SBML Model Report

Model name: "Blum2000_LHsecretion_1"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Enuo He[1] at November nineth 2006 at 5:07 p. m. and last time modified at April sixth 2014 at 9:48 p. m. Table 1 provides 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	8
events	1	constraints	0
reactions	5	function definitions	0
global parameters	2	unit definitions	3
rules	1	initial assignments	0

Model Notes

A mathematical model quantifying GnRH-induced LH secretion from gonadotropes by Blum et al (2000)

This paper includes three stages, and the model does not include the third stage. Also an event is included which remove the hormone GnRH at time=5min. Figure 1 and Figure 2 of the paper are reproduced, using SBML odeSolver. We choose to encode the model with the concentration of GnRH equal to 1.0nM.

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To cite BioModels Database, please use Le Novre N., Bornstein B., Broicher A., Courtot M., Donizelli M., Dharuri H., Li L., Sauro H., Schilstra M., Shapiro B., Snoep J.L., Hucka M. (2006) BioModels Database: A Free, Centralized Database of Curated, Published, Quantitative Kinetic Models of Biochemical and Cellular Systems Nucleic Acids Res., 34: D689-D691.

2 Unit Definitions

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

2.1 Unit `time`

Definition 60 s

2.2 Unit `substance`

Definition nmol

2.3 Unit `unitDefinition_3`

Name unit for beta

Definition $(60\ \mathrm{s})^{-1}$

2.4 Unit `volume`

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

Definition l

2.5 Unit `area`

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

Definition m^2

2.6 Unit `length`

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

Definition m

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 eight 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
H	H	cell	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
HR	HR	cell	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
R	R	cell	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
HRRH	HRRH	cell	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
E	E	cell	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
GQ	GQ	cell	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
IP3	IP3	cell	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CHO	CHO	cell	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains two global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`alpha`	alpha		2.0	nmol	☑
`beta`	beta		4.0	$(60\ \mathrm{s})^{-1}$	☑

6 Rule

This is an overview of one rule.

6.1 Rule `CHO`

Rule `CHO` is an assignment rule for species `CHO`:

$$\mathrm{CHO} = \frac{0.0010 \cdot \mathrm{alpha} \cdot [\mathrm{IP3}] \cdot (0.3 + 0.3 \cdot \mathrm{beta} \cdot \mathrm{time} \cdot \exp(1 - \mathrm{beta} \cdot \mathrm{time}))}{1 + 0.0010 \cdot \mathrm{alpha} \cdot [\mathrm{IP3}]} \tag{1}$$

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 `RemovalH`

Name removal of hormone

Trigger condition

$$\mathrm{time} > 5 \tag{2}$$

Assignment

$$\mathrm{H} = 0 \tag{3}$$

8 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	`reaction_0`	H binding to R	$\mathrm{H} + \mathrm{R} \rightleftharpoons \mathrm{HR}$	
2	`reaction_1`	HR forming HRRH	$2\,\mathrm{HR} \rightleftharpoons \mathrm{HRRH}$	
3	`reaction_2`	G protein react with dimer producing E	$\mathrm{HRRH} + \mathrm{GQ} \rightleftharpoons \mathrm{E}$	
4	`reaction_3`	IP3 converted into inactive metabolites	$\mathrm{IP3} \longrightarrow \emptyset$	
5	`reaction_4`	Production of IP3	$\emptyset \xrightarrow{\mathrm{E}} \mathrm{IP3}$	

8.1 Reaction reaction_0

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

Name H binding to R

Reaction equation

$$\mathrm{H} + \mathrm{R} \rightleftharpoons \mathrm{HR} \tag{4}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
H	H	
R	R	

Product

Table 7: Properties of each product.

Id	Name	SBO
HR	HR	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k1} \cdot [\mathrm{H}] \cdot [\mathrm{R}] - \mathrm{k2} \cdot [\mathrm{HR}]) \tag{5}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			2.5		☑
k2			5.0		☑

8.2 Reaction reaction_1

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

Name HR forming HRRH

Reaction equation

$$2\,\mathrm{HR} \rightleftharpoons \mathrm{HRRH} \tag{6}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
HR	HR	

Product

Table 10: Properties of each product.

Id	Name	SBO
HRRH	HRRH	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{cell}) \cdot \left(\mathrm{k1} \cdot [\mathrm{HR}]^2 - \mathrm{k2} \cdot [\mathrm{HRRH}]\right) \tag{7}$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			2500.0		☑
k2			5.0		☑

8.3 Reaction reaction_2

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

Name G protein react with dimer producing E

Reaction equation

$$\mathrm{HRRH} + \mathrm{GQ} \rightleftharpoons \mathrm{E} \tag{8}$$

Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
HRRH	HRRH	
GQ	GQ	

Product

Table 13: Properties of each product.

Id	Name	SBO
E	E	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k1} \cdot [\mathrm{HRRH}] \cdot [\mathrm{GQ}] - \mathrm{k2} \cdot [\mathrm{E}]) \tag{9}$$

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			4000.0		☑
k2			200.0		☑

8.4 Reaction reaction_3

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

Name IP3 converted into inactive metabolites

Reaction equation

$$\mathrm{IP3} \longrightarrow \emptyset \tag{10}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
IP3	IP3	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k1} \cdot [\mathrm{IP3}] \tag{11}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			10.0		☑

8.5 Reaction reaction_4

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

Name Production of IP3

Reaction equation

$$\emptyset \xrightarrow{\mathrm{E}} \mathrm{IP3} \tag{12}$$

Modifier

Table 17: Properties of each modifier.

Id	Name	SBO
E	E	

Product

Table 18: Properties of each product.

Id	Name	SBO
IP3	IP3	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k} \cdot [\mathrm{E}] \tag{13}$$

Table 19: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k			$2 \cdot 10^7$		☑

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 H

Name H

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

Involved in event RemovalH

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{H} = -v_1 \tag{14}$$

Furthermore, one event influences this species' rate of change.

9.2 Species HR

Name HR

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{HR} = v_1 - 2\,v_2 \tag{15}$$

9.3 Species R

Name R

Initial concentration $0.01\ \mathrm{nmol \cdot l^{-1}}$

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

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

9.4 Species HRRH

Name HRRH

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{HRRH} = v_2 - v_3 \tag{17}$$

9.5 Species E

Name E

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

This species takes part in two reactions (as a product in reaction_2 and as a modifier in reaction_4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E} = v_3 \tag{18}$$

9.6 Species GQ

Name GQ

Initial concentration $0.1\ \mathrm{nmol \cdot l^{-1}}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GQ} = -v_3 \tag{19}$$

9.7 Species IP3

Name IP3

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IP3} = v_5 - v_4 \tag{20}$$

9.8 Species CHO

Name CHO

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

Involved in rule CHO

One rule which determines this species' quantity.

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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