SBML Model Report

Model name: "Saucerman2006_PKA"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Harish Dharuri[1] at October third 2007 at 10:05 a. m. and last time modified at October tenth 2014 at 10:06 a. 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	3
species types	0	species	37
events	0	constraints	0
reactions	30	function definitions	0
global parameters	20	unit definitions	11
rules	8	initial assignments	0

Model Notes

The model reproduces Fig 2B of the paper. Model successfully tested on MathSBML

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commercially or not, in a restricted way or not.

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2 Unit Definitions

This is an overview of 13 unit definitions of which two are predefined by SBML and not mentioned in the model.

2.1 Unit substance

Definition µmol

2.2 Unit volume

Definition l

2.3 Unit area

Definition μm^2

2.4 Unit molecules

Definition item

2.5 Unit umol_litre_um_3

Definition $10^{-21} \cdot mol$

2.6 Unit um2

Definition μm^2

2.7 Unit uM_s_1

Definition $0.0010\ dimensionless \cdot m^{-3} \cdot mol \cdot s^{-1}$

2.8 Unit uM

Definition $0.0010\ dimensionless \cdot m^{-3} \cdot mol$

2.9 Unit s_1

Definition s^{-1}

2.10 Unit uM_1_s_1

Definition $1000\ \text{dimensionless} \cdot m^3 \cdot mol^{-1} \cdot s^{-1}$

2.11 Unit s

Definition s

2.12 Unit length

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

Definition m

2.13 Unit time

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

Definition s

3 Compartments

This model contains three compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
ec	ec		3	1		☑	
cell	cell		3	0.25		☑	membrane
membrane	membrane		2	0.25	μm^2	☑	ec

3.1 Compartment ec

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

Name ec

3.2 Compartment cell

This is a three dimensional compartment with a constant size of 0.25 litre, which is surrounded by membrane (membrane).

Name cell

3.3 Compartment `membrane`

This is a two dimensional compartment with a constant size of 0.25 μm^2, which is surrounded by `ec` (ec).

Name membrane

4 Species

This model contains 37 species. The boundary condition of one of these species is set to `true` so that this species' amount cannot be changed by any reaction. 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
Gsbg_cell	Gsbg	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
L_cell	L	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
Gsa_gdp_cell	Gsa_gdp	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
Gsa_gtp_cell	Gsa_gtp	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
b1AR_S464_cell	b1AR_S464	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
PDEcAMP_cell	PDEcAMP	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
PDE_cell	PDE	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
ATP_cell	ATP	cell	$\mu mol \cdot l^{-1}$	⊟	☑
b1AR_cell	b1AR	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
Gs_cell	Gs	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
A2RC_cell	A2RC	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
A2R_cell	A2R	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
PKAC_cell	PKAC	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
ARC_cell	ARC	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
PKAC_AKAR_cell	PKAC_AKAR	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
Propranolol_cell	Propranolol	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
b1ARinhib_cell	b1ARinhib	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
light_spot_cell	light_spot	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
AC_cell	AC	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
PKI_cell	PKI	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
PKAC_PKI_cell	PKAC_PKI	cell	$\mu mol \cdot l^{-1}$	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
RC_cell	RC	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
b1AR_Gs_cell	b1AR_Gs	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
cAMP_cell	cAMP	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
GsAC_cell	GsAC	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
IBMX_cell	IBMX	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
PDE_IBMX_cell	PDE_IBMX	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
Fsk_cell	Fsk	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
FskAC_cell	FskAC	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
b1AR_p_cell	b1AR_p	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
L_b1AR_cell	L_b1AR	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
AKAR_cell	AKAR	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
AKARp_cell	AKARp	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
PP_cell	PP	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
PP_AKARp_cell	PP_AKARp	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
DMNB_cAMP_cell	DMNB_cAMP	cell	$\mu mol \cdot l^{-1}$	⊟	⊟
L_b1AR_Gs_cell	L_b1AR_Gs	cell	$\mu mol \cdot l^{-1}$	⊟	⊟

5 Parameters

This model contains 20 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_ac_gsa_cAMP_synthesis_GsAC			2.5	s^{-1}	☑
Vmax_cAMP_synthesis_GsAC			0.0	0.0010 dimensionless $\cdot$ $m^{-3} \cdot mol \cdot s^{-1}$	⊟
ton_global_light_cAMP_photolysis			2160.0	s	☑
toff_global_light_cAMP_photolysis			2165.0	s	☑
ton_local_light_cAMP_photolysis			0.0	s	☑
toff_local_light_cAMP_photolysis			0.0	s	☑
light_cAMP_photolysis			0.0	0.0010 dimensionless $\cdot$ $m^{-3} \cdot mol$	⊟
kfsk_cAMP_synthesis_FskAC			7.3	s^{-1}	☑
Vmax_cAMP_synthesis_FskAC			0.0	0.0010 dimensionless $\cdot$ $m^{-3} \cdot mol \cdot s^{-1}$	⊟
Kf_inhibit_PDE			0.0	1000 dimensionless $\cdot$ $m^{3} \cdot mol^{-1} \cdot s^{-1}$	⊟
Kr_inhibit_PDE			0.0	s^{-1}	⊟
ar_for_add_propranolol			0.0		⊟
t_propadd			2420.0		☑
Propranolol_pipette			1.0		☑
tauPropranolol			1.0		☑

Id	Name	SBO	Value	Unit	Constant
ar_for_add-_Ligand			0.0		⊟
t_Ladd			2160.0		☑
L_pipette			0.1		☑
tauL			1.0		☑
Ratio_AKARp-_AKARtot			0.0		⊟

6 Rules

This is an overview of eight rules.

6.1 Rule Vmax_cAMP_synthesis_GsAC

Rule Vmax_cAMP_synthesis_GsAC is an assignment rule for parameter Vmax_cAMP_synthesis-_GsAC:

$$\text{Vmax\_cAMP\_synthesis\_GsAC} = \text{k\_ac\_gsa\_cAMP\_synthesis\_GsAC} \cdot [\text{GsAC\_cell}] \quad (1)$$

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

6.2 Rule light_cAMP_photolysis

Rule light_cAMP_photolysis is an assignment rule for parameter light_cAMP_photolysis:

$$\begin{aligned}&\text{light\_cAMP\_photolysis} \quad (2)\\ &= \begin{cases} 1 & \text{if } (\text{t} > \text{ton\_global\_light\_cAMP\_photolysis}) \wedge (\text{t} < \text{toff\_global\_light\_cAMP\_photolysis}) \\ 0 & \text{otherwise} \end{cases} \\ &\quad + \begin{cases} [\text{light\_spot\_cell}] & \text{if } (\text{t} > \text{ton\_local\_light\_cAMP\_photolysis}) \wedge (\text{t} < \text{toff\_local\_light\_cAMP\_photolysis}) \\ 0 & \text{otherwise} \end{cases}\end{aligned}$$

6.3 Rule Vmax_cAMP_synthesis_FskAC

Rule Vmax_cAMP_synthesis_FskAC is an assignment rule for parameter Vmax_cAMP_synthesis-_FskAC:

$$\text{Vmax\_cAMP\_synthesis\_FskAC} = \text{kfsk\_cAMP\_synthesis\_FskAC} \cdot [\text{FskAC\_cell}] \quad (3)$$

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

6.4 Rule Kf_inhibit_PDE

Rule Kf_inhibit_PDE is an assignment rule for parameter Kf_inhibit_PDE:

$$\text{Kf\_inhibit\_PDE} = \begin{cases} 1000 & \text{if t} > 1000 \\ 0 & \text{otherwise} \end{cases} \tag{4}$$

6.5 Rule Kr_inhibit_PDE

Rule Kr_inhibit_PDE is an assignment rule for parameter Kr_inhibit_PDE:

$$\text{Kr\_inhibit\_PDE} = \begin{cases} 30000 & \text{if t} > 1000 \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

6.6 Rule ar_for_add_propranolol

Rule ar_for_add_propranolol is an assignment rule for parameter ar_for_add_propranolol:

$$\text{ar\_for\_add\_propranolol} = \begin{cases} (\text{Propranolol\_pipette} + ([\text{Propranolol\_cell}])) \cdot \dfrac{1}{\text{tauPropranolol}} & \text{if t} > \text{t\_propadd} \\ 0 & \text{otherwise} \end{cases} \tag{6}$$

6.7 Rule ar_for_add_Ligand

Rule ar_for_add_Ligand is an assignment rule for parameter ar_for_add_Ligand:

$$\text{ar\_for\_add\_Ligand} = \begin{cases} (\text{L\_pipette} + ([\text{L\_cell}])) \cdot \dfrac{1}{\text{tauL}} & \text{if t} > \text{t\_Ladd} \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

6.8 Rule Ratio_AKARp_AKARtot

Rule Ratio_AKARp_AKARtot is an assignment rule for parameter Ratio_AKARp_AKARtot:

$$\text{Ratio\_AKARp\_AKARtot} = \frac{[\text{AKARp\_cell}]}{[\text{AKAR\_cell}] + [\text{AKARp\_cell}] + [\text{PKAC\_AKAR\_cell}] + [\text{PP\_AKARp\_cell}]} \tag{8}$$

Derived unit dimensionless

7 Reactions

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

Table 5: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	cAMP_synthesis_GsAC	cAMP_synthesis_GsAC	$\text{ATP\_cell} \xrightleftharpoons{\text{GsAC\_cell}} \text{cAMP\_cell}$	
2	bind_b1AR_propranolol	bind_b1AR_propranolol	$\text{Propranolol\_cell} + \text{b1AR\_cell} \rightleftharpoons \text{b1ARinhib\_cell}$	
3	add_propranolol	add_propranolol	$\emptyset \rightleftharpoons \text{Propranolol\_cell}$	
4	cAMP_photolysis	cAMP_photolysis	$\text{DMNB\_cAMP\_cell} \xrightleftharpoons{\text{light\_spot\_cell}} \text{cAMP\_cell}$	
5	LRG_activation	LRG_activation	$\text{L\_b1AR\_Gs\_cell} \rightleftharpoons \text{Gsa\_gtp\_cell} + \text{Gsbg\_cell} + \text{L\_b1AR\_cell}$	
6	bind_Lb1AR_Gs	bind_Lb1AR_Gs	$\text{Gs\_cell} + \text{L\_b1AR\_cell} \rightleftharpoons \text{L\_b1AR\_Gs\_cell}$	
7	desens_bark	desens_bark	$\text{L\_b1AR\_cell} \xrightleftharpoons{\text{L\_b1AR\_Gs\_cell}} \text{b1AR\_S464\_cell}$	
8	bind_cAMP_ARC	bind_cAMP_ARC	$\text{ARC\_cell} + \text{cAMP\_cell} \rightleftharpoons \text{A2RC\_cell}$	
9	bind_b1AR_Gs	bind_b1AR_Gs	$\text{b1AR\_cell} + \text{Gs\_cell} \rightleftharpoons \text{b1AR\_Gs\_cell}$	
10	bind_PDEcAMP	bind_PDEcAMP	$\text{PDE\_cell} + \text{cAMP\_cell} \rightleftharpoons \text{PDEcAMP\_cell}$	
11	Gs_gtp_hydrolysis	Gs_gtp_hydrolysis	$\text{Gsa\_gtp\_cell} \rightleftharpoons \text{Gsa\_gdp\_cell}$	
12	Gs_reassociation	Gs_reassociation	$\text{Gsbg\_cell} + \text{Gsa\_gdp\_cell} \rightleftharpoons \text{Gs\_cell}$	
13	bind_FskAC	bind_FskAC	$\text{AC\_cell} + \text{Fsk\_cell} \rightleftharpoons \text{FskAC\_cell}$	
14	bind_AKARp_PP	bind_AKARp_PP	$\text{PP\_cell} + \text{AKARp\_cell} \rightleftharpoons \text{PP\_AKARp\_cell}$	
15	desens_pka	desens_pka	$\text{b1AR\_cell} \xrightleftharpoons{\text{PKAC\_cell, L\_b1AR\_Gs\_cell, L\_b1AR\_cell}} \text{b1AR\_p\_cell}$	
16	bind_L_b1ARGs	bind_L_b1ARGs	$\text{b1AR\_Gs\_cell} + \text{L\_cell} \rightleftharpoons \text{L\_b1AR\_Gs\_cell}$	

№	Id	Name	Reaction Equation	SBO
17	bind_L_b1AR	bind_L_b1AR	$\mathrm{L\_cell} + \mathrm{b1AR\_cell} \rightleftharpoons \mathrm{L\_b1AR\_cell}$	
18	bind_A2R_PKAC	bind_A2R_PKAC	$\mathrm{A2RC\_cell} \rightleftharpoons \mathrm{A2R\_cell} + \mathrm{PKAC\_cell}$	
19	inhib_PKAC	inhib_PKAC	$\mathrm{PKAC\_cell} + \mathrm{PKI\_cell} \rightleftharpoons \mathrm{PKAC\_PKI\_cell}$	
20	bind_RC_cAMP	bind_RC_cAMP	$\mathrm{RC\_cell} + \mathrm{cAMP\_cell} \rightleftharpoons \mathrm{ARC\_cell}$	
21	cAMP_synthesis_FskAC	cAMP_synthesis_FskAC	$\mathrm{ATP\_cell} \overset{\mathrm{FskAC\_cell}}{\rightleftharpoons} \mathrm{cAMP\_cell}$	
22	add_Ligand	add_Ligand	$\emptyset \rightleftharpoons \mathrm{L\_cell}$	
23	bind_Gs_AC	bind_Gs_AC	$\mathrm{Gsa\_gtp\_cell} + \mathrm{AC\_cell} \rightleftharpoons \mathrm{GsAC\_cell}$	
24	resens_bark	resens_bark	$\mathrm{b1AR\_S464\_cell} \rightleftharpoons \mathrm{L\_b1AR\_cell}$	
25	bind_PKAC_AKAR	bind_PKAC_AKAR	$\mathrm{AKAR\_cell} + \mathrm{PKAC\_cell} \rightleftharpoons \mathrm{PKAC\_AKAR\_cell}$	
26	inhibit_PDE	inhibit_PDE	$\mathrm{PDE\_cell} + \mathrm{IBMX\_cell} \rightleftharpoons \mathrm{PDE\_IBMX\_cell}$	
27	AKARp_dephosph	AKARp_dephosph	$\mathrm{PP\_AKARp\_cell} \rightleftharpoons \mathrm{PP\_cell} + \mathrm{AKAR\_cell}$	
28	AKAR_phosph	AKAR_phosph	$\mathrm{PKAC\_AKAR\_cell} \rightleftharpoons \mathrm{AKARp\_cell} + \mathrm{PKAC\_cell}$	
29	RG_activation	RG_activation	$\mathrm{b1AR\_Gs\_cell} \rightleftharpoons \mathrm{Gsa\_gtp\_cell} + \mathrm{Gsbg\_cell} + \mathrm{b1AR\_cell}$	
30	cAMP_degradation	cAMP_degradation	$\mathrm{PDEcAMP\_cell} \rightleftharpoons \mathrm{PDE\_cell}$	

7.1 Reaction cAMP_synthesis_GsAC

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

Name cAMP_synthesis_GsAC

Reaction equation

$$\text{ATP\_cell} \xrightleftharpoons{\text{GsAC\_cell}} \text{cAMP\_cell} \tag{9}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
ATP_cell	ATP	

Modifier

Table 7: Properties of each modifier.

Id	Name	SBO
GsAC_cell	GsAC	

Product

Table 8: Properties of each product.

Id	Name	SBO
cAMP_cell	cAMP	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{Vmax\_cAMP\_synthesis\_GsAC} \cdot [\text{ATP\_cell}] \cdot \frac{1}{\text{Km} + [\text{ATP\_cell}]} \cdot \text{vol}\,(\text{cell}) \tag{10}$$

Table 9: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km			315.0	0.0010 dimensionless · $m^{-3} \cdot mol$	☑

7.2 Reaction bind_b1AR_propranolol

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

Name bind_b1AR_propranolol

Reaction equation

$$\text{Propranolol\_cell} + \text{b1AR\_cell} \rightleftharpoons \text{b1ARinhib\_cell} \tag{11}$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
Propranolol_cell	Propranolol	
b1AR_cell	b1AR	

Product

Table 11: Properties of each product.

Id	Name	SBO
b1ARinhib_cell	b1ARinhib	

Kinetic Law

Derived unit $m^3 \cdot s^{-1} \cdot l^{-1} \cdot \mu mol$

$$v_2 = (\text{Kf} \cdot [\text{Propranolol\_cell}] \cdot [\text{b1AR\_cell}] + ((\text{Kr} \cdot [\text{b1ARinhib\_cell}]))) \cdot \text{vol}(\text{cell}) \tag{12}$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kf			1000.0	1000 dimensionless$\cdot$ $\mathrm{m}^3 \cdot \mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑
Kr			8.0	s^{-1}	☑

7.3 Reaction add_propranolol

This is a reversible reaction of no reactant forming one product.

Name add_propranolol

Reaction equation

$$\emptyset \rightleftharpoons \text{Propranolol\_cell} \tag{13}$$

Product

Table 13: Properties of each product.

Id	Name	SBO
Propranolol_cell	Propranolol	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{ar\_for\_add\_propranolol} \cdot \text{vol}\,(\text{cell}) \tag{14}$$

7.4 Reaction cAMP_photolysis

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

Name cAMP_photolysis

Reaction equation

$$\text{DMNB\_cAMP\_cell} \overset{\text{light\_spot\_cell}}{\rightleftharpoons} \text{cAMP\_cell} \tag{15}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
DMNB_cAMP_cell	DMNB_cAMP	

Modifier

Table 15: Properties of each modifier.

Id	Name	SBO
light_spot_cell	light_spot	

Product

Table 16: Properties of each product.

Id	Name	SBO
cAMP_cell	cAMP	

Kinetic Law

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

$$v_4 = \mathrm{kphot} \cdot \mathrm{light\_cAMP\_photolysis} \cdot [\mathrm{DMNB\_cAMP\_cell}] \cdot \mathrm{vol}\,(\mathrm{cell}) \tag{16}$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kphot			0.1	$1000\,\mathrm{dimensionless} \cdot \mathrm{m}^3 \cdot \mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑

7.5 Reaction LRG_activation

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

Name LRG_activation

Reaction equation

$$\mathrm{L\_b1AR\_Gs\_cell} \rightleftharpoons \mathrm{Gsa\_gtp\_cell} + \mathrm{Gsbg\_cell} + \mathrm{L\_b1AR\_cell} \tag{17}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
L_b1AR_Gs_cell	L_b1AR_Gs	

Products

Table 19: Properties of each product.

Id	Name	SBO
Gsa_gtp_cell	Gsa_gtp	
Gsbg_cell	Gsbg	
L_b1AR_cell	L_b1AR	

Kinetic Law

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

$$v_5 = \mathrm{k\_gact} \cdot [\mathrm{L\_b1AR\_Gs\_cell}] \cdot \mathrm{vol}\,(\mathrm{cell}) \tag{18}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_gact			16.0	s^{-1}	☑

7.6 Reaction bind_Lb1AR_Gs

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

Name bind_Lb1AR_Gs

Reaction equation

$$\mathrm{Gs\_cell} + \mathrm{L\_b1AR\_cell} \rightleftharpoons \mathrm{L\_b1AR\_Gs\_cell} \tag{19}$$

Reactants

Table 21: Properties of each reactant.

Id	Name	SBO
Gs_cell	Gs	
L_b1AR_cell	L_b1AR	

Product

Table 22: Properties of each product.

Id	Name	SBO
L_b1AR_Gs_cell	L_b1AR_Gs	

Kinetic Law

Derived unit $\mathrm{m}^3 \cdot \mathrm{s}^{-1} \cdot \mathrm{l}^{-1} \cdot \mu\mathrm{mol}$

$$v_6 = (\mathrm{Kf} \cdot [\mathrm{Gs\_cell}] \cdot [\mathrm{L\_b1AR\_cell}] + ((\mathrm{Kr} \cdot [\mathrm{L\_b1AR\_Gs\_cell}]))) \cdot \mathrm{vol}(\mathrm{cell}) \tag{20}$$

Table 23: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kf			1000.0	$1000\,\mathrm{dimensionless} \cdot \mathrm{m}^3 \cdot \mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑
Kr			62.0	s^{-1}	☑

7.7 Reaction desens_bark

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

Name desens_bark

Reaction equation

$$\mathrm{L\_b1AR\_cell} \xrightleftharpoons{\mathrm{L\_b1AR\_Gs\_cell}} \mathrm{b1AR\_S464\_cell} \tag{21}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
L_b1AR_cell	L_b1AR	

Modifier

Table 25: Properties of each modifier.

Id	Name	SBO
L_b1AR_Gs_cell	L_b1AR_Gs	

Product

Table 26: Properties of each product.

Id	Name	SBO
b1AR_S464_cell	b1AR_S464	

Kinetic Law

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

$$v_7 = \mathrm{k\_barkp} \cdot ([\mathrm{L\_b1AR\_cell}] + [\mathrm{L\_b1AR\_Gs\_cell}]) \cdot \mathrm{vol}\,(\mathrm{cell}) \tag{22}$$

Table 27: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_barkp			0.001	s^{-1}	☑

7.8 Reaction bind_cAMP_ARC

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

Name bind_cAMP_ARC

Reaction equation

$$\mathrm{ARC\_cell} + \mathrm{cAMP\_cell} \rightleftharpoons \mathrm{A2RC\_cell} \tag{23}$$

Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
ARC_cell	ARC	
cAMP_cell	cAMP	

Product

Table 29: Properties of each product.

Id	Name	SBO
A2RC_cell	A2RC	

Kinetic Law

Derived unit $\mathrm{m}^3 \cdot \mathrm{s}^{-1} \cdot \mathrm{l}^{-1} \cdot \mu\mathrm{mol}$

$$v_8 = (\mathrm{Kf} \cdot [\mathrm{ARC\_cell}] \cdot [\mathrm{cAMP\_cell}] + ((\mathrm{Kr} \cdot [\mathrm{A2RC\_cell}]))) \cdot \mathrm{vol}\,(\mathrm{cell}) \tag{24}$$

Table 30: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kf			1000.0	1000 dimensionless$\cdot \mathrm{m}^3 \cdot \mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑
Kr			1640.0	s^{-1}	☑

7.9 Reaction bind_b1AR_Gs

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

Name bind_b1AR_Gs

Reaction equation

$$\mathrm{b1AR\_cell} + \mathrm{Gs\_cell} \rightleftharpoons \mathrm{b1AR\_Gs\_cell} \tag{25}$$

Reactants

Table 31: Properties of each reactant.

Id	Name	SBO
b1AR_cell	b1AR	
Gs_cell	Gs	

Product

Table 32: Properties of each product.

Id	Name	SBO
b1AR_Gs_cell	b1AR_Gs	

Kinetic Law

Derived unit $\mathrm{m}^3 \cdot \mathrm{s}^{-1} \cdot \mathrm{l}^{-1} \cdot \mu\mathrm{mol}$

$$v_9 = (\mathrm{Kf} \cdot [\mathrm{b1AR\_cell}] \cdot [\mathrm{Gs\_cell}] + ((\mathrm{Kr} \cdot [\mathrm{b1AR\_Gs\_cell}]))) \cdot \mathrm{vol}(\mathrm{cell}) \tag{26}$$

Table 33: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kf			1000.0	$1000\,\mathrm{dimensionless} \cdot \mathrm{m}^3 \cdot \mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑
Kr			33000.0	s^{-1}	☑

7.10 Reaction bind_PDEcAMP

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

Name bind_PDEcAMP

Reaction equation

$$\mathrm{PDE\_cell} + \mathrm{cAMP\_cell} \rightleftharpoons \mathrm{PDEcAMP\_cell} \tag{27}$$

Reactants

Table 34: Properties of each reactant.

Id	Name	SBO
PDE_cell	PDE	
cAMP_cell	cAMP	

Product

Table 35: Properties of each product.

Id	Name	SBO
PDEcAMP_cell	PDEcAMP	

Kinetic Law

Derived unit $\mathrm{m}^3 \cdot \mathrm{s}^{-1} \cdot \mathrm{l}^{-1} \cdot \mu\mathrm{mol}$

$$v_{10} = (\mathrm{Kf} \cdot [\mathrm{PDE\_cell}] \cdot [\mathrm{cAMP\_cell}] + ((\mathrm{Kr} \cdot [\mathrm{PDEcAMP\_cell}]))) \cdot \mathrm{vol}(\mathrm{cell}) \quad (28)$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kf			1000.0	$1000\,\mathrm{dimensionless} \cdot \mathrm{m}^3 \cdot \mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑
Kr			1300.0	s^{-1}	☑

7.11 Reaction Gs_gtp_hydrolysis

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

Name Gs_gtp_hydrolysis

Reaction equation

$$\mathrm{Gsa\_gtp\_cell} \rightleftharpoons \mathrm{Gsa\_gdp\_cell} \quad (29)$$

Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
Gsa_gtp_cell	Gsa_gtp	

Product

Table 38: Properties of each product.

Id	Name	SBO
Gsa_gdp_cell	Gsa_gdp	

Kinetic Law

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

$$v_{11} = \text{khyd} \cdot [\text{Gsa\_gtp\_cell}] \cdot \text{vol}(\text{cell}) \tag{30}$$

Table 39: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
khyd			0.8	s^{-1}	☑

7.12 Reaction Gs_reassociation

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

Name Gs_reassociation

Reaction equation

$$\text{Gsbg\_cell} + \text{Gsa\_gdp\_cell} \rightleftharpoons \text{Gs\_cell} \tag{31}$$

Reactants

Table 40: Properties of each reactant.

Id	Name	SBO
Gsbg_cell	Gsbg	
Gsa_gdp_cell	Gsa_gdp	

Product

Table 41: Properties of each product.

Id	Name	SBO
Gs_cell	Gs	

Kinetic Law

Derived unit $\mathrm{m}^3 \cdot \mathrm{s}^{-1} \cdot \mathrm{l}^{-1} \cdot \mu\mathrm{mol}$

$$v_{12} = \mathrm{k\_reassoc} \cdot [\mathrm{Gsa\_gdp\_cell}] \cdot [\mathrm{Gsbg\_cell}] \cdot \mathrm{vol}\,(\mathrm{cell}) \tag{32}$$

Table 42: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_reassoc			1210.0	1000 dimensionless $\cdot$ $\mathrm{m}^3 \cdot \mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑

7.13 Reaction bind_FskAC

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

Name bind_FskAC

Reaction equation

$$\mathrm{AC\_cell} + \mathrm{Fsk\_cell} \rightleftharpoons \mathrm{FskAC\_cell} \tag{33}$$

Reactants

Table 43: Properties of each reactant.

Id	Name	SBO
AC_cell	AC	
Fsk_cell	Fsk	

Product

Table 44: Properties of each product.

Id	Name	SBO
FskAC_cell	FskAC	

Kinetic Law

Derived unit $\mathrm{m}^3 \cdot \mathrm{s}^{-1} \cdot \mathrm{l}^{-1} \cdot \mu\mathrm{mol}$

$$v_{13} = (\mathrm{Kf} \cdot [\mathrm{AC\_cell}] \cdot [\mathrm{Fsk\_cell}] + ((\mathrm{Kr} \cdot [\mathrm{FskAC\_cell}]))) \cdot \mathrm{vol}(\mathrm{cell}) \tag{34}$$

Table 45: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kf			1000.0	$1000\,\mathrm{dimensionless} \cdot \mathrm{m}^3 \cdot \mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑
Kr			860000.0	s^{-1}	☑

7.14 Reaction bind_AKARp_PP

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

Name bind_AKARp_PP

Reaction equation

$$\mathrm{PP\_cell} + \mathrm{AKARp\_cell} \rightleftharpoons \mathrm{PP\_AKARp\_cell} \tag{35}$$

Reactants

Table 46: Properties of each reactant.

Id	Name	SBO
PP_cell	PP	
AKARp_cell	AKARp	

Product

Table 47: Properties of each product.

Id	Name	SBO
PP_AKARp_cell	PP_AKARp	

Kinetic Law

Derived unit $\mathrm{m}^3 \cdot \mathrm{s}^{-1} \cdot \mathrm{l}^{-1} \cdot \mu\mathrm{mol}$

$$v_{14} = (\mathrm{Kf} \cdot [\mathrm{PP\_cell}] \cdot [\mathrm{AKARp\_cell}] + ((\mathrm{Kr} \cdot [\mathrm{PP\_AKARp\_cell}]))) \cdot \mathrm{vol}(\mathrm{cell}) \quad (36)$$

Table 48: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kf			1000.0	$1000\,\mathrm{dimensionless} \cdot \mathrm{m}^3 \cdot \mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑
Kr			7000.0	s^{-1}	☑

7.15 Reaction desens_pka

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

Name desens_pka

Reaction equation

$$\mathrm{b1AR\_cell} \xrightleftharpoons{\mathrm{PKAC\_cell},\ \mathrm{L\_b1AR\_Gs\_cell},\ \mathrm{L\_b1AR\_cell}} \mathrm{b1AR\_p\_cell} \quad (37)$$

Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
b1AR_cell	b1AR	

Modifiers

Table 50: Properties of each modifier.

Id	Name	SBO
PKAC_cell	PKAC	

Id	Name	SBO
L_b1AR_Gs_cell	L_b1AR_Gs	
L_b1AR_cell	L_b1AR	

Product

Table 51: Properties of each product.

Id	Name	SBO
b1AR_p_cell	b1AR_p	

Kinetic Law

Derived unit $\mathrm{m}^3 \cdot \mathrm{s}^{-1} \cdot \mathrm{l}^{-1} \cdot \mu\mathrm{mol}$

$$v_{15} = (\mathrm{kpkap} \cdot [\mathrm{PKAC\_cell}] \cdot ([\mathrm{L\_b1AR\_Gs\_cell}] + [\mathrm{b1AR\_cell}] + [\mathrm{L\_b1AR\_cell}]) + ((\mathrm{kpkam} \cdot [\mathrm{b1AR\_p\_cell}]))) \cdot \mathrm{vol}(\mathrm{cell}) \quad (38)$$

Table 52: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kpkap			0.004	$1000\,\mathrm{dimensionless} \cdot \mathrm{m}^3 \cdot \mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑
kpkam			0.002	s^{-1}	☑

7.16 Reaction bind_L_b1ARGs

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

Name bind_L_b1ARGs

Reaction equation

$$\mathrm{b1AR\_Gs\_cell} + \mathrm{L\_cell} \rightleftharpoons \mathrm{L\_b1AR\_Gs\_cell} \quad (39)$$

Reactants

Table 53: Properties of each reactant.

Id	Name	SBO
b1AR_Gs_cell	b1AR_Gs	
L_cell	L	

Product

Table 54: Properties of each product.

Id	Name	SBO
L_b1AR_Gs_cell	L_b1AR_Gs	

Kinetic Law

Derived unit $\mathrm{m}^3 \cdot \mathrm{s}^{-1} \cdot \mathrm{l}^{-1} \cdot \mu\mathrm{mol}$

$$v_{16} = (\mathrm{Kf} \cdot [\mathrm{b1AR\_Gs\_cell}] \cdot [\mathrm{L\_cell}] + ((\mathrm{Kd} \cdot [\mathrm{L\_b1AR\_Gs\_cell}]))) \cdot \mathrm{vol}(\mathrm{cell}) \quad (40)$$

Table 55: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kf			1000.000	$1000\,\mathrm{dimensionless} \cdot \mathrm{m}^3 \cdot \mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑
Kd			0.536	s^{-1}	☑

7.17 Reaction bind_L_b1AR

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

Name bind_L_b1AR

Reaction equation

$$\mathrm{L\_cell} + \mathrm{b1AR\_cell} \rightleftharpoons \mathrm{L\_b1AR\_cell} \quad (41)$$

Reactants

Table 56: Properties of each reactant.

Id	Name	SBO
L_cell	L	
b1AR_cell	b1AR	

Product

Table 57: Properties of each product.

Id	Name	SBO
L_b1AR_cell	L_b1AR	

Kinetic Law

Derived unit $\mathrm{m}^3 \cdot \mathrm{s}^{-1} \cdot \mathrm{l}^{-1} \cdot \mu\mathrm{mol}$

$$v_{17} = (\mathrm{Kf} \cdot [\mathrm{L\_cell}] \cdot [\mathrm{b1AR\_cell}] + ((\mathrm{Kr} \cdot [\mathrm{L\_b1AR\_cell}]))) \cdot \mathrm{vol}(\mathrm{cell}) \tag{42}$$

Table 58: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kf			1000.0	$1000\,\mathrm{dimensionless} \cdot \mathrm{m}^3 \cdot \mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑
Kr			285.0	s^{-1}	☑

7.18 Reaction bind_A2R_PKAC

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

Name bind_A2R_PKAC

Reaction equation

$$\mathrm{A2RC\_cell} \rightleftharpoons \mathrm{A2R\_cell} + \mathrm{PKAC\_cell} \tag{43}$$

Reactant

Table 59: Properties of each reactant.

Id	Name	SBO
A2RC_cell	A2RC	

Products

Table 60: Properties of each product.

Id	Name	SBO
A2R_cell	A2R	
PKAC_cell	PKAC	

Kinetic Law

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

$$v_{18} = (\mathrm{Kf} \cdot [\mathrm{A2RC\_cell}] + ((\mathrm{Kr} \cdot [\mathrm{A2R\_cell}] \cdot [\mathrm{PKAC\_cell}]))) \cdot \mathrm{vol}(\mathrm{cell}) \tag{44}$$

Table 61: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kf			4375.0	s^{-1}	☑
Kr			1000.0	$1000\,\mathrm{dimensionless} \cdot \mathrm{m}^3 \cdot \mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑

7.19 Reaction inhib_PKAC

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

Name inhib_PKAC

Reaction equation

$$\mathrm{PKAC\_cell} + \mathrm{PKI\_cell} \rightleftharpoons \mathrm{PKAC\_PKI\_cell} \tag{45}$$

Reactants

Table 62: Properties of each reactant.

Id	Name	SBO
PKAC_cell	PKAC	
PKI_cell	PKI	

Product

Table 63: Properties of each product.

Id	Name	SBO
PKAC_PKI_cell	PKAC_PKI	

Kinetic Law

Derived unit $\mathrm{m}^3 \cdot \mathrm{s}^{-1} \cdot \mathrm{l}^{-1} \cdot \mu\mathrm{mol}$

$$v_{19} = (\mathrm{Kf} \cdot [\mathrm{PKAC\_cell}] \cdot [\mathrm{PKI\_cell}] + ((\mathrm{Kr} \cdot [\mathrm{PKAC\_PKI\_cell}]))) \cdot \mathrm{vol}(\mathrm{cell}) \quad (46)$$

Table 64: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kf			1000.0	$1000\,\mathrm{dimensionless} \cdot \mathrm{m}^3 \cdot \mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑
Kr			0.2	s^{-1}	☑

7.20 Reaction bind_RC_cAMP

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

Name bind_RC_cAMP

Reaction equation

$$\mathrm{RC\_cell} + \mathrm{cAMP\_cell} \rightleftharpoons \mathrm{ARC\_cell} \quad (47)$$

Reactants

Table 65: Properties of each reactant.

Id	Name	SBO
RC_cell	RC	
cAMP_cell	cAMP	

Product

Table 66: Properties of each product.

Id	Name	SBO
ARC_cell	ARC	

Kinetic Law

Derived unit $\mathrm{m}^3 \cdot \mathrm{s}^{-1} \cdot \mathrm{l}^{-1} \cdot \mu\mathrm{mol}$

$$v_{20} = (\mathrm{Kf} \cdot [\mathrm{RC\_cell}] \cdot [\mathrm{cAMP\_cell}] + ((\mathrm{Kr} \cdot [\mathrm{ARC\_cell}]))) \cdot \mathrm{vol}(\mathrm{cell}) \tag{48}$$

Table 67: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kf			1000.0	$1000\,\mathrm{dimensionless} \cdot \mathrm{m}^3 \cdot \mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑
Kr			9140.0	s^{-1}	☑

7.21 Reaction cAMP_synthesis_FskAC

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

Name cAMP_synthesis_FskAC

Reaction equation

$$\mathrm{ATP\_cell} \overset{\mathrm{FskAC\_cell}}{\rightleftharpoons} \mathrm{cAMP\_cell} \tag{49}$$

Reactant

Table 68: Properties of each reactant.

Id	Name	SBO
ATP_cell	ATP	

Modifier

Table 69: Properties of each modifier.

Id	Name	SBO
FskAC_cell	FskAC	

Product

Table 70: Properties of each product.

Id	Name	SBO
cAMP_cell	cAMP	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \text{Vmax\_cAMP\_synthesis\_FskAC} \cdot [\text{ATP\_cell}] \cdot \frac{1}{\text{Km} + [\text{ATP\_cell}]} \cdot \text{vol}(\text{cell}) \qquad (50)$$

Table 71: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km			860.0	$0.0010\,\text{dimensionless} \cdot \text{m}^{-3} \cdot \text{mol}$	☑

7.22 Reaction add_Ligand

This is a reversible reaction of no reactant forming one product.

Name add_Ligand

Reaction equation

$$\emptyset \rightleftharpoons \text{L\_cell} \qquad (51)$$

Product

Table 72: Properties of each product.

Id	Name	SBO
L_cell	L	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \text{ar\_for\_add\_Ligand} \cdot \text{vol}(\text{cell}) \tag{52}$$

7.23 Reaction bind_Gs_AC

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

Name bind_Gs_AC

Reaction equation

$$\text{Gsa\_gtp\_cell} + \text{AC\_cell} \rightleftharpoons \text{GsAC\_cell} \tag{53}$$

Reactants

Table 73: Properties of each reactant.

Id	Name	SBO
Gsa_gtp_cell	Gsa_gtp	
AC_cell	AC	

Product

Table 74: Properties of each product.

Id	Name	SBO
GsAC_cell	GsAC	

Kinetic Law

Derived unit $\text{m}^3 \cdot \text{s}^{-1} \cdot \text{l}^{-1} \cdot \mu\text{mol}$

$$v_{23} = (\text{Kf} \cdot [\text{Gsa\_gtp\_cell}] \cdot [\text{AC\_cell}] + ((\text{Kr} \cdot [\text{GsAC\_cell}]))) \cdot \text{vol}(\text{cell}) \tag{54}$$

Table 75: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kf			1000.0	1000 dimensionless $\cdot$ $m^3 \cdot mol^{-1} \cdot s^{-1}$	☑
Kr			400.0	s^{-1}	☑

7.24 Reaction resens_bark

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

Name resens_bark

Reaction equation

$$\text{b1AR\_S464\_cell} \rightleftharpoons \text{L\_b1AR\_cell} \tag{55}$$

Reactant

Table 76: Properties of each reactant.

Id	Name	SBO
b1AR_S464_cell	b1AR_S464	

Product

Table 77: Properties of each product.

Id	Name	SBO
L_b1AR_cell	L_b1AR	

Kinetic Law

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

$$v_{24} = \text{k\_barkm} \cdot [\text{b1AR\_S464\_cell}] \cdot \text{vol}(\text{cell}) \tag{56}$$

Table 78: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_barkm			0.002	s^{-1}	☑

7.25 Reaction bind_PKAC_AKAR

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

Name bind_PKAC_AKAR

Reaction equation

$$\mathrm{AKAR\_cell} + \mathrm{PKAC\_cell} \rightleftharpoons \mathrm{PKAC\_AKAR\_cell} \tag{57}$$

Reactants

Table 79: Properties of each reactant.

Id	Name	SBO
AKAR_cell	AKAR	
PKAC_cell	PKAC	

Product

Table 80: Properties of each product.

Id	Name	SBO
PKAC_AKAR_cell	PKAC_AKAR	

Kinetic Law

Derived unit $\mathrm{m}^3 \cdot \mathrm{s}^{-1} \cdot \mathrm{l}^{-1} \cdot \mu\mathrm{mol}$

$$v_{25} = (\mathrm{Kf} \cdot [\mathrm{AKAR\_cell}] \cdot [\mathrm{PKAC\_cell}] + ((\mathrm{Kr} \cdot [\mathrm{PKAC\_AKAR\_cell}]))) \cdot \mathrm{vol}(\mathrm{cell}) \tag{58}$$

Table 81: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kf			1000.0	$1000\,\mathrm{dimensionless} \cdot \mathrm{m}^3 \cdot \mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑
Kr			21000.0	s^{-1}	☑

7.26 Reaction inhibit_PDE

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

Name inhibit_PDE

Reaction equation

$$\text{PDE\_cell} + \text{IBMX\_cell} \rightleftharpoons \text{PDE\_IBMX\_cell} \tag{59}$$

Reactants

Table 82: Properties of each reactant.

Id	Name	SBO
PDE_cell	PDE	
IBMX_cell	IBMX	

Product

Table 83: Properties of each product.

Id	Name	SBO
PDE_IBMX_cell	PDE_IBMX	

Kinetic Law

Derived unit $\mathrm{m}^3 \cdot \mathrm{s}^{-1} \cdot \mathrm{l}^{-1} \cdot \mu\mathrm{mol}$

$$\begin{aligned} v_{26} = (&\text{Kf\_inhibit\_PDE} \cdot [\text{PDE\_cell}] \cdot [\text{IBMX\_cell}] \\ &+ ((\text{Kr\_inhibit\_PDE} \cdot [\text{PDE\_IBMX\_cell}]))) \cdot \text{vol}(\text{cell}) \end{aligned} \tag{60}$$

7.27 Reaction AKARp_dephosph

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

Name AKARp_dephosph

Reaction equation

$$\text{PP\_AKARp\_cell} \rightleftharpoons \text{PP\_cell} + \text{AKAR\_cell} \tag{61}$$

Reactant

Table 84: Properties of each reactant.

Id	Name	SBO
PP_AKARp_cell	PP_AKARp	

Products

Table 85: Properties of each product.

Id	Name	SBO
PP_cell	PP	
AKAR_cell	AKAR	

Kinetic Law

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

$$v_{27} = \text{kcat\_PP\_AKARp} \cdot [\text{PP\_AKARp\_cell}] \cdot \text{vol}(\text{cell}) \tag{62}$$

Table 86: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcat_PP-_AKARp			8.5	s^{-1}	☑

7.28 Reaction AKAR_phosph

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

Name AKAR_phosph

Reaction equation

$$\text{PKAC\_AKAR\_cell} \rightleftharpoons \text{AKARp\_cell} + \text{PKAC\_cell} \tag{63}$$

Reactant

Table 87: Properties of each reactant.

Id	Name	SBO
PKAC_AKAR_cell	PKAC_AKAR	

Products

Table 88: Properties of each product.

Id	Name	SBO
AKARp_cell	AKARp	
PKAC_cell	PKAC	

Kinetic Law

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

$$v_{28} = \mathrm{kpka\_akar} \cdot [\mathrm{PKAC\_AKAR\_cell}] \cdot \mathrm{vol}\,(\mathrm{cell}) \tag{64}$$

Table 89: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kpka_akar			54.0	s^{-1}	☑

7.29 Reaction RG_activation

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

Name RG_activation

Reaction equation

$$\mathrm{b1AR\_Gs\_cell} \rightleftharpoons \mathrm{Gsa\_gtp\_cell} + \mathrm{Gsbg\_cell} + \mathrm{b1AR\_cell} \tag{65}$$

Reactant

Table 90: Properties of each reactant.

Id	Name	SBO
b1AR_Gs_cell	b1AR_Gs	

Products

Table 91: Properties of each product.

Id	Name	SBO
Gsa_gtp_cell	Gsa_gtp	
Gsbg_cell	Gsbg	
b1AR_cell	b1AR	

Kinetic Law

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

$$v_{29} = \text{k\_gact} \cdot [\text{b1AR\_Gs\_cell}] \cdot \text{vol}(\text{cell}) \tag{66}$$

Table 92: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_gact			16.0	s^{-1}	☑

7.30 Reaction cAMP_degradation

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

Name cAMP_degradation

Reaction equation

$$\text{PDEcAMP\_cell} \rightleftharpoons \text{PDE\_cell} \tag{67}$$

Reactant

Table 93: Properties of each reactant.

Id	Name	SBO
PDEcAMP_cell	PDEcAMP	

Product

Table 94: Properties of each product.

Id	Name	SBO
PDE_cell	PDE	

Kinetic Law

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

$$v_{30} = \mathrm{kpde} \cdot [\mathrm{PDEcAMP\_cell}] \cdot \mathrm{vol}\,(\mathrm{cell}) \tag{68}$$

Table 95: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kpde			5.0	s^{-1}	☑

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.

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.

8.1 Species `Gsbg_cell`

Name Gsbg

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

This species takes part in three reactions (as a reactant in `Gs_reassociation` and as a product in `LRG_activation`, `RG_activation`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gsbg\_cell} = v_5 + v_{29} - v_{12} \tag{69}$$

8.2 Species `L_cell`

Name L

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

This species takes part in three reactions (as a reactant in `bind_L_b1ARGs`, `bind_L_b1AR` and as a product in `add_Ligand`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{L\_cell} = v_{22} - v_{16} - v_{17} \tag{70}$$

8.3 Species Gsa_gdp_cell

Name Gsa_gdp

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

This species takes part in two reactions (as a reactant in Gs_reassociation and as a product in Gs_gtp_hydrolysis).

$$\frac{\text{d}}{\text{d}t}\text{Gsa\_gdp\_cell} = v_{11} - v_{12} \tag{71}$$

8.4 Species Gsa_gtp_cell

Name Gsa_gtp

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

This species takes part in four reactions (as a reactant in Gs_gtp_hydrolysis, bind_Gs_AC and as a product in LRG_activation, RG_activation).

$$\frac{\text{d}}{\text{d}t}\text{Gsa\_gtp\_cell} = v_5 + v_{29} - v_{11} - v_{23} \tag{72}$$

8.5 Species b1AR_S464_cell

Name b1AR_S464

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

This species takes part in two reactions (as a reactant in resens_bark and as a product in desens_bark).

$$\frac{\text{d}}{\text{d}t}\text{b1AR\_S464\_cell} = v_7 - v_{24} \tag{73}$$

8.6 Species PDEcAMP_cell

Name PDEcAMP

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

This species takes part in two reactions (as a reactant in cAMP_degradation and as a product in bind_PDEcAMP).

$$\frac{\text{d}}{\text{d}t}\text{PDEcAMP\_cell} = v_{10} - v_{30} \tag{74}$$

8.7 Species PDE_cell

Name PDE

Initial concentration $0.014\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in three reactions (as a reactant in bind_PDEcAMP, inhibit_PDE and as a product in cAMP_degradation).

$$\frac{\text{d}}{\text{d}t}\text{PDE\_cell} = v_{30} - v_{10} - v_{26} \tag{75}$$

8.8 Species ATP_cell

Name ATP

Initial concentration $5000\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in two reactions (as a reactant in cAMP_synthesis_GsAC, cAMP_synthesis_FskAC), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\text{d}}{\text{d}t}\text{ATP\_cell} = 0 \tag{76}$$

8.9 Species b1AR_cell

Name b1AR

Initial concentration $0.0132\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in five reactions (as a reactant in bind_b1AR_propranolol, bind_b1AR_Gs, desens_pka, bind_L_b1AR and as a product in RG_activation).

$$\frac{\text{d}}{\text{d}t}\text{b1AR\_cell} = v_{29} - v_2 - v_9 - v_{15} - v_{17} \tag{77}$$

8.10 Species Gs_cell

Name Gs

Initial concentration $3.83\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in three reactions (as a reactant in bind_Lb1AR_Gs, bind_b1AR_Gs and as a product in Gs_reassociation).

$$\frac{\text{d}}{\text{d}t}\text{Gs\_cell} = v_{12} - v_6 - v_9 \tag{78}$$

8.11 Species A2RC_cell

Name A2RC

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

This species takes part in two reactions (as a reactant in bind_A2R_PKAC and as a product in bind_cAMP_ARC).

$$\frac{\text{d}}{\text{d}t}\text{A2RC\_cell} = v_8 - v_{18} \tag{79}$$

8.12 Species A2R_cell

Name A2R

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

This species takes part in one reaction (as a product in bind_A2R_PKAC).

$$\frac{\text{d}}{\text{d}t}\text{A2R\_cell} = v_{18} \tag{80}$$

8.13 Species PKAC_cell

Name PKAC

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

This species takes part in five reactions (as a reactant in inhib_PKAC, bind_PKAC_AKAR and as a product in bind_A2R_PKAC, AKAR_phosph and as a modifier in desens_pka).

$$\frac{\text{d}}{\text{d}t}\text{PKAC\_cell} = v_{18} + v_{28} - v_{19} - v_{25} \tag{81}$$

8.14 Species ARC_cell

Name ARC

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

This species takes part in two reactions (as a reactant in bind_cAMP_ARC and as a product in bind_RC_cAMP).

$$\frac{\text{d}}{\text{d}t}\text{ARC\_cell} = v_{20} - v_8 \tag{82}$$

8.15 Species PKAC_AKAR_cell

Name PKAC_AKAR

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

This species takes part in two reactions (as a reactant in AKAR_phosph and as a product in bind_PKAC_AKAR).

$$\frac{\text{d}}{\text{d}t}\text{PKAC\_AKAR\_cell} = v_{25} - v_{28} \tag{83}$$

8.16 Species Propranolol_cell

Name Propranolol

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

This species takes part in two reactions (as a reactant in bind_b1AR_propranolol and as a product in add_propranolol).

$$\frac{\text{d}}{\text{d}t}\text{Propranolol\_cell} = v_3 - v_2 \tag{84}$$

8.17 Species b1ARinhib_cell

Name b1ARinhib

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

This species takes part in one reaction (as a product in bind_b1AR_propranolol).

$$\frac{\text{d}}{\text{d}t}\text{b1ARinhib\_cell} = v_2 \tag{85}$$

8.18 Species light_spot_cell

Name light_spot

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

This species takes part in one reaction (as a modifier in cAMP_photolysis).

$$\frac{\text{d}}{\text{d}t}\text{light\_spot\_cell} = 0 \tag{86}$$

8.19 Species AC_cell

Name AC

Initial concentration $0.0497\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in two reactions (as a reactant in bind_FskAC, bind_Gs_AC).

$$\frac{\text{d}}{\text{d}t}\text{AC\_cell} = -v_{13} - v_{23} \tag{87}$$

8.20 Species PKI_cell

Name PKI

Initial concentration $0.18\ \mu\text{mol}\cdot\text{l}^{-1}$

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

$$\frac{\text{d}}{\text{d}t}\text{PKI\_cell} = -v_{19} \tag{88}$$

8.21 Species PKAC_PKI_cell

Name PKAC_PKI

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

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

$$\frac{\text{d}}{\text{d}t}\text{PKAC\_PKI\_cell} = v_{19} \tag{89}$$

8.22 Species RC_cell

Name RC

Initial concentration $1.18\ \mu\text{mol}\cdot\text{l}^{-1}$

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

$$\frac{\text{d}}{\text{d}t}\text{RC\_cell} = -v_{20} \tag{90}$$

8.23 Species b1AR_Gs_cell

Name b1AR_Gs

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

This species takes part in three reactions (as a reactant in bind_L_b1ARGs, RG_activation and as a product in bind_b1AR_Gs).

$$\frac{\text{d}}{\text{d}t}\text{b1AR\_Gs\_cell} = v_9 - v_{16} - v_{29} \tag{91}$$

8.24 Species cAMP_cell

Name cAMP

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

This species takes part in six reactions (as a reactant in bind_cAMP_ARC, bind_PDEcAMP, bind_RC_cAMP and as a product in cAMP_synthesis_GsAC, cAMP_photolysis, cAMP_synthesis_FskAC).

$$\frac{\text{d}}{\text{d}t}\text{cAMP\_cell} = v_1 + v_4 + v_{21} - v_8 - v_{10} - v_{20} \tag{92}$$

8.25 Species GsAC_cell

Name GsAC

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

This species takes part in two reactions (as a product in bind_Gs_AC and as a modifier in cAMP_synthesis_GsAC).

$$\frac{\text{d}}{\text{d}t}\text{GsAC\_cell} = v_{23} \tag{93}$$

8.26 Species IBMX_cell

Name IBMX

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

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

$$\frac{\text{d}}{\text{d}t}\text{IBMX\_cell} = -v_{26} \tag{94}$$

8.27 Species PDE_IBMX_cell

Name PDE_IBMX

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

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

$$\frac{\text{d}}{\text{d}t}\text{PDE\_IBMX\_cell} = v_{26} \tag{95}$$

8.28 Species Fsk_cell

Name Fsk

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Fsk\_cell} = -\ v_{13} \tag{96}$$

8.29 Species FskAC_cell

Name FskAC

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

This species takes part in two reactions (as a product in bind_FskAC and as a modifier in cAMP-_synthesis_FskAC).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{FskAC\_cell} = v_{13} \tag{97}$$

8.30 Species b1AR_p_cell

Name b1AR_p

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{b1AR\_p\_cell} = v_{15} \tag{98}$$

8.31 Species L_b1AR_cell

Name L_b1AR

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

This species takes part in six reactions (as a reactant in bind_Lb1AR_Gs, desens_bark and as a product in LRG_activation, bind_L_b1AR, resens_bark and as a modifier in desens_pka).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{L\_b1AR\_cell} = v_5 + v_{17} + v_{24} - v_6 - v_7 \tag{99}$$

8.32 Species AKAR_cell

Name AKAR

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

This species takes part in two reactions (as a reactant in bind_PKAC_AKAR and as a product in AKARp_dephosph).

$$\frac{\text{d}}{\text{d}t}\text{AKAR\_cell} = v_{27} - v_{25} \tag{100}$$

8.33 Species AKARp_cell

Name AKARp

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

This species takes part in two reactions (as a reactant in bind_AKARp_PP and as a product in AKAR_phosph).

$$\frac{\text{d}}{\text{d}t}\text{AKARp\_cell} = v_{28} - v_{14} \tag{101}$$

8.34 Species PP_cell

Name PP

Initial concentration $0.67\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in bind_AKARp_PP and as a product in AKARp_dephosph).

$$\frac{\text{d}}{\text{d}t}\text{PP\_cell} = v_{27} - v_{14} \tag{102}$$

8.35 Species PP_AKARp_cell

Name PP_AKARp

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

This species takes part in two reactions (as a reactant in AKARp_dephosph and as a product in bind_AKARp_PP).

$$\frac{\text{d}}{\text{d}t}\text{PP\_AKARp\_cell} = v_{14} - v_{27} \tag{103}$$

8.36 Species DMNB_cAMP_cell

Name DMNB_cAMP

Initial concentration $3.01\ \mu\text{mol}\cdot\text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{DMNB\_cAMP\_cell} = -v_4 \tag{104}$$

8.37 Species L_b1AR_Gs_cell

Name L_b1AR_Gs

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

This species takes part in five reactions (as a reactant in LRG_activation and as a product in bind_Lb1AR_Gs, bind_L_b1ARGs and as a modifier in desens_bark, desens_pka).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{L\_b1AR\_Gs\_cell} = v_6 + v_{16} - v_5 \tag{105}$$

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