

SBML Model Report

Model name: “Bray1995_chemotaxis-receptorlinkedcomplex”



May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by the following three authors: Lukas Endler¹, Vijayalakshmi Chelliah² and Dennis Bray³ at November seventh 2008 at 10:55 a.m. and last time modified at June third 2014 at 2:51 p.m. Table 1 gives 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	22
events	0	constraints	0
reactions	34	function definitions	0
global parameters	2	unit definitions	5
rules	1	initial assignments	0

Model Notes

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2 Unit Definitions

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

2.1 Unit perMpersec

Name perMpersec

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

2.2 Unit persec

Name persec

Definition s^{-1}

2.3 Unit volume

Name femtolitre

Definition fl

2.4 Unit M

Name M

Definition $\text{mol} \cdot \text{l}^{-1}$

2.5 Unit Mpersec

Name Mpersec

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

2.6 Unit substance

Notes Mole is the predefined SBML unit for substance.

Definition mol

2.7 Unit area

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

Definition m^2

2.8 Unit length

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

Definition m

2.9 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		3	1.41	fl	<input checked="" type="checkbox"/>	

3.1 Compartment cell

This is a three dimensional compartment with a constant size of 1.41 fl.

Name cell

4 Species

This model contains 22 species. Section 8 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
AA	AA	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
AAp	AAp	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
W	W	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
WAA	WAA	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
WAAp	WAAp	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
WWAA	WWAA	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
WWAAp	WWAAp	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
TT	TT	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
TTW	TTW	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
TTWW	TTWW	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
TTWAA	TTWAA	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
TTWAAp	TTWAAp	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
TTAA	TTAA	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
TTAAp	TTAAp	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
TTWWAA	TTWWAA	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
TTWWAAp	TTWWAAp	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
Y	Y	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
Yp	Yp	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
Z	Z	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
B	B	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
Bp	Bp	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square
SetYp	setYp	cell	$\text{mol} \cdot \text{fl}^{-1}$	\square	\square

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion

5 Parameters

This model contains two global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Hill	Hill		4.0		<input checked="" type="checkbox"/>
Bias	Bias		0.0	dimensionless	<input type="checkbox"/>

6 Rule

This is an overview of one rule.

6.1 Rule Bias

Rule Bias is an assignment rule for parameter Bias:

$$\text{Bias} = 1 - \frac{[\text{Yp}]^{\text{Hill}}}{2.333 \cdot [\text{SetYp}]^{\text{Hill}} + [\text{Yp}]^{\text{Hill}}} \quad (1)$$

7 Reactions

This model contains 34 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	complex_r1	complex_r1	$TTW \rightleftharpoons TT + W$	
2	complex_r2	complex_r2	$WAA \rightleftharpoons W + AA$	
3	complex_r3	complex_r3	$TTWAA \rightleftharpoons TT + WAA$	
4	complex_r4	complex_r4	$TTWWAA \rightleftharpoons TTW + WAA$	
5	complex_r5	complex_r5	$TTWWAA \rightleftharpoons TTWW + AA$	
6	complex_r6	complex_r6	$TTWWAA \rightleftharpoons TT + WWAA$	
7	complex_r7	complex_r7	$TTAA \rightleftharpoons TT + AA$	
8	complex_r8	complex_r8	$TTWAA \rightleftharpoons TTW + AA$	
9	complex_r9	complex_r9	$TTWWAA \rightleftharpoons TTWAA + W$	
10	complex_r10	complex_r10	$TTWW \rightleftharpoons TTW + W$	
11	complex_r11	complex_r11	$WWAA \rightleftharpoons W + WAA$	
12	complex_r12	complex_r12	$TTWAA \rightleftharpoons TTAA + W$	
13	phosphorylation- _r1	phosphorylation_r1	$TTWWAA \longrightarrow TTWWA\text{Ap}$	
14	phosphorylation- _r2	phosphorylation_r2	$AA \longrightarrow A\text{Ap}$	
15	phosphorylation- _r3	phosphorylation_r3	$WAA \longrightarrow W\text{AAp}$	
16	phosphorylation- _r4	phosphorylation_r4	$WWAA \longrightarrow WW\text{AAp}$	
17	phosphorylation- _r5	phosphorylation_r5	$TTAA \longrightarrow T\text{TAAp}$	

Nº	Id	Name	Reaction Equation	SBO
18	phosphorylation- _r6	phosphorylation_r6	$TTWAA \longrightarrow TTWAAp$	
19	phosphorylation- _r7	phosphorylation_r7	$Y \longrightarrow Yp$	
20	phosphorylation- _r8	phosphorylation_r8	$Yp \longrightarrow Y$	
21	phosphorylation- _r9	phosphorylation_r9	$Yp + Z \longrightarrow Y + Z$	
22	phosphorylation- _r10	phosphorylation_r10	$Bp \longrightarrow B$	
23	phosphotransfer- _r1	phosphotransfer_r1	$B + AA_p \longrightarrow Bp + AA$	
24	phosphotransfer- _r2	phosphotransfer_r2	$B + WAA_p \longrightarrow Bp + WAA$	
25	phosphotransfer- _r3	phosphotransfer_r3	$B + WWAA_p \longrightarrow Bp + WWAA$	
26	phosphotransfer- _r4	phosphotransfer_r4	$B + TTAA_p \longrightarrow Bp + TTAA$	
27	phosphotransfer- _r5	phosphotransfer_r5	$B + TTWAA_p \longrightarrow Bp + TTWAA$	
28	phosphotransfer- _r6	phosphotransfer_r6	$B + TTWWAA_p \longrightarrow Bp + TTWWAA$	
29	phosphotransfer- _r7	phosphotransfer_r7	$Y + AA_p \longrightarrow Yp + AA$	
30	phosphotransfer- _r8	phosphotransfer_r8	$Y + WAA_p \longrightarrow Yp + WAA$	
31	phosphotransfer- _r9	phosphotransfer_r9	$Y + WWAA_p \longrightarrow Yp + WWAA$	

Nº	Id	Name	Reaction Equation	SBO
32	phosphotransfer- _r10	phosphotransfer_r10	$Y + \text{TTAAp} \longrightarrow Y_p + \text{TTAA}$	
33	phosphotransfer- _r11	phosphotransfer_r11	$Y + \text{TTWAAp} \longrightarrow Y_p + \text{TTWAA}$	
34	phosphotransfer- _r12	phosphotransfer_r12	$Y + \text{TTWWAAp} \longrightarrow Y_p + \text{TTWWAA}$	

7.1 Reaction `complex_r1`

This is a reversible reaction of one reactant forming two products.

Name `complex_r1`

Reaction equation



Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
TTW	TTW	

Products

Table 7: Properties of each product.

Id	Name	SBO
TT	TT	
W	W	

Kinetic Law

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

$$v_1 = \text{vol}(\text{cell}) \cdot (k_1 \cdot [\text{TTW}] - k_2 \cdot [\text{TT}] \cdot [\text{W}]) \quad (3)$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.004	s^{-1}	<input checked="" type="checkbox"/>
k2			1000000.000	$\text{l} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.2 Reaction `complex_r2`

This is a reversible reaction of one reactant forming two products.

Name `complex_r2`

Reaction equation



Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
WAA	WAA	

Products

Table 10: Properties of each product.

Id	Name	SBO
W	W	
AA	AA	

Kinetic Law

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

$$v_2 = \text{vol}(\text{cell}) \cdot (k_1 \cdot [\text{WAA}] - k_2 \cdot [\text{W}] \cdot [\text{AA}]) \quad (5)$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.009	s^{-1}	<input checked="" type="checkbox"/>
k2			1000000.000	$\text{l} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.3 Reaction `complex_r3`

This is a reversible reaction of one reactant forming two products.

Name `complex_r3`

Reaction equation



Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
TTWAA	TTWAA	

Products

Table 13: Properties of each product.

Id	Name	SBO
TT	TT	
WAA	WAA	

Kinetic Law

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

$$v_3 = \text{vol}(\text{cell}) \cdot (k_1 \cdot [\text{TTWAA}] - k_2 \cdot [\text{TT}] \cdot [\text{WAA}]) \quad (7)$$

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			297.0	s^{-1}	<input checked="" type="checkbox"/>
k2			1000000.0	$\text{l} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.4 Reaction `complex_r4`

This is a reversible reaction of one reactant forming two products.

Name `complex_r4`

Reaction equation



Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
TTWWAA	TTWWAA	

Products

Table 16: Properties of each product.

Id	Name	SBO
TTW	TTW	
WAA	WAA	

Kinetic Law

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

$$v_4 = \text{vol}(\text{cell}) \cdot (k_1 \cdot [\text{TTWWAA}] - k_2 \cdot [\text{TTW}] \cdot [\text{WAA}]) \quad (9)$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.64	s^{-1}	<input checked="" type="checkbox"/>
k2			1000000.00	$\text{l} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.5 Reaction `complex_r5`

This is a reversible reaction of one reactant forming two products.

Name `complex_r5`

Reaction equation



Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
TTWWAA	TTWWAA	

Products

Table 19: Properties of each product.

Id	Name	SBO
TTWW	TTWW	
AA	AA	

Kinetic Law

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

$$v_5 = \text{vol}(\text{cell}) \cdot (k_1 \cdot [\text{TTWWAA}] - k_2 \cdot [\text{TTWW}] \cdot [\text{AA}]) \quad (11)$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.112	s^{-1}	<input checked="" type="checkbox"/>
k2			1000000.000	$\text{l} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.6 Reaction `complex_r6`

This is a reversible reaction of one reactant forming two products.

Name `complex_r6`

Reaction equation



Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
TTWWAA	TTWWAA	

Products

Table 22: Properties of each product.

Id	Name	SBO
TT	TT	
WWAA	WWAA	

Kinetic Law

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

$$v_6 = \text{vol}(\text{cell}) \cdot (k_1 \cdot [\text{TTWWAA}] - k_2 \cdot [\text{TT}] \cdot [\text{WWAA}]) \quad (13)$$

Table 23: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.023	s^{-1}	<input checked="" type="checkbox"/>
k2			1000000.000	$\text{l} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.7 Reaction `complex_r7`

This is a reversible reaction of one reactant forming two products.

Name `complex_r7`

Reaction equation



Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
TTAA	TTAA	

Products

Table 25: Properties of each product.

Id	Name	SBO
TT	TT	

Id	Name	SBO
AA	AA	

Kinetic Law

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

$$v_7 = \text{vol}(\text{cell}) \cdot (k_1 \cdot [\text{TTAA}] - k_2 \cdot [\text{TT}] \cdot [\text{AA}]) \quad (15)$$

Table 26: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			39.3	s^{-1}	<input checked="" type="checkbox"/>
k2			1000000.0	$\text{l} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.8 Reaction `complex_r8`

This is a reversible reaction of one reactant forming two products.

Name `complex_r8`

Reaction equation



Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
TTWAA	TTWAA	

Products

Table 28: Properties of each product.

Id	Name	SBO
TTW	TTW	
AA	AA	

Kinetic Law

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

$$v_8 = \text{vol}(\text{cell}) \cdot (k_1 \cdot [\text{TTWAA}] - k_2 \cdot [\text{TTW}] \cdot [\text{AA}]) \quad (17)$$

Table 29: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			727.0	s^{-1}	<input checked="" type="checkbox"/>
k2			1000000.0	$1 \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.9 Reaction `complex_r9`

This is a reversible reaction of one reactant forming two products.

Name `complex_r9`

Reaction equation



Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
TTWWAA	TTWWAA	

Products

Table 31: Properties of each product.

Id	Name	SBO
TTWAA	TTWAA	
W	W	

Kinetic Law

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

$$v_9 = \text{vol}(\text{cell}) \cdot (k_1 \cdot [\text{TTWWAA}] - k_2 \cdot [\text{TTWAA}] \cdot [\text{W}]) \quad (19)$$

Table 32: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			$7.87 \cdot 10^{-6}$	s^{-1}	<input checked="" type="checkbox"/>
k2			1000000.000	$l \cdot mol^{-1} \cdot s^{-1}$	<input checked="" type="checkbox"/>

7.10 Reaction `complex_r10`

This is a reversible reaction of one reactant forming two products.

Name `complex_r10`

Reaction equation



Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
TTWW	TTWW	

Products

Table 34: Properties of each product.

Id	Name	SBO
TTW	TTW	
W	W	

Kinetic Law

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

$$v_{10} = \text{vol}(\text{cell}) \cdot (k1 \cdot [TTWW] - k2 \cdot [TTW] \cdot [W]) \quad (21)$$

Table 35: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.051	s^{-1}	<input checked="" type="checkbox"/>
k2			1000000.000	$l \cdot mol^{-1} \cdot s^{-1}$	<input checked="" type="checkbox"/>

7.11 Reaction `complex_r11`

This is a reversible reaction of one reactant forming two products.

Name `complex_r11`

Reaction equation



Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
WWAA	WWAA	

Products

Table 37: Properties of each product.

Id	Name	SBO
W	W	
WAA	WAA	

Kinetic Law

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

$$v_{11} = \text{vol}(\text{cell}) \cdot (k_1 \cdot [\text{WWAA}] - k_2 \cdot [\text{W}] \cdot [\text{WAA}]) \quad (23)$$

Table 38: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.102	s^{-1}	<input checked="" type="checkbox"/>
k2			1000000.000	$\text{l} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.12 Reaction `complex_r12`

This is a reversible reaction of one reactant forming two products.

Name `complex_r12`

Reaction equation



Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
TTWAA	TTWAA	

Products

Table 40: Properties of each product.

Id	Name	SBO
TTAA	TTAA	
W	W	

Kinetic Law

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

$$v_{12} = \text{vol}(\text{cell}) \cdot (k_1 \cdot [\text{TTWAA}] - k_2 \cdot [\text{TTAA}] \cdot [\text{W}]) \quad (25)$$

Table 41: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.068	s^{-1}	<input checked="" type="checkbox"/>
k2			1000000.000	$\text{l} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.13 Reaction phosphorylation_r1

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

Name phosphorylation_r1

Reaction equation



Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
TTWWAA	TTWWAA	

Product

Table 43: Properties of each product.

Id	Name	SBO
TTWWAAp	TTWWAAp	

Kinetic Law

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

$$v_{13} = \text{vol}(\text{cell}) \cdot k_1 \cdot [\text{TTWWAA}] \quad (27)$$

Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			15.5	s^{-1}	<input checked="" type="checkbox"/>

7.14 Reaction phosphorylation_r2

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

Name phosphorylation_r2

Reaction equation



Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
AA	AA	

Product

Table 46: Properties of each product.

Id	Name	SBO
AAp	AAp	

Kinetic Law

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

$$v_{14} = \text{vol}(\text{cell}) \cdot k_1 \cdot [\text{AA}] \quad (29)$$

Table 47: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.023	s^{-1}	<input checked="" type="checkbox"/>

7.15 Reaction phosphorylation_r3

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

Name phosphorylation_r3

Reaction equation



Reactant

Table 48: Properties of each reactant.

Id	Name	SBO
WAA	WAA	

Product

Table 49: Properties of each product.

Id	Name	SBO
WAAp	WAAp	

Id	Name	SBO
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Kinetic Law

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

$$v_{15} = \text{vol}(\text{cell}) \cdot k1 \cdot [\text{WAA}] \quad (31)$$

Table 50: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.023	s^{-1}	<input checked="" type="checkbox"/>

7.16 Reaction phosphorylation_r4

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

Name phosphorylation_r4

Reaction equation



Reactant

Table 51: Properties of each reactant.

Id	Name	SBO
WWAA	WWAA	

Product

Table 52: Properties of each product.

Id	Name	SBO
WWAAp	WWAAp	

Kinetic Law

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

$$v_{16} = \text{vol}(\text{cell}) \cdot k_1 \cdot [\text{WWAA}] \quad (33)$$

Table 53: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.023	s ⁻¹	<input checked="" type="checkbox"/>

7.17 Reaction phosphorylation_r5

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

Name phosphorylation_r5

Reaction equation



Reactant

Table 54: Properties of each reactant.

Id	Name	SBO
TTAA	TTAA	

Product

Table 55: Properties of each product.

Id	Name	SBO
TTAAp	TTAAp	

Kinetic Law

Derived unit s⁻¹ · mol

$$v_{17} = \text{vol}(\text{cell}) \cdot k_1 \cdot [\text{TTAA}] \quad (35)$$

Table 56: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.023	s ⁻¹	<input checked="" type="checkbox"/>

7.18 Reaction phosphorylation_r6

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

Name phosphorylation_r6

Reaction equation



Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
TTWAA	TTWAA	

Product

Table 58: Properties of each product.

Id	Name	SBO
TTWAAp	TTWAAp	

Kinetic Law

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

$$v_{18} = \text{vol}(\text{cell}) \cdot k_1 \cdot [\text{TTWAA}] \quad (37)$$

Table 59: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.023	s^{-1}	<input checked="" type="checkbox"/>

7.19 Reaction phosphorylation_r7

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

Name phosphorylation_r7

Reaction equation



Reactant

Table 60: Properties of each reactant.

Id	Name	SBO
Y	Y	

Product

Table 61: Properties of each product.

Id	Name	SBO
Yp	Yp	

Kinetic Law

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

$$v_{19} = \text{vol}(\text{cell}) \cdot k_1 \cdot [Y] \quad (39)$$

Table 62: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.001	s^{-1}	<input checked="" type="checkbox"/>

7.20 Reaction phosphorylation_r8

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

Name phosphorylation_r8

Reaction equation



Reactant

Table 63: Properties of each reactant.

Id	Name	SBO
Yp	Yp	

Product

Table 64: Properties of each product.

Id	Name	SBO
Y	Y	

Kinetic Law

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

$$v_{20} = \text{vol}(\text{cell}) \cdot k1 \cdot [\text{Yp}] \quad (41)$$

Table 65: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.037	s^{-1}	<input checked="" type="checkbox"/>

7.21 Reaction phosphorylation_r9

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

Name phosphorylation_r9

Reaction equation



Reactants

Table 66: Properties of each reactant.

Id	Name	SBO
Yp	Yp	
Z	Z	

Products

Table 67: Properties of each product.

Id	Name	SBO
Y	Y	
Z	Z	

Kinetic Law

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

$$v_{21} = \text{vol}(\text{cell}) \cdot k1 \cdot [\text{Yp}] \cdot [\text{Z}] \quad (43)$$

Table 68: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			500000.0	$\text{l} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.22 Reaction phosphorylation_r10

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

Name phosphorylation_r10

Reaction equation



Reactant

Table 69: Properties of each reactant.

Id	Name	SBO
Bp	Bp	

Product

Table 70: Properties of each product.

Id	Name	SBO
B	B	

Kinetic Law

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

$$v_{22} = \text{vol}(\text{cell}) \cdot k_1 \cdot [\text{Bp}] \quad (45)$$

Table 71: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.35	s^{-1}	<input checked="" type="checkbox"/>

7.23 Reaction `phosphotransfer_r1`

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

Name `phosphotransfer_r1`

Reaction equation



Reactants

Table 72: Properties of each reactant.

Id	Name	SBO
B	B	
AAp	AAp	

Products

Table 73: Properties of each product.

Id	Name	SBO
Bp	Bp	
AA	AA	

Kinetic Law

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

$$v_{23} = \text{vol}(\text{cell}) \cdot k1 \cdot [\text{B}] \cdot [\text{AAp}] \quad (47)$$

Table 74: Properties of each parameter.

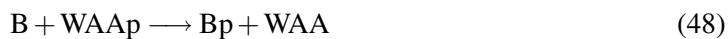
Id	Name	SBO	Value	Unit	Constant
k1			6000000.0	$1 \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.24 Reaction phosphotransfer_r2

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

Name phosphotransfer_r2

Reaction equation



Reactants

Table 75: Properties of each reactant.

Id	Name	SBO
B	B	
WAAp	WAAp	

Products

Table 76: Properties of each product.

Id	Name	SBO
Bp	Bp	
WAA	WAA	

Kinetic Law

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

$$v_{24} = \text{vol}(\text{cell}) \cdot k1 \cdot [\text{B}] \cdot [\text{WAAp}] \quad (49)$$

Table 77: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			6000000.0	$1 \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.25 Reaction phosphotransfer_r3

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

Name phosphotransfer_r3

Reaction equation



Reactants

Table 78: Properties of each reactant.

Id	Name	SBO
B	B	
WWAAp	WWAAp	

Products

Table 79: Properties of each product.

Id	Name	SBO
Bp	Bp	
WWAA	WWAA	

Kinetic Law

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

$$v_{25} = \text{vol}(\text{cell}) \cdot k1 \cdot [\text{B}] \cdot [\text{WWAAp}] \quad (51)$$

Table 80: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			6000000.0	$1 \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.26 Reaction [phosphotransfer_r4](#)

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

Name phosphotransfer_r4

Reaction equation



Reactants

Table 81: Properties of each reactant.

Id	Name	SBO
B	B	
TTAAp	TTAAp	

Products

Table 82: Properties of each product.

Id	Name	SBO
Bp	Bp	
TTAA	TTAA	

Kinetic Law

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

$$v_{26} = \text{vol}(\text{cell}) \cdot k1 \cdot [\text{B}] \cdot [\text{TTAAp}] \quad (53)$$

Table 83: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			6000000.0	$\text{l} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.27 Reaction [phosphotransfer_r5](#)

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

Name phosphotransfer_r5

Reaction equation



Reactants

Table 84: Properties of each reactant.

Id	Name	SBO
B	B	
TTWAAp	TTWAAp	

Products

Table 85: Properties of each product.

Id	Name	SBO
Bp	Bp	
TTWAA	TTWAA	

Kinetic Law

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

$$v_{27} = \text{vol}(\text{cell}) \cdot k_1 \cdot [\text{B}] \cdot [\text{TTWAAp}] \quad (55)$$

Table 86: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			6000000.0	$1 \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.28 Reaction `phosphotransfer_r6`

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

Name `phosphotransfer_r6`

Reaction equation



Reactants

Table 87: Properties of each reactant.

Id	Name	SBO
B	B	
TTWWAAp	TTWWAAp	

Products

Table 88: Properties of each product.

Id	Name	SBO
Bp	Bp	
TTWWAA	TTWWAA	

Kinetic Law

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

$$v_{28} = \text{vol}(\text{cell}) \cdot k1 \cdot [\text{B}] \cdot [\text{TTWWAAp}] \quad (57)$$

Table 89: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			6000000.0	$\text{l} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.29 Reaction phosphotransfer_r7

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

Name phosphotransfer_r7

Reaction equation



Reactants

Table 90: Properties of each reactant.

Id	Name	SBO
Y	Y	
AAp	AAp	

Products

Table 91: Properties of each product.

Id	Name	SBO
Yp	Yp	
AA	AA	

Kinetic Law

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

$$v_{29} = \text{vol}(\text{cell}) \cdot k1 \cdot [\text{Y}] \cdot [\text{AAp}] \quad (59)$$

Table 92: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			$3 \cdot 10^7$	$1 \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.30 Reaction `phosphotransfer_r8`

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

Name `phosphotransfer_r8`

Reaction equation



Reactants

Table 93: Properties of each reactant.

Id	Name	SBO
Y	Y	

Id	Name	SBO
WAAp	WAAp	

Products

Table 94: Properties of each product.

Id	Name	SBO
Yp	Yp	
WAA	WAA	

Kinetic Law

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

$$v_{30} = \text{vol}(\text{cell}) \cdot k1 \cdot [\text{Y}] \cdot [\text{WAAp}] \quad (61)$$

Table 95: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			$3 \cdot 10^7$	$1 \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.31 Reaction `phosphotransfer_r9`

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

Name `phosphotransfer_r9`

Reaction equation



Reactants

Table 96: Properties of each reactant.

Id	Name	SBO
Y	Y	
WAAp	WAAp	

Products

Table 97: Properties of each product.

Id	Name	SBO
Yp	Yp	
WWAA	WWAA	

Kinetic Law

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

$$v_{31} = \text{vol}(\text{cell}) \cdot k1 \cdot [\text{Y}] \cdot [\text{WWAAp}] \quad (63)$$

Table 98: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			$3 \cdot 10^7$	$\text{l} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.32 Reaction phosphotransfer_r10

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

Name phosphotransfer_r10

Reaction equation



Reactants

Table 99: Properties of each reactant.

Id	Name	SBO
Y	Y	
TTAAp	TTAAp	

Products

Table 100: Properties of each product.

Id	Name	SBO
Yp	Yp	
TTAA	TTAA	

Kinetic Law

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

$$v_{32} = \text{vol}(\text{cell}) \cdot k1 \cdot [\text{Y}] \cdot [\text{TTAAp}] \quad (65)$$

Table 101: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			$3 \cdot 10^7$	$\text{l} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.33 Reaction [phosphotransfer_r11](#)

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

Name [phosphotransfer_r11](#)

Reaction equation



Reactants

Table 102: Properties of each reactant.

Id	Name	SBO
Y	Y	
TTWAAp	TTWAAp	

Products

Table 103: Properties of each product.

Id	Name	SBO
Yp	Yp	

Id	Name	SBO
TTWAA	TTWAA	

Kinetic Law

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

$$v_{33} = \text{vol}(\text{cell}) \cdot k1 \cdot [\text{Y}] \cdot [\text{TTWAAp}] \quad (67)$$

Table 104: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			$3 \cdot 10^7$	$1 \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

7.34 Reaction [phosphotransfer_r12](#)

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

Name [phosphotransfer_r12](#)

Reaction equation



Reactants

Table 105: Properties of each reactant.

Id	Name	SBO
Y	Y	
TTWWAAp	TTWWAAp	

Products

Table 106: Properties of each product.

Id	Name	SBO
Yp	Yp	
TTWWAA	TTWWAA	

Kinetic Law

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

$$v_{34} = \text{vol}(\text{cell}) \cdot k1 \cdot [\text{Y}] \cdot [\text{TTWWAAp}] \quad (69)$$

Table 107: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			$3 \cdot 10^7$	$\text{l} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>

8 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.

8.1 Species AA

Name AA

Initial concentration $2.5 \cdot 10^{-6} \text{ mol} \cdot \text{fl}^{-1}$

This species takes part in seven reactions (as a reactant in [phosphorylation_r2](#) and as a product in [complex_r2](#), [complex_r5](#), [complex_r7](#), [complex_r8](#), [phosphotransfer_r1](#), [phosphotransfer_r7](#)).

$$\frac{d}{dt} \text{AA} = v_2 + v_5 + v_7 + v_8 + v_{23} + v_{29} - v_{14} \quad (70)$$

8.2 Species AAp

Name AAp

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

This species takes part in three reactions (as a reactant in [phosphotransfer_r1](#), [phosphotransfer_r7](#) and as a product in [phosphorylation_r2](#)).

$$\frac{d}{dt} \text{AAp} = v_{14} - v_{23} - v_{29} \quad (71)$$

8.3 Species W

Name W

Initial concentration $5 \cdot 10^{-6} \text{ mol} \cdot \text{fl}^{-1}$

This species takes part in six reactions (as a product in [complex_r1](#), [complex_r2](#), [complex_r9](#), [complex_r10](#), [complex_r11](#), [complex_r12](#)).

$$\frac{d}{dt}W = v_1 + v_2 + v_9 + v_{10} + v_{11} + v_{12} \quad (72)$$

8.4 Species WAA

Name WAA

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

This species takes part in seven reactions (as a reactant in [complex_r2](#), [phosphorylation_r3](#) and as a product in [complex_r3](#), [complex_r4](#), [complex_r11](#), [phosphotransfer_r2](#), [phosphotransfer_r8](#)).

$$\frac{d}{dt}WAA = v_3 + v_4 + v_{11} + v_{24} + v_{30} - v_2 - v_{15} \quad (73)$$

8.5 Species WAAp

Name WAAp

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

This species takes part in three reactions (as a reactant in [phosphotransfer_r2](#), [phosphotransfer_r8](#) and as a product in [phosphorylation_r3](#)).

$$\frac{d}{dt}WAAp = v_{15} - v_{24} - v_{30} \quad (74)$$

8.6 Species WWAA

Name WWAA

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

This species takes part in five reactions (as a reactant in [complex_r11](#), [phosphorylation_r4](#) and as a product in [complex_r6](#), [phosphotransfer_r3](#), [phosphotransfer_r9](#)).

$$\frac{d}{dt}WWAA = v_6 + v_{25} + v_{31} - v_{11} - v_{16} \quad (75)$$

8.7 Species WWAAp

Name WWAAp

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

This species takes part in three reactions (as a reactant in [phosphotransfer_r3](#), [phosphotransfer_r9](#) and as a product in [phosphorylation_r4](#)).

$$\frac{d}{dt} \text{WWAAp} = v_{16} - v_{25} - v_{31} \quad (76)$$

8.8 Species TT

Name TT

Initial concentration $2.5 \cdot 10^{-6} \text{ mol} \cdot \text{fl}^{-1}$

This species takes part in four reactions (as a product in [complex_r1](#), [complex_r3](#), [complex_r6](#), [complex_r7](#)).

$$\frac{d}{dt} \text{TT} = v_1 + v_3 + v_6 + v_7 \quad (77)$$

8.9 Species TTW

Name TTW

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

This species takes part in four reactions (as a reactant in [complex_r1](#) and as a product in [complex_r4](#), [complex_r8](#), [complex_r10](#)).

$$\frac{d}{dt} \text{TTW} = v_4 + v_8 + v_{10} - v_1 \quad (78)$$

8.10 Species TTWW

Name TTWW

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

This species takes part in two reactions (as a reactant in [complex_r10](#) and as a product in [complex_r5](#)).

$$\frac{d}{dt} \text{TTWW} = v_5 - v_{10} \quad (79)$$

8.11 Species TTWAA

Name TTWAA

Initial concentration 0 mol · fl⁻¹

This species takes part in seven reactions (as a reactant in [complex_r3](#), [complex_r8](#), [complex_r12](#), [phosphorylation_r6](#) and as a product in [complex_r9](#), [phosphotransfer_r5](#), [phosphotransfer_r11](#)).

$$\frac{d}{dt}TTWAA = v_9 + v_{27} + v_{33} - v_3 - v_8 - v_{12} - v_{18} \quad (80)$$

8.12 Species TTWAAp

Name TTWAAp

Initial concentration 0 mol · fl⁻¹

This species takes part in three reactions (as a reactant in [phosphotransfer_r5](#), [phosphotransfer_r11](#) and as a product in [phosphorylation_r6](#)).

$$\frac{d}{dt}TTWAAp = v_{18} - v_{27} - v_{33} \quad (81)$$

8.13 Species TTAA

Name TTAA

Initial concentration 0 mol · fl⁻¹

This species takes part in five reactions (as a reactant in [complex_r7](#), [phosphorylation_r5](#) and as a product in [complex_r12](#), [phosphotransfer_r4](#), [phosphotransfer_r10](#)).

$$\frac{d}{dt}TTAA = v_{12} + v_{26} + v_{32} - v_7 - v_{17} \quad (82)$$

8.14 Species TTAAp

Name TTAAp

Initial concentration 0 mol · fl⁻¹

This species takes part in three reactions (as a reactant in [phosphotransfer_r4](#), [phosphotransfer_r10](#) and as a product in [phosphorylation_r5](#)).

$$\frac{d}{dt}TTAAp = v_{17} - v_{26} - v_{32} \quad (83)$$

8.15 Species TTWWAA

Name TTWWAA

Initial concentration 0 mol · fl⁻¹

This species takes part in seven reactions (as a reactant in [complex_r4](#), [complex_r5](#), [complex_r6](#), [complex_r9](#), [phosphorylation_r1](#) and as a product in [phosphotransfer_r6](#), [phosphotransfer_r12](#)).

$$\frac{d}{dt}TTWWAA = v_{28} + v_{34} - v_4 - v_5 - v_6 - v_9 - v_{13} \quad (84)$$

8.16 Species TTWWAAp

Name TTWWAAp

Initial concentration 0 mol · fl⁻¹

This species takes part in three reactions (as a reactant in [phosphotransfer_r6](#), [phosphotransfer_r12](#) and as a product in [phosphorylation_r1](#)).

$$\frac{d}{dt}TTWWAAp = v_{13} - v_{28} - v_{34} \quad (85)$$

8.17 Species Y

Name Y

Initial concentration 10⁻⁵ mol · fl⁻¹

This species takes part in nine reactions (as a reactant in [phosphorylation_r7](#), [phosphotransfer_r7](#), [phosphotransfer_r8](#), [phosphotransfer_r9](#), [phosphotransfer_r10](#), [phosphotransfer_r11](#), [phosphotransfer_r12](#) and as a product in [phosphorylation_r8](#), [phosphorylation_r9](#)).

$$\frac{d}{dt}Y = v_{20} + v_{21} - v_{19} - v_{29} - v_{30} - v_{31} - v_{32} - v_{33} - v_{34} \quad (86)$$

8.18 Species Yp

Name Yp

Initial concentration 0 mol · fl⁻¹

This species takes part in nine reactions (as a reactant in [phosphorylation_r8](#), [phosphorylation_r9](#) and as a product in [phosphorylation_r7](#), [phosphotransfer_r7](#), [phosphotransfer_r8](#), [phosphotransfer_r9](#), [phosphotransfer_r10](#), [phosphotransfer_r11](#), [phosphotransfer_r12](#)).

$$\frac{d}{dt}Yp = v_{19} + v_{29} + v_{30} + v_{31} + v_{32} + v_{33} + v_{34} - v_{20} - v_{21} \quad (87)$$

8.19 Species Z

Name Z

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

This species takes part in two reactions (as a reactant in [phosphorylation_r9](#) and as a product in [phosphorylation_r9](#)).

$$\frac{d}{dt}Z = v_{21} - v_{21} \quad (88)$$

8.20 Species B

Name B

Initial concentration $2 \cdot 10^{-6} \text{ mol} \cdot \text{fl}^{-1}$

This species takes part in seven reactions (as a reactant in [phosphotransfer_r1](#), [phosphotransfer_r2](#), [phosphotransfer_r3](#), [phosphotransfer_r4](#), [phosphotransfer_r5](#), [phosphotransfer_r6](#) and as a product in [phosphorylation_r10](#)).

$$\frac{d}{dt}B = v_{22} - v_{23} - v_{24} - v_{25} - v_{26} - v_{27} - v_{28} \quad (89)$$

8.21 Species Bp

Name Bp

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

This species takes part in seven reactions (as a reactant in [phosphorylation_r10](#) and as a product in [phosphotransfer_r1](#), [phosphotransfer_r2](#), [phosphotransfer_r3](#), [phosphotransfer_r4](#), [phosphotransfer_r5](#), [phosphotransfer_r6](#)).

$$\frac{d}{dt}Bp = v_{23} + v_{24} + v_{25} + v_{26} + v_{27} + v_{28} - v_{22} \quad (90)$$

8.22 Species SetYp

Name setYp

Initial concentration $1.63 \cdot 10^{-6} \text{ mol} \cdot \text{fl}^{-1}$

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{d}{dt}\text{SetYp} = 0 \quad (91)$$

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