SBML Model Report

Model name: "Thomsen1988-_AdenylateCyclase_Inhibition"

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1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Enuo He[1] at September 26th 2006 at 6:47 p. m. and last time modified at February thirteenth 2014 at 3:49 p. m. Table 1 shows 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	10
events	0	constraints	0
reactions	6	function definitions	0
global parameters	0	unit definitions	0
rules	0	initial assignments	0

Model Notes

This model was created according to the paper *Inhibition of Adenylate Cyclase Is Mediated by the High Affinity Conformation of the alpha2-Adrenergic Receptor* published in 1988.

The figure4 (steady state curve) in the paper has been simulated having the same plot with Copasi 4.0.19 (development) and roadRunner(online).Because the initial concentration of R and D were not given in the paper ,so we gave it 1e-9 Mol/L and 1e-8 Mol/L respectively.

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Pay attention that the simulations of steady state concentration of species in arbitrary units are shown for figure4 and figure6 in the paper.

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 l

2.3 Unit `area`

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

Definition m^2

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		3	1	litre	☑	

3.1 Compartment `cell`

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

Name cell

4 Species

This model contains ten species. Section 6 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
agonist	D	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DR	DR	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DRG_GDP	DRG_GDP	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DRG	DRG	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
GDP	GDP	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DRG_GTP	DRG_GTP	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
GTP	GTP	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Recptor	R	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
G_GDP	G_GDP	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
G_GTP	G_GTP	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Reactions

This model contains six 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 4: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	`Forming`	Forming DR	agonist + Recptor $\rightleftharpoons$ DR	
2	`reaction_1`	DR binding with G_GDP produc DRG_GDP	DR + G_GDP $\rightleftharpoons$ DRG_GDP	
3	`reaction_2`	GDP releasing	DRG_GDP $\rightleftharpoons$ GDP + DRG	
4	`reaction_3`	GTP binding with DRG	DRG + GTP $\rightleftharpoons$ DRG_GTP	
5	`reaction_4`	DRG_GTP dissociates(G protein activation)	DRG_GTP $\longrightarrow$ G_GTP + DR	
6	`reaction_5`	G protein inactivated	G_GTP $\longrightarrow$ G_GDP	

5.1 Reaction `Forming`

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

Name Forming DR

Reaction equation

$$\text{agonist} + \text{Recptor} \rightleftharpoons \text{DR} \tag{1}$$

Reactants

Table 5: Properties of each reactant.

Id	Name	SBO
`agonist`	D	
`Recptor`	R	

Product

Table 6: Properties of each product.

Id	Name	SBO
`DR`	DR	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}\,(\text{cell}) \cdot (\text{k1} \cdot [\text{agonist}] \cdot [\text{Recptor}] - \text{k7} \cdot [\text{DR}]) \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`k1`			5000000.0		☑
`k7`	k7		0.5		☑

5.2 Reaction `reaction_1`

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

Name DR binding with G_GDP produc DRG_GDP

Reaction equation

$$\mathrm{DR} + \mathrm{G\_GDP} \rightleftharpoons \mathrm{DRG\_GDP} \tag{3}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
DR	DR	
G_GDP	G_GDP	

Product

Table 9: Properties of each product.

Id	Name	SBO
DRG_GDP	DRG_GDP	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k2} \cdot [\mathrm{DR}] \cdot [\mathrm{G\_GDP}] - \mathrm{k8} \cdot [\mathrm{DRG\_GDP}]) \tag{4}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k2			10^8		☑
k8	k8		0.100		☑

5.3 Reaction reaction_2

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

Name GDP releasing

Reaction equation

$$\mathrm{DRG\_GDP} \rightleftharpoons \mathrm{GDP} + \mathrm{DRG} \tag{5}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
DRG_GDP	DRG_GDP	

Products

Table 12: Properties of each product.

Id	Name	SBO
GDP	GDP	
DRG	DRG	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k3} \cdot [\mathrm{DRG\_GDP}] - \mathrm{k9} \cdot [\mathrm{DRG}] \cdot [\mathrm{GDP}]) \tag{6}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k3			0.1		☑
k9	k9		100000.0		☑

5.4 Reaction reaction_3

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

Name GTP binding with DRG

Reaction equation

$$\mathrm{DRG} + \mathrm{GTP} \rightleftharpoons \mathrm{DRG\_GTP} \tag{7}$$

Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
DRG	DRG	
GTP	GTP	

Product

Table 15: Properties of each product.

Id	Name	SBO
DRG_GTP	DRG_GTP	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k4} \cdot [\mathrm{DRG}] \cdot [\mathrm{GTP}] - \mathrm{k10} \cdot [\mathrm{DRG\_GTP}]) \tag{8}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k4			10^7		☑
k10	k10		0.100		☑

5.5 Reaction reaction_4

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

Name DRG_GTP dissociates(G protein activation)

Reaction equation

$$\mathrm{DRG\_GTP} \longrightarrow \mathrm{G\_GTP} + \mathrm{DR} \tag{9}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
DRG_GTP	DRG_GTP	

Products

Table 18: Properties of each product.

Id	Name	SBO
G_GTP	G_GTP	
DR	DR	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k5} \cdot [\mathrm{DRG\_GTP}] \tag{10}$$

Table 19: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k5			0.05		☑

5.6 Reaction reaction_5

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

Name G protein inactivated

Reaction equation

$$\mathrm{G\_GTP} \longrightarrow \mathrm{G\_GDP} \tag{11}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
G_GTP	G_GTP	

Product

Table 21: Properties of each product.

Id	Name	SBO
G_GDP	G_GDP	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k6} \cdot [\mathrm{G\_GTP}] \tag{12}$$

Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k6			0.1		☑

6 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.

6.1 Species agonist

Name D

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{agonist} = -\,v_1 \tag{13}$$

6.2 Species DR

Name DR

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

This species takes part in three reactions (as a reactant in reaction_1 and as a product in Forming, reaction_4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DR} = v_1 + v_5 - v_2 \tag{14}$$

6.3 Species DRG_GDP

Name DRG_GDP

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

This species takes part in two reactions (as a reactant in reaction_2 and as a product in reaction_1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DRG\_GDP} = v_2 - v_3 \tag{15}$$

6.4 Species DRG

Name DRG

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

This species takes part in two reactions (as a reactant in reaction_3 and as a product in reaction_2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DRG} = v_3 - v_4 \tag{16}$$

6.5 Species GDP

Name GDP

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

This species takes part in one reaction (as a product in reaction_2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GDP} = v_3 \tag{17}$$

6.6 Species DRG_GTP

Name DRG_GTP

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

This species takes part in two reactions (as a reactant in reaction_4 and as a product in reaction_3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DRG\_GTP} = v_4 - v_5 \tag{18}$$

6.7 Species GTP

Name GTP

Initial concentration $10^{-5}\,\mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a reactant in reaction_3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GTP} = -\,v_4 \tag{19}$$

6.8 Species Recptor

Name R

Initial concentration $10^{-9}\,\mathrm{mol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Recptor} = -\,v_1 \tag{20}$$

6.9 Species G_GDP

Name G_GDP

Initial concentration $10^{-9}\,\mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in reaction_1 and as a product in reaction_5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G\_GDP} = v_6 - v_2 \tag{21}$$

6.10 Species G_GTP

Name G_GTP

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

This species takes part in two reactions (as a reactant in reaction_5 and as a product in reaction_4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G\_GTP} = v_5 - v_6 \tag{22}$$

SBML2LaTeX was developed by Andreas Dräger[a], Hannes Planatscher[a], Dieudonné M Wouamba[a], Adrian Schröder[a], Michael Hucka[b], Lukas Endler[c], Martin Golebiewski[d] and Andreas Zell[a]. Please see http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX for more information.

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