappa}{3} \cdot [MYpYp] \right)}{vol (cell)}$$
 (2)

# **6.3 Function definition** function\_4\_motor\_r3

Name function\_4\_motor\_r3

Arguments [MYpYp], [MYpYpYp], [Yp], alpha, vol (cell), ka, kappa

#### **Mathematical Expression**

$$\frac{ka \cdot \left( [MYpYp] \cdot [Yp] - \frac{3 \cdot alpha \cdot alpha \cdot kappa}{2} \cdot [MYpYpYp] \right)}{\text{vol (cell)}}$$
(3)

#### **6.4 Function definition** function\_4\_motor\_r4

Name function\_4\_motor\_r4

Arguments [MYpYpYp], [MYpYpYpYp], [Yp], alpha, vol (cell), ka, kappa

#### **Mathematical Expression**

$$\frac{ka \cdot ([MYpYpYp] \cdot [Yp] - 4 \cdot alpha \cdot alpha \cdot alpha \cdot kappa \cdot [MYpYpYpYp])}{vol(cell)}(4)$$

### 6.5 Function definition Autophosphorylation

Name Autophosphorylation

**Arguments** kcat, correction, E

#### **Mathematical Expression**

$$kcat \cdot correction \cdot E$$
 (5)

## **6.6 Function definition** ModAutophosphorylation

Name ModAutophosphorylation

Arguments [M], S, kcat, correction

# **Mathematical Expression**

$$[M] \cdot S \cdot kcat \cdot correction$$
 (6)

#### 7 Rules

This is an overview of two rules.

#### 7.1 Rule Bias

Rule Bias is an assignment rule for parameter Bias:

$$Bias = \frac{[M] + [MYp]}{[M] + [MYp] + [MYpYp] + [MYpYpYp] + [MYpYpYpYp]}$$
 (7)

**Derived unit** dimensionless

### 7.2 Rule parameter\_2

Rule parameter\_2 is an assignment rule for parameter parameter\_2:

$$parameter_2 = \frac{[species_1]}{[species_1] + parameter_3}$$
 (8)

# 8 Events

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

#### 8.1 Event event\_1

Name Add ASP

time 
$$\geq 5$$
 (9)

# **Assignment**

$$asp = parameter_1 \tag{10}$$

# **8.2 Event** event\_2

Name Remove ASP

$$time \ge 10 \tag{11}$$

$$asp = 0 (12)$$

# 9 Reactions

This model contains 35 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

N⁰	Id	Name	Reaction Equation	SBO
1	phosphorylation- _r1	A->Ap	$A \longrightarrow Ap$	0000216
2	phosphorylation- _r2	TWA+A->TWA+Ap	$A \xrightarrow{TWA} Ap$	0000216
3	phosphorylation- _r3	Tni_WA+A->Tni_WA+Ap	$A \xrightarrow{\mathbf{Tni}_{-}\mathbf{WA}} \mathbf{Ap}$	0000216
4	phosphorylation- _r4	Tasp_WA+Yp->Tasp_WA+Y	$Tasp\_WA + Yp \longrightarrow Tasp\_WA + Y$	0000330
5	phosphorylation- _r5	Ap+Y->A+Yp	$Ap + Y \longrightarrow A + Yp$	0000216
6	phosphorylation- _r6	Y ->Yp	$Y \longrightarrow Yp$	0000216
7	phosphorylation- r7	Yp->Y	$Yp \longrightarrow Y$	0000330
8	phosphorylation- _r8	Yp+Z->Y+Z	$Yp + Z \longrightarrow Y + Z$	0000330
9	phosphorylation- r9	Ap+B->A+Bp	$Ap + B \longrightarrow A + Bp$	0000402
10	phosphorylation- _r10	Bp->B	$Bp \longrightarrow B$	0000330
11 12		T+asp<->Tasp T+ni<->Tni	$T + asp \Longrightarrow Tasp$ $T + ni \Longrightarrow Tni$	0000177 0000177

N⁰	Id	Name	Reaction Equation	SBO
13	regulatory_r3	T+W<->TW	$T + W \Longrightarrow TW$	0000177
14	regulatory_r4	T+A<->TA	$T + A \rightleftharpoons TA$	0000177
15	regulatory_r5	W+A<->WA	$W + A \Longrightarrow WA$	0000177
16	regulatory_r6	TW+A<->TWA	$TW + A \Longrightarrow TWA$	0000177
17	regulatory_r7	TA+W<->TWA	$TA + W \Longrightarrow TWA$	0000177
18	regulatory_r8	T+WA<->TWA	$T + WA \Longrightarrow TWA$	0000177
19	regulatory_r9	Tasp+W<->Tasp_W	$Tasp + W \Longrightarrow Tasp_W$	0000177
20	regulatory_r10	Tasp+A<->Tasp_A	$Tasp + A \rightleftharpoons Tasp\_A$	0000177
21	regulatory_r11	Tasp_W+A<->Tasp_WA	$Tasp_W + A \Longrightarrow Tasp_WA$	0000177
22	regulatory_r12	Tasp_A+W<->Tasp_WA	$Tasp_A + W \Longrightarrow Tasp_WA$	0000177
23	regulatory_r13	Tasp+WA<->Tasp_WA	$Tasp + WA \Longrightarrow Tasp_WA$	0000177
24	regulatory_r14	Tni+W<->Tni_W	$Tni + W \Longrightarrow Tni_W$	0000177
25	regulatory_r15	Tni+A<->Tni_A	$Tni + A \Longrightarrow Tni\_A$	0000177
26	regulatory_r16	$Tni_W+A<->Tni_WA$	$Tni_W + A \rightleftharpoons Tni_WA$	0000177
27	regulatory_r17	Tni_A+W<->Tni_WA	$Tni_A + W \Longrightarrow Tni_WA$	0000177
28	regulatory_r18	Tni+WA<->Tni_WA	$Tni + WA \Longrightarrow Tni_WA$	0000177
29	motor_r1	M+Yp<->MYp	$M + Yp \Longrightarrow MYp$	0000177
30	motor_r2	MYp+Yp<->MYpYp	$MYp + Yp \Longrightarrow MYpYp$	0000177
31	motor_r3	MYpYp+Yp<->MYpYpYp	$MYpYp + Yp \Longrightarrow MYpYpYp$	0000177
32	motor_r4	MYpYpYp+Yp<->MYpYpYpYp	$MYpYpYp + Yp \Longrightarrow MYpYpYpYp$	0000177
33	${\tt reaction\_1}$	$TA + asp < -> Tasp_A$	$TA + asp \Longrightarrow Tasp\_A$	0000177
34	${\tt reaction\_2}$	TW+asp <-> Tasp_W	$TW + asp \Longrightarrow Tasp_W$	0000177
35	$reaction_3$	TWA+asp <-> Tasp_WA	$TWA + asp \Longrightarrow Tasp_WA$	0000177

# **9.1 Reaction** phosphorylation\_r1

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

Name A->Ap

SBO:0000216 phosphorylation

# **Reaction equation**

$$A \longrightarrow Ap$$
 (13)

#### Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
A	A	

#### **Product**

Table 7: Properties of each product.

Id	Name	SBO
Ap	Ap	

#### **Kinetic Law**

$$v_1 = \text{vol}(\text{cell}) \cdot \text{Autophosphorylation}(\text{kcat}, \text{parameter}\_2, [A])$$
 (14)

Autophosphorylation (kcat, correction, 
$$E$$
) = kcat · correction ·  $E$  (15)

Autophosphorylation (kcat, correction, 
$$E$$
) = kcat · correction ·  $E$  (16)

Table 8: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
kcat	kcat	0.001	

# **9.2 Reaction** phosphorylation\_r2

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

Name TWA+A->TWA+Ap

SBO:0000216 phosphorylation

# **Reaction equation**

$$A \xrightarrow{TWA} Ap \tag{17}$$

#### Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
Α	A	

#### **Modifier**

Table 10: Properties of each modifier.

Id	Name	SBO
TWA	TWA	

#### **Product**

Table 11: Properties of each product.

Id	Name	SBO
Ap	Ap	

#### **Kinetic Law**

$$v_2 = \text{vol}(\text{cell}) \cdot \text{ModAutophosphorylation}([\text{TWA}], [\text{A}], \text{kcat}, \text{parameter}\_2)$$
 (18)

$$ModAutophosphorylation([M], S, kcat, correction) = [M] \cdot S \cdot kcat \cdot correction$$
 (19)

$$ModAutophosphorylation([M], S, kcat, correction) = [M] \cdot S \cdot kcat \cdot correction \qquad (20)$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcat	kcat	7	5000.0		

# **9.3 Reaction** phosphorylation\_r3

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

Name  $Tni_WA+A->Tni_WA+Ap$ 

SBO:0000216 phosphorylation

# **Reaction equation**

$$A \xrightarrow{Tni\_WA} Ap \tag{21}$$

#### Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
A	A	

#### **Modifier**

Table 14: Properties of each modifier.

Id	Name	SBO
Tni_WA	Tni_WA	

#### **Product**

Table 15: Properties of each product.

Id	Name	SBO
Ap	Ap	

#### **Kinetic Law**

$$v_3 = \text{vol}(\text{cell}) \cdot \text{ModAutophosphorylation}([\text{Tni\_WA}], [A], \text{kcat}, \text{parameter\_2})$$
 (22)

$$ModAutophosphorylation ([M], S, kcat, correction) = [M] \cdot S \cdot kcat \cdot correction$$
 (23)

$$ModAutophosphorylation ([M], S, kcat, correction) = [M] \cdot S \cdot kcat \cdot correction \tag{24}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcat	kcat		200000.0		

# **9.4 Reaction** phosphorylation\_r4

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

Name  $Tasp_WA+Yp->Tasp_WA+Y$ 

SBO:0000330 dephosphorylation

#### **Reaction equation**

$$Tasp\_WA + Yp \longrightarrow Tasp\_WA + Y \tag{25}$$

#### **Reactants**

Table 17: Properties of each reactant.

Id	Name	SBO
${\tt Tasp\_WA}$	Tasp_WA	
Yp	Yp	

#### **Products**

Table 18: Properties of each product.

Id	Name	SBO
Tasp_WA	Tasp_WA	
Y	Y	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_4 = \text{vol}\left(\text{cell}\right) \cdot \text{k1} \cdot \left[\text{Tasp\_WA}\right] \cdot \left[\text{Yp}\right] \tag{26}$$

Table 19: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	$10^{8}$	$\checkmark$

# **9.5 Reaction** phosphorylation\_r5

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

Name Ap+Y->A+Yp

SBO:0000216 phosphorylation

# **Reaction equation**

$$Ap + Y \longrightarrow A + Yp \tag{27}$$

#### **Reactants**

Table 20: Properties of each reactant.

Id	Name	SBO
Ap Y	Ap Y	

#### **Products**

Table 21: Properties of each product.

Id	Name	SBO
Α	A	
Υp	Yp	

#### **Kinetic Law**

$$v_5 = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{Ap}] \cdot [\text{Y}]$$
 (28)

Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		200000.0		$\overline{Z}$

# **9.6 Reaction** phosphorylation\_r6

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

Name  $Y \rightarrow Yp$ 

SBO:0000216 phosphorylation

# **Reaction equation**

$$Y \longrightarrow Yp$$
 (29)

#### Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
Y	Y	

#### **Product**

Table 24: Properties of each product.

Id	Name	SBO
Yр	Yp	

#### **Kinetic Law**

$$v_6 = \text{vol}(\text{cell}) \cdot \text{Autophosphorylation}(\text{kcat}, \text{parameter}\_2, [Y])$$
 (30)

Autophosphorylation (kcat, correction, 
$$E$$
) = kcat · correction ·  $E$  (31)

Autophosphorylation (kcat, correction, 
$$E$$
) = kcat · correction ·  $E$  (32)

Table 25: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
kcat	kcat	0.0	

# **9.7 Reaction** phosphorylation\_r7

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

Name Yp->Y

SBO:0000330 dephosphorylation

# **Reaction equation**

$$Yp \longrightarrow Y$$
 (33)

#### Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
Υр	Yp	

# **Product**

Table 27: Properties of each product.

Id	Name	SBO
Y	Y	

#### **Kinetic Law**

$$v_7 = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{Yp}] \tag{34}$$

Table 28: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.037	

# **9.8 Reaction** phosphorylation\_r8

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

Name Yp+Z->Y+Z

SBO:0000330 dephosphorylation

# **Reaction equation**

$$Yp + Z \longrightarrow Y + Z$$
 (35)

#### **Reactants**

Table 29: Properties of each reactant.

Id	Name	SBO
Υp	Yp	
Z	Z	

#### **Products**

Table 30: Properties of each product.

Id	Name	SBO
Y	Y	
Z	Z	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_8 = vol\left(cell\right) \cdot k1 \cdot [Yp] \cdot [Z] \tag{36}$$

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	5	0.00000		$\overline{Z}$

# **9.9 Reaction** phosphorylation\_r9

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

Name Ap+B->A+Bp

SBO:0000402 transfer of a chemical group

# **Reaction equation**

$$Ap + B \longrightarrow A + Bp$$
 (37)

#### **Reactants**

Table 32: Properties of each reactant.

Id	Name	SBO
Ap	Ap	
В	В	

#### **Products**

Table 33: Properties of each product.

Id	Name	SBO
Α	A	
Вр	Bp	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_9 = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{Ap}] \cdot [\text{B}]$$
(38)

Table 34: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	10	0.000000		Ø

# **9.10 Reaction** phosphorylation\_r10

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

Name Bp->B

SBO:0000330 dephosphorylation

# **Reaction equation**

$$Bp \longrightarrow B$$
 (39)

#### Reactant

Table 35: Properties of each reactant.

Id	Name	SBO
Вр	Bp	

#### **Product**

Table 36: Properties of each product.

Id	Name	SBO
В	В	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{10} = \text{vol}(\text{cell}) \cdot \text{k1} \cdot [\text{Bp}] \tag{40}$$

Table 37: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	1.0	$\checkmark$

# **9.11 Reaction** regulatory\_r1

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

Name T+asp<->Tasp

SBO:0000177 non-covalent binding

# **Reaction equation**

$$T + asp \Longrightarrow Tasp$$
 (41)

Table 38: Properties of each reactant.

Id	Name	SBO
Т	Т	
asp	asp	

Table 39: Properties of each product.

Id	Name	SBO
Tasp	Tasp	

# **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{11} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{T}] \cdot [\text{asp}] - \text{k2} \cdot [\text{Tasp}])$$
(42)

Table 40: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	1000000.0	$\square$
k2	k2	1.0	$\square$

# **9.12 Reaction** regulatory\_r2

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

Name T+ni<->Tni

SBO:0000177 non-covalent binding

# **Reaction equation**

$$T + ni \rightleftharpoons Tni$$
 (43)

Table 41: Properties of each reactant.

Id	Name	SBO
Т	T	
ni	ni	

Table 42: Properties of each product.

Id	Name	SBO
Tni	Tni	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{12} = \text{vol}\left(\text{cell}\right) \cdot \left(\text{k1} \cdot [\text{T}] \cdot [\text{ni}] - \text{k2} \cdot [\text{Tni}]\right) \tag{44}$$

Table 43: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	1000.0	Ø
k2	k2	1.0	

# **9.13 Reaction** regulatory\_r3

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

Name T+W<->TW

SBO:0000177 non-covalent binding

# **Reaction equation**

$$T + W \rightleftharpoons TW$$
 (45)

Table 44: Properties of each reactant.

Id	Name	SBO
Т	T	
W	W	

Table 45: Properties of each product.

Id	Name	SBO
TW	TW	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$\nu_{13} = vol\left(cell\right) \cdot \left(k1 \cdot [T] \cdot [W] - k2 \cdot [TW]\right) \tag{46}$$

Table 46: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	100000.0	
k2	k2	1.0	$\square$

# **9.14 Reaction** regulatory\_r4

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

Name T+A <-> TA

SBO:0000177 non-covalent binding

# **Reaction equation**

$$T + A \rightleftharpoons TA$$
 (47)

Table 47: Properties of each reactant.

Id	Name	SBO
Т	T	
Α	A	

Table 48: Properties of each product.

Id	Name	SBO
TA	TA	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{14} = \text{vol}\left(\text{cell}\right) \cdot \left(\text{k1} \cdot [\text{T}] \cdot [\text{A}] - \text{k2} \cdot [\text{TA}]\right) \tag{48}$$

Table 49: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	10000.0	lacksquare
k2	k2	1.0	Ø

# **9.15 Reaction** regulatory\_r5

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

Name W+A<->WA

SBO:0000177 non-covalent binding

# **Reaction equation**

$$W + A \Longrightarrow WA$$
 (49)

Table 50: Properties of each reactant.

Id	Name	SBO
W	W	
A	A	

Table 51: Properties of each product.

Id	Name	SBO
WA	WA	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{15} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{W}] \cdot [\text{A}] - \text{k2} \cdot [\text{WA}])$$
(50)

Table 52: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	100000.0	
k2	k2	1.0	$\square$

# **9.16 Reaction** regulatory\_r6

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

Name TW+A<->TWA

SBO:0000177 non-covalent binding

# **Reaction equation**

$$TW + A \rightleftharpoons TWA$$
 (51)

Table 53: Properties of each reactant.

Id	Name	SBO
TW	TW	
Α	A	

Table 54: Properties of each product.

Id	Name	SBO
TWA	TWA	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{16} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{TW}] \cdot [\text{A}] - \text{k2} \cdot [\text{TWA}])$$
(52)

Table 55: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	400000.0	
k2	k2	1.0	$\square$

# **9.17 Reaction** regulatory\_r7

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

Name TA+W<->TWA

SBO:0000177 non-covalent binding

# **Reaction equation**

$$TA + W \rightleftharpoons TWA$$
 (53)

Table 56: Properties of each reactant.

Id	Name	SBO
TA	TA	
W	$\mathbf{W}$	

Table 57: Properties of each product.

Id	Name	SBO
TWA	TWA	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{17} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{TA}] \cdot [\text{W}] - \text{k2} \cdot [\text{TWA}])$$
(54)

Table 58: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	400000.0	
k2	k2	1.0	$\square$

# **9.18 Reaction** regulatory\_r8

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

Name T+WA < -> TWA

SBO:0000177 non-covalent binding

# **Reaction equation**

$$T + WA \Longrightarrow TWA$$
 (55)

Table 59: Properties of each reactant.

Id	Name	SBO
Т	T	
WA	WA	

Table 60: Properties of each product.

Id	Name	SBO
TWA	TWA	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{18} = \text{vol}\left(\text{cell}\right) \cdot \left(\text{k1} \cdot [\text{T}] \cdot [\text{WA}] - \text{k2} \cdot [\text{TWA}]\right) \tag{56}$$

Table 61: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	400000.0	
k2	k2	1.0	$\square$

# **9.19 Reaction** regulatory\_r9

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

Name  $Tasp+W<->Tasp_W$ 

SBO:0000177 non-covalent binding

# **Reaction equation**

$$Tasp + W \Longrightarrow Tasp_W \tag{57}$$

Table 62: Properties of each reactant.

Id	Name	SBO
Tasp W	Tasp W	

Table 63: Properties of each product.

Id	Name	SBO
Tasp_W	Tasp_W	

# **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{19} = \text{vol}\left(\text{cell}\right) \cdot \left(\text{k1} \cdot [\text{Tasp}] \cdot [\text{W}] - \text{k2} \cdot [\text{Tasp}_{-}\text{W}]\right) \tag{58}$$

Table 64: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	100000.0	
k2	k2	1.0	$\square$

# **9.20 Reaction** regulatory\_r10

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

Name Tasp+A<->Tasp\_A

SBO:0000177 non-covalent binding

# **Reaction equation**

$$Tasp + A \Longrightarrow Tasp\_A \tag{59}$$

Table 65: Properties of each reactant.

Id	Name	SBO
Tasp	Tasp	
A	A	

Table 66: Properties of each product.

Id	Name	SBO
Tasp_A	Tasp_A	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{20} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{Tasp}] \cdot [\text{A}] - \text{k2} \cdot [\text{Tasp\_A}])$$
(60)

Table 67: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	10000.0	lacksquare
k2	k2	1.0	Ø

# **9.21 Reaction** regulatory\_r11

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

Name  $Tasp_W+A<->Tasp_WA$ 

SBO:0000177 non-covalent binding

# **Reaction equation**

$$Tasp_W + A \Longrightarrow Tasp_WA \tag{61}$$

Table 68: Properties of each reactant.

SBO	Name	Id
	Tasp_W	Tasp_W
	A	Α

Table 69: Properties of each product.

Id	Name	SBO
${\tt Tasp\_WA}$	Tasp_WA	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{21} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{Tasp\_W}] \cdot [\text{A}] - \text{k2} \cdot [\text{Tasp\_WA}])$$
(62)

Table 70: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	400000.0	$\overline{Z}$
k2	k2	1.0	

# **9.22 Reaction** regulatory\_r12

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

Name Tasp\_A+W<->Tasp\_WA

SBO:0000177 non-covalent binding

# **Reaction equation**

$$Tasp\_A + W \Longrightarrow Tasp\_WA \tag{63}$$

Table 71: Properties of each reactant.

Name	SBO
Tasp_A W	
	Tasp_A

Table 72: Properties of each product.

Id	Name	SBO
${\tt Tasp\_WA}$	Tasp_WA	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{22} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{Tasp\_A}] \cdot [\text{W}] - \text{k2} \cdot [\text{Tasp\_WA}])$$
(64)

Table 73: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	400000.0	
k2	k2	1.0	$\square$

# **9.23 Reaction** regulatory\_r13

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

Name Tasp+WA<->Tasp\_WA

SBO:0000177 non-covalent binding

# **Reaction equation**

$$Tasp + WA \Longrightarrow Tasp_WA \tag{65}$$

Table 74: Properties of each reactant.

Id	Name	SBO
Tasp WA	Tasp WA	

Table 75: Properties of each product.

Id	Name	SBO
Tasp_WA	Tasp_WA	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{23} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{Tasp}] \cdot [\text{WA}] - \text{k2} \cdot [\text{Tasp}_{-}\text{WA}])$$
(66)

Table 76: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	400000.0	$\overline{Z}$
k2	k2	1.0	

# **9.24 Reaction** regulatory\_r14

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

Name  $Tni+W < -> Tni_W$ 

SBO:0000177 non-covalent binding

# **Reaction equation**

$$Tni + W \rightleftharpoons Tni_W$$
 (67)

Table 77: Properties of each reactant.

Id	Name	SBO
Tni	Tni	
W	W	

Table 78: Properties of each product.

Id	Name	SBO
Tni_W	$Tni_{-}W$	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{24} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{Tni}] \cdot [\text{W}] - \text{k2} \cdot [\text{Tni}_{-}\text{W}])$$
(68)

Table 79: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.1	
k2	k2	1.0	

# **9.25 Reaction** regulatory\_r15

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

Name  $Tni+A < -> Tni\_A$ 

SBO:0000177 non-covalent binding

# **Reaction equation**

$$Tni + A \rightleftharpoons Tni A$$
 (69)

Table 80: Properties of each reactant.

Id	Name	SBO
Tni	Tni	
Α	A	

Table 81: Properties of each product.

Id	Name	SBO
Tni_A	Tni_A	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{25} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{Tni}] \cdot [\text{A}] - \text{k2} \cdot [\text{Tni}\_{\text{A}}])$$
(70)

Table 82: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.01	
k2	k2	1.00	

# **9.26 Reaction** regulatory\_r16

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

Name  $Tni_W+A<->Tni_WA$ 

SBO:0000177 non-covalent binding

# **Reaction equation**

$$Tni_W + A \Longrightarrow Tni_WA$$
 (71)

Table 83: Properties of each reactant.

Id	Name	SBO
Tni_W	Tni_W	
A	A	

Table 84: Properties of each product.

Id	Name	SBO
Tni_WA	Tni_WA	

### **Kinetic Law**

Derived unit contains undeclared units

$$v_{26} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{Tni}_{-}\text{W}] \cdot [\text{A}] - \text{k2} \cdot [\text{Tni}_{-}\text{WA}])$$
(72)

Table 85: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.4	
k2	k2	1.0	

# **9.27 Reaction** regulatory\_r17

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

Name  $Tni_A+W<->Tni_WA$ 

SBO:0000177 non-covalent binding

# **Reaction equation**

$$Tni_A + W \Longrightarrow Tni_WA$$
 (73)

Table 86: Properties of each reactant.

Id	Name	SBO
Tni_A	Tni_A	
W	W	

Table 87: Properties of each product.

Id	Name	SBO
Tni_WA	Tni_WA	

### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{27} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{Tni}\_\text{A}] \cdot [\text{W}] - \text{k2} \cdot [\text{Tni}\_\text{WA}])$$
(74)

Table 88: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.4	$\overline{Z}$
k2	k2	1.0	

# 9.28 Reaction regulatory\_r18

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

Name Tni+WA<->Tni\_WA

SBO:0000177 non-covalent binding

# **Reaction equation**

$$Tni + WA \Longrightarrow Tni_WA$$
 (75)

Table 89: Properties of each reactant.

Id	Name	SBO
Tni	Tni	
WA	WA	

Table 90: Properties of each product.

Id	Name	SBO
Tni_WA	Tni_WA	

### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{28} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{Tni}] \cdot [\text{WA}] - \text{k2} \cdot [\text{Tni}_{\text{W}}])$$
(76)

Table 91: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.4	Ø
k2	k2	1.0	$\square$

# 9.29 Reaction motor\_r1

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

Name M+Yp<->MYp

SBO:0000177 non-covalent binding

# **Reaction equation**

$$M + Yp \rightleftharpoons MYp$$
 (77)

Table 92: Properties of each reactant.

Id	Name	SBO
M	M	
Yр	Yp	

Table 93: Properties of each product.

Id	Name	SBO
МҮр	MYp	-

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_{29} = \text{vol}(\text{cell}) \cdot \text{function\_4\_motor\_r1}([M], [MYp], [Yp], \text{vol}(\text{cell}), \text{ka}, \text{kappa})$$
 (78)

$$\begin{aligned} & \text{function\_4\_motor\_r1}\left([M],[MYp],[Yp],\text{vol}\left(\text{cell}\right),\text{ka},\text{kappa}\right) \\ & = \frac{\text{ka}\cdot\left([M]\cdot[Yp] - \frac{\text{kappa}}{4}\cdot[MYp]\right)}{\text{vol}\left(\text{cell}\right)} \end{aligned} \tag{79}$$

$$\begin{split} & \text{function\_4\_motor\_r1}\left([M],[MYp],[Yp],\text{vol}\left(\text{cell}\right),\text{ka},\text{kappa}\right) \\ & = \frac{\text{ka}\cdot\left([M]\cdot[Yp] - \frac{\text{kappa}}{4}\cdot[MYp]\right)}{\text{vol}\left(\text{cell}\right)} \end{split} \tag{80}$$

### 9.30 Reaction motor\_r2

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

Name MYp+Yp<->MYpYp

SBO:0000177 non-covalent binding

### **Reaction equation**

$$MYp + Yp \rightleftharpoons MYpYp$$
 (81)

Table 94: Properties of each reactant.

Id	Name	SBO
МҮр	MYp	
Yр	Yp	

Table 95: Properties of each product.

Id	Name	SBO
МҮрҮр	MYpYp	

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_{30} = \text{vol}(\text{cell}) \cdot \text{function\_4\_motor\_r2}([\text{MYp}], [\text{MYpYp}], [\text{Yp}], \text{alpha}, \text{vol}(\text{cell}), \text{ka}, \text{kappa})$$
 (82)

$$\begin{aligned} & \text{function\_4\_motor\_r2} \left( [MYp], [MYpYp], [Yp], \text{alpha}, \text{vol} \left( \text{cell} \right), \text{ka}, \text{kappa} \right) \\ &= \frac{\text{ka} \cdot \left( [MYp] \cdot [Yp] - \frac{2 \cdot \text{alpha} \cdot \text{kappa}}{3} \cdot [MYpYp] \right)}{\text{vol} \left( \text{cell} \right)} \end{aligned} \tag{83}$$

$$\begin{aligned} & \text{function\_4\_motor\_r2} \left( [MYp], [MYpYp], [Yp], \text{alpha}, \text{vol} \left( \text{cell} \right), \text{ka}, \text{kappa} \right) \\ &= \frac{\text{ka} \cdot \left( [MYp] \cdot [Yp] - \frac{2 \cdot \text{alpha} \cdot \text{kappa}}{3} \cdot [MYpYp] \right)}{\text{vol} \left( \text{cell} \right)} \end{aligned} \tag{84}$$

### 9.31 Reaction motor\_r3

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

Name MYpYp+Yp<->MYpYpYp

SBO:0000177 non-covalent binding

### **Reaction equation**

$$MYpYp + Yp \rightleftharpoons MYpYpYp \tag{85}$$

Table 96: Properties of each reactant.

Id	Name	SBO
МҮрҮр	MYpYp	
Yр	Yp	

Table 97: Properties of each product.

Id	Name	SBO
МҮрҮрҮр	MYpYpYp	

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_{31} = \text{vol} (\text{cell}) \cdot \text{function\_4\_motor\_r3} ([\text{MYpYp}], [\text{MYpYpYp}], [\text{Yp}], \text{alpha}, \text{vol} (\text{cell}), \text{ka}, \text{kappa})$$
(86)

$$\begin{aligned} & \text{function\_4\_motor\_r3}\left([MYpYp],[MYpYpYp],[Yp],\text{alpha},\text{vol}\left(\text{cell}\right),\text{ka},\text{kappa}\right) \\ & = \frac{\text{ka}\cdot\left([MYpYp]\cdot[Yp] - \frac{3\cdot\text{alpha}\cdot\text{alpha}\cdot\text{kappa}}{2}\cdot[MYpYpYp]\right)}{\text{vol}\left(\text{cell}\right)} \end{aligned} \tag{87}$$

$$function\_4\_motor\_r3\left([MYpYp],[MYpYpYp],[Yp],alpha,vol\left(cell\right),ka,kappa\right) \\ = \frac{ka\cdot\left([MYpYp]\cdot[Yp] - \frac{3\cdot alpha\cdot alpha\cdot kappa}{2}\cdot[MYpYpYp]\right)}{vol\left(cell\right)}$$
 (88)

### 9.32 Reaction motor\_r4

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

Name MYpYpYp+Yp<->MYpYpYpYp

SBO:0000177 non-covalent binding

### **Reaction equation**

$$MYpYpYp + Yp \Longrightarrow MYpYpYpYp$$
 (89)

Table 98: Properties of each reactant.

Id	Name	SBO
МҮрҮрҮр	MYpYpYp	
Yp	Yp	

Table 99: Properties of each product.

Id	Name	SBO
МҮрҮрҮр	MYpYpYpYp	

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_{32} = \text{vol}(\text{cell}) \cdot \text{function\_4\_motor\_r4}([\text{MYpYpYp}], [\text{MYpYpYpYp}], [\text{Yp}], \text{alpha}, vol(\text{cell}), ka, kappa)$$

$$(90)$$

$$\begin{aligned} & \text{function\_4\_motor\_r4}([MYpYpYp],[MYpYpYp],[Yp],alpha,vol(cell),ka,kappa)} \\ & = \frac{ka \cdot ([MYpYpYp] \cdot [Yp] - 4 \cdot alpha \cdot alpha \cdot alpha \cdot kappa \cdot [MYpYpYpYp])}{\text{vol}(cell)} \end{aligned} \tag{91}$$

$$\begin{split} & \text{function\_4\_motor\_r4} \left( [MYpYpYp], [MYpYpYpYp], [Yp], alpha, vol\left(cell\right), ka, kappa \right) \\ & = \frac{ka \cdot \left( [MYpYpYp] \cdot [Yp] - 4 \cdot alpha \cdot alpha \cdot alpha \cdot kappa \cdot [MYpYpYpYp] \right)}{\text{vol}\left(cell\right)} \end{aligned} \tag{92}$$

#### 9.33 Reaction reaction\_1

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

Name  $TA + asp <-> Tasp_A$ 

SBO:0000177 non-covalent binding

### **Reaction equation**

$$TA + asp \Longrightarrow Tasp\_A$$
 (93)

Table 100: Properties of each reactant.

Id	Name	SBO
TA	TA	
asp	asp	

Table 101: Properties of each product.

Id	Name	SBO
Tasp_A	Tasp_A	

### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{33} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{TA}] \cdot [\text{asp}] - \text{k2} \cdot [\text{Tasp\_A}])$$
(94)

Table 102: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	1000000.0	Ø
k2	k2	1.0	

# 9.34 Reaction reaction\_2

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

Name  $TW+asp <-> Tasp_W$ 

SBO:0000177 non-covalent binding

# **Reaction equation**

$$TW + asp \Longrightarrow Tasp_{-}W \tag{95}$$

Table 103: Properties of each reactant.

Id	Name	SBO
TW	TW	
asp	asp	

Table 104: Properties of each product.

Id	Name	SBO
Tasp_W	Tasp_W	

### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{34} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{TW}] \cdot [\text{asp}] - \text{k2} \cdot [\text{Tasp}_{-}\text{W}])$$
(96)

Table 105: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	1000000.0	Ø
k2	k2	1.0	

# 9.35 Reaction reaction\_3

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

Name TWA+asp <-> Tasp\_WA

SBO:0000177 non-covalent binding

# **Reaction equation**

$$TWA + asp \Longrightarrow Tasp\_WA \tag{97}$$

Table 106: Properties of each reactant.

Id	Name	SBO
TWA	TWA	
asp	asp	

Table 107: Properties of each product.

Id	Name	SBO
Tasp_WA	Tasp_WA	

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_{35} = \text{vol}(\text{cell}) \cdot (\text{k1} \cdot [\text{TWA}] \cdot [\text{asp}] - \text{k2} \cdot [\text{Tasp}_{-}\text{WA}])$$
(98)

Table 108: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	1000000.0	Ø
k2	k2	1.0	

# 10 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.

# 10.1 Species asp

Name asp

SBO:0000247 simple chemical

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

Involved in events event\_1, event\_2

This species takes part in four reactions (as a reactant in regulatory\_r1, reaction\_1, reaction\_2, reaction\_3). Not these but two events influence the species' quantity because this species is on the boundary of the reaction system.

# 10.2 Species ni

Name ni

SBO:0000247 simple chemical

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

This species takes part in one reaction (as a reactant in regulatory\_r2), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ni} = 0 \tag{99}$$

### 10.3 Species T

Name T

SBO:0000245 macromolecule

Initial concentration  $3.12 \cdot 10^{-6} \ mol \cdot l^{-1}$ 

This species takes part in five reactions (as a reactant in regulatory\_r1, regulatory\_r2, regulatory\_r3, regulatory\_r4, regulatory\_r8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{T} = -|v_{11}| - |v_{12}| - |v_{13}| - |v_{14}| - |v_{18}| \tag{100}$$

### 10.4 Species Tasp

Name Tasp

SBO:0000253 non-covalent complex

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

This species takes part in four reactions (as a reactant in regulatory\_r9, regulatory\_r10, regulatory\_r13 and as a product in regulatory\_r1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tasp} = |v_{11}| - |v_{19}| - |v_{20}| - |v_{23}| \tag{101}$$

### 10.5 Species Tni

Name Tni

SBO:0000253 non-covalent complex

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

This species takes part in four reactions (as a reactant in regulatory\_r14, regulatory\_r15, regulatory\_r18 and as a product in regulatory\_r2).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{Tni} = |v_{12}| - |v_{24}| - |v_{25}| - |v_{28}| \tag{102}$$

# 10.6 Species W

Name W

SBO:0000245 macromolecule

Initial concentration  $2.89 \cdot 10^{-6} \ mol \cdot l^{-1}$ 

This species takes part in seven reactions (as a reactant in regulatory\_r3, regulatory\_r5, regulatory\_r7, regulatory\_r9, regulatory\_r12, regulatory\_r14, regulatory\_r17).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{W} = -|v_{13}| - |v_{15}| - |v_{17}| - |v_{19}| - |v_{22}| - |v_{24}| - |v_{27}| \tag{103}$$

#### 10.7 Species TW

Name TW

SBO:0000253 non-covalent complex

Initial concentration  $5.91 \cdot 10^{-7} \text{ mol} \cdot l^{-1}$ 

This species takes part in three reactions (as a reactant in regulatory\_r6, reaction\_2 and as a product in regulatory\_r3).

$$\frac{d}{dt}TW = v_{13} - v_{16} - v_{34} \tag{104}$$

#### 10.8 Species Tasp\_W

Name Tasp\_W

SBO:0000253 non-covalent complex

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

This species takes part in three reactions (as a reactant in regulatory\_r11 and as a product in regulatory\_r9, reaction\_2).

$$\frac{d}{dt} \text{Tasp}_{-}W = |v_{19}| + |v_{34}| - |v_{21}| \tag{105}$$

### 10.9 Species Tni\_W

Name Tni\_W

SBO:0000253 non-covalent complex

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

This species takes part in two reactions (as a reactant in regulatory\_r16 and as a product in regulatory\_r14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tni}_{-}\mathrm{W} = |v_{24}| - |v_{26}| \tag{106}$$

# 10.10 Species TA

Name TA

SBO:0000253 non-covalent complex

Initial concentration  $4.44 \cdot 10^{-7} \text{ mol} \cdot l^{-1}$ 

This species takes part in three reactions (as a reactant in regulatory\_r7, reaction\_1 and as a product in regulatory\_r4).

$$\frac{d}{dt}TA = |v_{14}| - |v_{17}| - |v_{33}| \tag{107}$$

### 10.11 Species Tasp\_A

Name Tasp\_A

SBO:0000253 non-covalent complex

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

This species takes part in three reactions (as a reactant in regulatory\_r12 and as a product in regulatory\_r10, reaction\_1).

$$\frac{d}{dt} \text{Tasp\_A} = |v_{20}| + |v_{33}| - |v_{22}|$$
 (108)

### 10.12 Species Tni\_A

Name Tni\_A

SBO:0000253 non-covalent complex

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

This species takes part in two reactions (as a reactant in regulatory\_r17 and as a product in regulatory\_r15).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tni}_{A} = v_{25} - v_{27} \tag{109}$$

### 10.13 Species WA

Name WA

SBO:0000253 non-covalent complex

Initial concentration  $6.78 \cdot 10^{-7} \text{ mol} \cdot l^{-1}$ 

This species takes part in four reactions (as a reactant in regulatory\_r8, regulatory\_r13, regulatory\_r18 and as a product in regulatory\_r5).

$$\frac{d}{dt}WA = |v_{15}| - |v_{18}| - |v_{23}| - |v_{28}| \tag{110}$$

### 10.14 Species TWA

Name TWA

SBO:0000253 non-covalent complex

Initial concentration  $8.47 \cdot 10^{-7} \text{ mol} \cdot l^{-1}$ 

This species takes part in five reactions (as a reactant in reaction\_3 and as a product in regulatory\_r6, regulatory\_r7, regulatory\_r8 and as a modifier in phosphorylation\_r2).

$$\frac{d}{dt}TWA = v_{16} + v_{17} + v_{18} - v_{35}$$
 (111)

### 10.15 Species Tasp\_WA

Name Tasp\_WA

SBO:0000253 non-covalent complex

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

This species takes part in six reactions (as a reactant in phosphorylation\_r4 and as a product in phosphorylation\_r4, regulatory\_r11, regulatory\_r12, regulatory\_r13, reaction\_3).

$$\frac{d}{dt} \text{Tasp\_WA} = |v_4| + |v_{21}| + |v_{22}| + |v_{23}| + |v_{35}| - |v_4|$$
(112)

### 10.16 Species Tni\_WA

Name Tni\_WA

SBO:0000253 non-covalent complex

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

This species takes part in four reactions (as a product in regulatory\_r16, regulatory\_r17, regulatory\_r18 and as a modifier in phosphorylation\_r3).

$$\frac{d}{dt} \text{Tni}_{-} WA = |v_{26}| + |v_{27}| + |v_{28}| \tag{113}$$

#### 10.17 Species A

Name A

SBO:0000245 macromolecule

Initial concentration  $3 \cdot 10^{-6} \text{ mol} \cdot l^{-1}$ 

This species takes part in twelve reactions (as a reactant in phosphorylation\_r1, phosphorylation\_r2, phosphorylation\_r3, regulatory\_r4, regulatory\_r5, regulatory\_r6, regulatory\_r10, regulatory\_r11, regulatory\_r15, regulatory\_r16 and as a product in phosphorylation\_r5, phosphorylation\_r9).

$$\frac{d}{dt}A = v_5 + v_9 - v_1 - v_2 - v_3 - v_{14} - v_{15} - v_{16} - v_{20} - v_{21} - v_{25} - v_{26}$$
 (114)

# 10.18 Species Ap

Name Ap

SBO:0000245 macromolecule

Initial concentration  $3.48 \cdot 10^{-8} \text{ mol} \cdot l^{-1}$ 

This species takes part in five reactions (as a reactant in phosphorylation\_r5, phosphorylation\_r9 and as a product in phosphorylation\_r1, phosphorylation\_r2, phosphorylation\_r3).

$$\frac{d}{dt}Ap = |v_1| + |v_2| + |v_3| - |v_5| - |v_9|$$
(115)

### 10.19 Species B

Name B

SBO:0000245 macromolecule

Initial concentration  $1.93 \cdot 10^{-6} \text{ mol} \cdot l^{-1}$ 

This species takes part in two reactions (as a reactant in phosphorylation\_r9 and as a product in phosphorylation\_r10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{B} = |v_{10}| - |v_9| \tag{116}$$

### 10.20 Species Bp

Name Bp

Initial concentration  $6.87 \cdot 10^{-8} \text{ mol} \cdot 1^{-1}$ 

This species takes part in two reactions (as a reactant in phosphorylation\_r10 and as a product in phosphorylation\_r9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Bp} = |v_9| - |v_{10}| \tag{117}$$

### **10.21 Species Z**

Name Z

SBO:0000245 macromolecule

Initial concentration  $2 \cdot 10^{-5} \text{ mol} \cdot l^{-1}$ 

This species takes part in two reactions (as a reactant in phosphorylation\_r8 and as a product in phosphorylation\_r8).

$$\frac{\mathrm{d}}{\mathrm{d}t}Z = v_8 - v_8 \tag{118}$$

### 10.22 Species Y

Name Y

SBO:0000245 macromolecule

Initial concentration  $9.9 \cdot 10^{-6} \text{ mol} \cdot l^{-1}$ 

This species takes part in five reactions (as a reactant in phosphorylation\_r5, phosphorylation\_r6 and as a product in phosphorylation\_r4, phosphorylation\_r7, phosphorylation\_r8).

$$\frac{\mathrm{d}}{\mathrm{d}t}Y = v_4 + v_7 + v_8 - v_5 - v_6 \tag{119}$$

### 10.23 Species Yp

Name Yp

Initial concentration  $7 \cdot 10^{-9} \text{ mol} \cdot l^{-1}$ 

This species takes part in nine reactions (as a reactant in phosphorylation\_r4, phosphorylation\_r7, phosphorylation\_r8, motor\_r1, motor\_r2, motor\_r3, motor\_r4 and as a product in phosphorylation\_r5, phosphorylation\_r6).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathbf{Y} \mathbf{p} = |v_5| + |v_6| - |v_4| - |v_7| - |v_8| - |v_{29}| - |v_{30}| - |v_{31}| - |v_{32}| \tag{120}$$

### 10.24 Species M

Name M

SBO:0000245 macromolecule

Initial concentration  $6.24 \cdot 10^{-9} \text{ mol} \cdot l^{-1}$ 

This species takes part in one reaction (as a reactant in motor\_r1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{M} = -v_{29} \tag{121}$$

# 10.25 Species MYp

Name MYp

SBO:0000253 non-covalent complex

Initial concentration  $7.77 \cdot 10^{-10} \; mol \cdot l^{-1}$ 

This species takes part in two reactions (as a reactant in motor\_r2 and as a product in motor\_r1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{MYp} = |v_{29}| - |v_{30}| \tag{122}$$

### 10.26 Species MYpYp

Name MYpYp

SBO:0000253 non-covalent complex

Initial concentration  $2.99 \cdot 10^{-10} \text{ mol} \cdot l^{-1}$ 

This species takes part in two reactions (as a reactant in motor\_r3 and as a product in motor\_r2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{MYpYp} = |v_{30}| - |v_{31}| \tag{123}$$

# 10.27 Species MYpYpYp

Name MYpYpYp

SBO:0000253 non-covalent complex

Initial concentration  $3.78 \cdot 10^{-10} \text{ mol} \cdot l^{-1}$ 

This species takes part in two reactions (as a reactant in motor\_r4 and as a product in motor\_r3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{MYpYpYp} = |v_{31}| - |v_{32}| \tag{124}$$

### 10.28 Species MYpYpYpYp

Name MYpYpYpYp

SBO:0000253 non-covalent complex

Initial concentration  $2.31 \cdot 10^{-9} \text{ mol} \cdot 1^{-1}$ 

This species takes part in one reaction (as a product in motor\_r4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{MYpYpYpYp} = v_{32} \tag{125}$$

### 10.29 Species species\_1

Name ATP

SBO:0000247 simple chemical

Initial concentration  $0.1 \text{ mol} \cdot l^{-1}$ 

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species}_{-}1 = 0 \tag{126}$$

# A Glossary of Systems Biology Ontology Terms

**SBO:0000177 non-covalent binding:** Interaction between several biochemical entities that results in the formation of a non-covalent comple

**SBO:0000216 phosphorylation:** Addition of a phosphate group (-H2PO4) to a chemical entity

**SBO:0000245** macromolecule: Molecular entity mainly built-up by the repetition of pseudo-identical units. CHEBI:3383

- SBO:0000247 simple chemical: Simple, non-repetitive chemical entity
- **SBO:0000253 non-covalent complex:** Entity composed of several independant components that are not linked by covalent bonds
- **SBO:0000290 physical compartment:** Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions
- **SBO:0000330 dephosphorylation:** Removal of a phosphate group (-H2PO4) from a chemical entity.
- **SBO:0000402** transfer of a chemical group: Covalent reaction that results in the transfer of a chemical group from one molecule to another

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