SBML Model Report

Model name: "Yi2003_GproteinCycle"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Enuo He[1] at October 17th 2006 at 3:12 p. m. and last time modified at February 24th 2015 at 8:25 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	7
events	0	constraints	0
reactions	7	function definitions	0
global parameters	0	unit definitions	1
rules	0	initial assignments	0

Model Notes

The paper describes both wild-type and mutant cells of G protein cycle by using different values of G protein deactivation. We chosed the wild-type, k=0.11 s-1.

The unit of the concentration for the proteins are numbers of molecules per cell.

Figure5(A) was reproduced with COPASI 4.0 (Build 18) and SBML_odeSolver. Figure5(B) was reproduced with COPASI 4.0 (Build 18).

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2 Unit Definitions

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

2.1 Unit `substance`

Definition item

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 seven 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
L	Ligand	cell	$\text{item} \cdot \text{l}^{-1}$	⊟	⊟
R	Receptor	cell	$\text{item} \cdot \text{l}^{-1}$	⊟	⊟
G	Inactive heterotrimeric G-protein	cell	$\text{item} \cdot \text{l}^{-1}$	⊟	⊟
Gbg	Free levels of G-beta-gamma	cell	$\text{item} \cdot \text{l}^{-1}$	⊟	⊟
Gd	G-alpha-GDP	cell	$\text{item} \cdot \text{l}^{-1}$	⊟	⊟
Ga	G-alpha-GTP	cell	$\text{item} \cdot \text{l}^{-1}$	⊟	⊟
RL	Receptor-Ligand	cell	$\text{item} \cdot \text{l}^{-1}$	⊟	⊟

5 Reactions

This model contains seven 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	`reaction_0`	Ligand-Receptor Association	$L + R \rightleftharpoons RL$	
2	`reaction_1`	Receptor Synthesis	$\emptyset \longrightarrow R$	
3	`reaction_2`	Receptor Degradation	$R \longrightarrow \emptyset$	
4	`reaction_3`	Heterotrimeric G-Protein Formation	$Gd + Gbg \longrightarrow G$	
5	`reaction_4`	G-protein Activation	$G \xrightarrow{RL} Ga + Gbg$	
6	`reaction_5`	Receptor-Ligand Degradation	$RL \longrightarrow \emptyset$	
7	`reaction_6`	G-protein Inactivation	$Ga \longrightarrow Gd$	

5.1 Reaction reaction_0

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

Name Ligand-Receptor Association

Reaction equation

$$\mathrm{L} + \mathrm{R} \rightleftharpoons \mathrm{RL} \tag{1}$$

Reactants

Table 5: Properties of each reactant.

Id	Name	SBO
L	Ligand	
R	Receptor	

Product

Table 6: Properties of each product.

Id	Name	SBO
RL	Receptor-Ligand	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k1} \cdot [\mathrm{L}] \cdot [\mathrm{R}] - \mathrm{k2} \cdot [\mathrm{RL}]) \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			$3.32 \cdot 10^{-18}$		☑
k2			0.010		☑

5.2 Reaction reaction_1

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

Name Receptor Synthesis

Reaction equation

$$\emptyset \longrightarrow \mathrm{R} \tag{3}$$

Product

Table 8: Properties of each product.

Id	Name	SBO
R	Receptor	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{v} \tag{4}$$

Table 9: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v			4.0		☑

5.3 Reaction `reaction_2`

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

Name Receptor Degradation

Reaction equation

$$\mathrm{R} \longrightarrow \emptyset \tag{5}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
R	Receptor	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k1} \cdot [\mathrm{R}] \tag{6}$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			$4 \cdot 10^{-4}$		☑

5.4 Reaction reaction_3

This is an irreversible reaction of two reactants forming one product.

Name Heterotrimeric G-Protein Formation

Reaction equation

$$\mathrm{Gd} + \mathrm{Gbg} \longrightarrow \mathrm{G} \tag{7}$$

Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
Gd	G-alpha-GDP	
Gbg	Free levels of G-beta-gamma	

Product

Table 13: Properties of each product.

Id	Name	SBO
G	Inactive heterotrimeric G-protein	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k1} \cdot [\mathrm{Gd}] \cdot [\mathrm{Gbg}] \tag{8}$$

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			1.0		☑

5.5 Reaction reaction_4

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

Name G-protein Activation

Reaction equation

$$\mathrm{G} \xrightarrow{\mathrm{RL}} \mathrm{Ga} + \mathrm{Gbg} \tag{9}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
G	Inactive heterotrimeric G-protein	

Modifier

Table 16: Properties of each modifier.

Id	Name	SBO
RL	Receptor-Ligand	

Products

Table 17: Properties of each product.

Id	Name	SBO
Ga	G-alpha-GTP	
Gbg	Free levels of G-beta-gamma	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k1} \cdot [\mathrm{RL}] \cdot [\mathrm{G}] \tag{10}$$

Table 18: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			10^{-5}		☑

5.6 Reaction reaction_5

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

Name Receptor-Ligand Degradation

Reaction equation

$$\mathrm{RL} \longrightarrow \emptyset \tag{11}$$

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
RL	Receptor-Ligand	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k1} \cdot [\mathrm{RL}] \tag{12}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.004		☑

5.7 Reaction reaction_6

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

Name G-protein Inactivation

Reaction equation

$$\mathrm{Ga} \longrightarrow \mathrm{Gd} \tag{13}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
Ga	G-alpha-GTP	

Product

Table 22: Properties of each product.

Id	Name	SBO
Gd	G-alpha-GDP	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k1} \cdot [\mathrm{Ga}] \tag{14}$$

Table 23: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.11		☑

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 L

Name Ligand

Initial concentration $6.02 \cdot 10^{17}$ item $\cdot$ l^{-1}

This species takes part in one reaction (as a reactant in reaction_0).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{L} = -v_1 \tag{15}$$

6.2 Species R

Name Receptor

Initial concentration 10000 item $\cdot$ l^{-1}

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R} = v_2 - v_1 - v_3 \tag{16}$$

6.3 Species G

Name Inactive heterotrimeric G-protein

Initial concentration 7000 item $\cdot$ l^{-1}

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G} = v_4 - v_5 \tag{17}$$

6.4 Species Gbg

Name Free levels of G-beta-gamma

Initial concentration 3000 item $\cdot$ l^{-1}

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

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

6.5 Species Gd

Name G-alpha-GDP

Initial concentration 3000 item $\cdot$ l^{-1}

This species takes part in two reactions (as a reactant in reaction_3 and as a product in reaction_6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gd} = v_7 - v_4 \tag{19}$$

6.6 Species Ga

Name G-alpha-GTP

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

This species takes part in two reactions (as a reactant in reaction_6 and as a product in reaction_4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ga} = v_5 - v_7 \tag{20}$$

6.7 Species RL

Name Receptor-Ligand

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

This species takes part in three reactions (as a reactant in reaction_5 and as a product in reaction_0 and as a modifier in reaction_4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{RL} = v_1 - v_6 \tag{21}$$

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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