SBML Model Report

Model name: "Bertram2006_Endothelin"

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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 August third 2007 at 1:17 p. m. and last time modified at July fifth 2012 at 4:31 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	3
events	1	constraints	0
reactions	3	function definitions	0
global parameters	50	unit definitions	1
rules	20	initial assignments	0

Model Notes

The model is according to the paper *Endothelin Action on Pituitary Lactotrophs: One Receptor, Many GTP-Binding Proteins* Figure 1 has been simulated by MathSBML. The figure for the [Ca2+]i and [Ca2+]ER have been normalized in the paper.Original model comes from http://www.math.fsu.edu//software/pituitary

The units for parameters and species are varied from one to another, so I omit the unit definition here . Conductances in pS; currents in fA; Ca concentrations in uM; time in ms

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2 Unit Definitions

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

2.1 Unit `ms`

Name millisecond

Definition ms

2.2 Unit `substance`

Notes Mole is the predefined SBML unit for `substance`.

Definition mol

2.3 Unit `volume`

Notes Litre is the predefined SBML unit for `volume`.

Definition l

2.4 Unit `area`

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

Definition m^2

2.5 Unit `length`

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

Definition m

2.6 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`			3	1	litre	☑	

3.1 Compartment `cell`

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

4 Species

This model contains three species. Section 9 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
c	cytosolic calcium concentration	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
cer	ER calcium concentration	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
cAMP		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 50 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vh			−20.000		☑
sh			70.000		☑
tauh			20.000		☑
kserca			0.400		☑
sigmav			10.000		☑
kc			0.150		☑
vn			−16.000		☑
vk			−75.000		☑
taun			20.000		☑
gk			3500.000		☑
sn			5.000		☑
vca			25.000		☑
gca			2000.000		☑
vm			−20.000		☑
sm			12.000		☑
lambda			1.250		☑
cm			5300.000		☑
f			0.010		☑
fer			0.010		☑
alpha			$4.5 \cdot 10^{-6}$		☑
perl			$5 \cdot 10^{-4}$		☑
dact			0.350		☑
dip3			0.500		☑
dinh			0.400		☑
ninf			0.000		☐
minf			0.000		☐
hinf			0.000		☐
ica			0.000		☐
igirk			0.000		☐
ik			0.000		☐
girk			1000.000		☐
IP3			0.000		☐
ainf			0.000		☐
hinfer			0.000		☐
jerp			0.000		☐
binf			0.000		☐
o			0.000		☐

Id	Name	SBO	Value	Unit	Constant
jerleak			0.000		☐
jerip3			0.000		☐
jertot			0.000		☐
jmemtot			0.000		☐
ki			0.500		☑
perl_inf			0.000		☐
taudir			20000.000		☑
cAMPlow			0.200		☑
ETswitch			0.000		☐
h			0.000		☐
inh	variable for direct inhibition of secretion		1.000		☐
V	voltage		−60.000		☐
n	delayed rectifier activation		0.000		☐

6 Rules

This is an overview of 20 rules.

6.1 Rule minf

Rule minf is an assignment rule for parameter minf:

$$\text{minf} = \frac{1}{1 + \exp\left(\frac{\text{vm}-\text{V}}{\text{sm}}\right)} \tag{1}$$

6.2 Rule ninf

Rule ninf is an assignment rule for parameter ninf:

$$\text{ninf} = \frac{1}{1 + \exp\left(\frac{\text{vn}-\text{V}}{\text{sn}}\right)} \tag{2}$$

6.3 Rule hinf

Rule hinf is an assignment rule for parameter hinf:

$$\text{hinf} = \frac{1}{1 + \exp\left(\frac{\text{vh}-\text{V}}{\text{sh}}\right)} \tag{3}$$

6.4 Rule `ica`

Rule `ica` is an assignment rule for parameter `ica`:

$$\text{ica} = \text{gca} \cdot \text{minf} \cdot (\text{V} - \text{vca}) \tag{4}$$

6.5 Rule `igirk`

Rule `igirk` is an assignment rule for parameter `igirk`:

$$\text{igirk} = \text{girk} \cdot \text{h} \cdot (\text{V} - \text{vk}) \tag{5}$$

6.6 Rule `ik`

Rule `ik` is an assignment rule for parameter `ik`:

$$\text{ik} = \text{gk} \cdot \text{n} \cdot (\text{V} - \text{vk}) \tag{6}$$

6.7 Rule `ainf`

Rule `ainf` is an assignment rule for parameter `ainf`:

$$\text{ainf} = \frac{1}{1 + \frac{\text{dact}}{[\text{c}]}} \tag{7}$$

6.8 Rule `hinfer`

Rule `hinfer` is an assignment rule for parameter `hinfer`:

$$\text{hinfer} = \frac{1}{1 + \frac{[\text{c}]}{\text{dinh}}} \tag{8}$$

6.9 Rule `jerp`

Rule `jerp` is an assignment rule for parameter `jerp`:

$$\text{jerp} = \text{kserca} \cdot [\text{c}] \tag{9}$$

6.10 Rule `binf`

Rule `binf` is an assignment rule for parameter `binf`:

$$\text{binf} = \frac{\text{IP3}}{\text{IP3} + \text{dip3}} \tag{10}$$

6.11 Rule `o`

Rule `o` is an assignment rule for parameter `o`:

$$\text{o} = \text{ainf}^3 \cdot \text{binf}^3 \cdot \text{hinfer}^3 \tag{11}$$

6.12 Rule jmemtot

Rule jmemtot is an assignment rule for parameter jmemtot:

$$\text{jmemtot} = (\text{alpha} \cdot \text{ica} + \text{kc} \cdot [\text{c}]) \tag{12}$$

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

6.13 Rule jerleak

Rule jerleak is an assignment rule for parameter jerleak:

$$\text{jerleak} = \text{perl} \cdot ([\text{cer}] - [\text{c}]) \tag{13}$$

6.14 Rule jerip3

Rule jerip3 is an assignment rule for parameter jerip3:

$$\text{jerip3} = \text{o} \cdot ([\text{cer}] - [\text{c}]) \tag{14}$$

6.15 Rule jertot

Rule jertot is an assignment rule for parameter jertot:

$$\text{jertot} = \text{jerleak} + \text{jerip3} - \text{jerp} \tag{15}$$

6.16 Rule perl_inf

Rule perl_inf is an assignment rule for parameter perl_inf:

$$\text{perl\_inf} = \frac{\text{inh} \cdot [\text{cAMP}] \cdot [\text{c}]^4}{\text{ki}^4 + [\text{c}]^4} \tag{16}$$

6.17 Rule h

Rule h is a rate rule for parameter h:

$$\frac{\text{d}}{\text{d}t}\text{h} = \frac{\text{hinf} - \text{h}}{\text{tauh}} \tag{17}$$

6.18 Rule inh

Rule inh is a rate rule for parameter inh:

$$\frac{\text{d}}{\text{d}t}\text{inh} = \text{ETswitch} \cdot \frac{0.2 - \text{inh}}{\text{taudir}} \tag{18}$$

6.19 Rule V

Rule V is a rate rule for parameter V:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{V} = \frac{\mathrm{ica} - \mathrm{ik} - \mathrm{igirk}}{\mathrm{cm}} \tag{19}$$

6.20 Rule n

Rule n is a rate rule for parameter n:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{n} = \frac{\mathrm{lambda} \cdot (\mathrm{ninf} - \mathrm{n})}{\mathrm{taun}} \tag{20}$$

7 Event

This is an overview of one event. Each event is initiated whenever its trigger condition switches from false to true. A delay function postpones the effects of an event to a later time point. At the time of execution, an event can assign values to species, parameters or compartments if these are not set to constant.

7.1 Event event_0000001

Name ET-1 switch

Notes At time 1 minute a nanomolar concentration of endothelin is added.

Trigger condition

$$\mathrm{time} > 60000 \tag{21}$$

Assignments

$$\mathrm{IP3} = 0.3 \tag{22}$$

$$\mathrm{girk} = 3000 \tag{23}$$

$$\mathrm{ETswitch} = 1 \tag{24}$$

8 Reactions

This model contains three 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	reaction_0000001		$\emptyset \longrightarrow c$	
2	reaction_0000002		$\emptyset \longrightarrow cer$	
3	reaction_000003		$\emptyset \longrightarrow cAMP$	

8.1 Reaction reaction_0000001

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

Reaction equation

$$\emptyset \longrightarrow \mathrm{c} \tag{25}$$

Product

Table 6: Properties of each product.

Id	Name	SBO
c	cytosolic calcium concentration	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{f} \cdot (\mathrm{jertot} + \mathrm{jmemtot}) \tag{26}$$

8.2 Reaction reaction_0000002

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

Reaction equation

$$\emptyset \longrightarrow \mathrm{cer} \tag{27}$$

Product

Table 7: Properties of each product.

Id	Name	SBO
cer	ER calcium concentration	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{fer} \cdot \mathrm{sigmav} \cdot \mathrm{jertot} \cdot \mathrm{vol}\,(\mathrm{cell}) \tag{28}$$

8.3 Reaction reaction_000003

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

Reaction equation

$$\emptyset \longrightarrow \mathrm{cAMP} \tag{29}$$

Product

Table 8: Properties of each product.

Id	Name	SBO
cAMP		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{ETswitch} \cdot \frac{\mathrm{cAMPlow} - [\mathrm{cAMP}]}{\mathrm{taudir}} \tag{30}$$

9 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.

9.1 Species c

Name cytosolic calcium concentration

Initial concentration $0.3\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a product in reaction_0000001).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{c} = v_1 \tag{31}$$

9.2 Species cer

Name ER calcium concentration

Initial concentration $260\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a product in reaction_0000002).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cer} = v_2 \tag{32}$$

9.3 Species cAMP

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

This species takes part in one reaction (as a product in reaction_000003).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{cAMP} = v_3 \tag{33}$$

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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