SBML Model Report

Model name: “Sneyd2002_IP3_Receptor”

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 May 30th 2006 at 12:07 a. m. and last time modified at February 24th 2015 at 8:32 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	6
events	0	constraints	0
reactions	5	function definitions	0
global parameters	27	unit definitions	1
rules	8	initial assignments	0

Model Notes

This model was successfully tested on Jarnac and MathSBML. The model reproduces the time profile of „Open Probability„ of the receptor as shown in Figure 4 of the publication. The value of calcium ion concentration „c„ in this model is 10 microM.

[1] California Institute of Technology, hdharuri@cds.caltech.edu

In summary, you are entitled to use this encoded model in absolutely any manner you deem suitable, verbatim, or with modification, alone or embedded it in a larger context, redistribute it, commercially or not, in a restricted way or not.

To cite BioModels Database, please use: Li C, Donizelli M, Rodriguez N, Dharuri H, Endler L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novre N, Laibe C (2010) BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models. BMC Syst Biol., 4:92.

2 Unit Definitions

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

2.1 Unit `substance`

Name micromole

Definition µmol

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
`compartment`			3	1	litre	☑	

3.1 Compartment `compartment`

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

4 Species

This model contains six 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
R	Receptor	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
O	Open State	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
I1	Inactivated State 1	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
S	Shut State	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
A	Activated State	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
I2	Inactivated State 2	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟

5 Parameters

This model contains 27 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
open_probability			0.000		☐
Phi1			0.000		☐
k1			0.640		☑
L1			0.120		☑
l2			1.700		☑
lminus2			0.800		☑
c			10.000		☑
L3			0.025		☑
Phi2			0.000		☐
k2			37.400		☑
l4			1.700		☑
Phi_minus2			0.000		☐
kminus1			0.040		☑
kminus2			1.400		☑
kminus3			29.800		☑
lminus4			2.500		☑
L5			54.700		☑
Phi3			0.000		☐
k3			0.110		☑
Phi4			0.000		☐
k4			4.000		☑
l6			4707.000		☑
Phi_minus4			0.000		☐
kminus4			0.540		☑
lminus6			11.400		☑
Phi5			0.000		☐
IP3	IP3		10.000		☑

6 Rules

This is an overview of eight rules.

6.1 Rule open_probability

Rule open_probability is an assignment rule for parameter open_probability:

$$\text{open\_probability} = (0.1 \cdot [\text{O}] + 0.9 \cdot [\text{A}])^4 \tag{1}$$

6.2 Rule Phi1

Rule Phi1 is an assignment rule for parameter Phi1:

$$\text{Phi1} = \frac{(\text{k1} \cdot \text{L1} + \text{l2}) \cdot \text{c}}{\text{L1} + \text{c} \cdot \left(1 + \frac{\text{L1}}{\text{L3}}\right)} \tag{2}$$

6.3 Rule Phi2

Rule Phi2 is an assignment rule for parameter Phi2:

$$\text{Phi2} = \frac{\text{k2} \cdot \text{L3} + \text{l4} \cdot \text{c}}{\text{L3} + \text{c} \cdot \left(1 + \frac{\text{L3}}{\text{L1}}\right)} \tag{3}$$

6.4 Rule Phi_minus2

Rule Phi_minus2 is an assignment rule for parameter Phi_minus2:

$$\text{Phi\_minus2} = \frac{\text{kminus2} + \text{lminus4} \cdot \text{c}}{1 + \frac{\text{c}}{\text{L5}}} \tag{4}$$

6.5 Rule Phi3

Rule Phi3 is an assignment rule for parameter Phi3:

$$\text{Phi3} = \frac{\text{k3} \cdot \text{L5}}{\text{L5} + \text{c}} \tag{5}$$

6.6 Rule Phi4

Rule Phi4 is an assignment rule for parameter Phi4:

$$\text{Phi4} = \frac{(\text{k4} \cdot \text{L5} + \text{l6}) \cdot \text{c}}{\text{L5} + \text{c}} \tag{6}$$

6.7 Rule Phi_minus4

Rule Phi_minus4 is an assignment rule for parameter Phi_minus4:

$$\text{Phi\_minus4} = \frac{\text{L1} \cdot (\text{kminus4} + \text{lminus6})}{\text{L1} + \text{c}} \tag{7}$$

6.8 Rule Phi5

Rule Phi5 is an assignment rule for parameter Phi5:

$$\mathrm{Phi5} = \frac{(\mathrm{k1} \cdot \mathrm{L1} + \mathrm{l2}) \cdot \mathrm{c}}{\mathrm{L1} + \mathrm{c}} \tag{8}$$

7 Reactions

This model contains five 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	v1	Receptor-Open state transition	R $\rightleftharpoons$ O	
2	v2	Receptor-Inactivated state 1 transition	R $\rightleftharpoons$ I1	
3	v3	Open-Shut state transition	O $\rightleftharpoons$ S	
4	v4	Open-Activated state transition	O $\rightleftharpoons$ A	
5	v5	Activated-Inactivated state 2 transition	A $\rightleftharpoons$ I2	

7.1 Reaction v1

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

Name Receptor-Open state transition

Reaction equation

$$\mathrm{R} \rightleftharpoons \mathrm{O} \tag{9}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
R	Receptor	

Product

Table 7: Properties of each product.

Id	Name	SBO
O	Open State	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{Phi2} \cdot \mathrm{IP3} \cdot [\mathrm{R}] - \mathrm{Phi\_minus2} \cdot [\mathrm{O}]) \tag{10}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
IP3			10.0		☑

7.2 Reaction v2

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

Name Receptor-Inactivated state 1 transition

Reaction equation

$$\mathrm{R} \rightleftharpoons \mathrm{I1} \tag{11}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
R	Receptor	

Product

Table 10: Properties of each product.

Id	Name	SBO
I1	Inactivated State 1	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{Phi1} \cdot [\mathrm{R}] - (\mathrm{kminus1} + \mathrm{lminus2}) \cdot [\mathrm{I1}]) \tag{12}$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kminus1			0.04		☑
lminus2			0.80		☑

7.3 Reaction v3

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

Name Open-Shut state transition

Reaction equation

$$\mathrm{O} \rightleftharpoons \mathrm{S} \tag{13}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
O	Open State	

Product

Table 13: Properties of each product.

Id	Name	SBO
S	Shut State	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{Phi3} \cdot [\mathrm{O}] - \mathrm{kminus3} \cdot [\mathrm{S}]) \tag{14}$$

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kminus3			29.8		☑

7.4 Reaction v4

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

Name Open-Activated state transition

Reaction equation

$$\mathrm{O} \rightleftharpoons \mathrm{A} \tag{15}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
O	Open State	

Product

Table 16: Properties of each product.

Id	Name	SBO
A	Activated State	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{Phi4} \cdot [\mathrm{O}] - \mathrm{Phi\_minus4} \cdot [\mathrm{A}]) \tag{16}$$

7.5 Reaction v5

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

Name Activated-Inactivated state 2 transition

Reaction equation

$$\mathrm{A} \rightleftharpoons \mathrm{I2} \tag{17}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
A	Activated State	

Product

Table 18: Properties of each product.

Id	Name	SBO
I2	Inactivated State 2	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{Phi5} \cdot [\mathrm{A}] - (\mathrm{kminus1} + \mathrm{lminus2}) \cdot [\mathrm{I2}]) \tag{18}$$

Table 19: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kminus1			0.04		☑
lminus2			0.80		☑

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 R

Name Receptor

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

This species takes part in two reactions (as a reactant in v1, v2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R} = -v_1 - v_2 \tag{19}$$

8.2 Species O

Name Open State

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

This species takes part in three reactions (as a reactant in v3, v4 and as a product in v1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{O} = v_1 - v_3 - v_4 \tag{20}$$

8.3 Species I1

Name Inactivated State 1

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

This species takes part in one reaction (as a product in v2).

$$\frac{\text{d}}{\text{d}t}\text{I1} = v_2 \tag{21}$$

8.4 Species S

Name Shut State

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

This species takes part in one reaction (as a product in v3).

$$\frac{\text{d}}{\text{d}t}\text{S} = v_3 \tag{22}$$

8.5 Species A

Name Activated State

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

This species takes part in two reactions (as a reactant in v5 and as a product in v4).

$$\frac{\text{d}}{\text{d}t}\text{A} = v_4 - v_5 \tag{23}$$

8.6 Species I2

Name Inactivated State 2

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

This species takes part in one reaction (as a product in v5).

$$\frac{\text{d}}{\text{d}t}\text{I2} = v_5 \tag{24}$$

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.

[a]Center for Bioinformatics Tübingen (ZBIT), Germany
[b]California Institute of Technology, Beckman Institute BNMC, Pasadena, United States
[c]European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom
[d]EML Research gGmbH, Heidelberg, Germany