SBML Model Report

Model name: "Hornberg2005_ERKcascade"

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 December eleventh 2006 at 10:48 a. m. and last time modified at May 14th 2012 at 12:15 a. 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	8
events	0	constraints	0
reactions	8	function definitions	0
global parameters	0	unit definitions	1
rules	0	initial assignments	0

Model Notes

SBML level 2 code generated for the JWS Online project by Jacky Snoep using PySCeS
Run this model online at http://jjj.biochem.sun.ac.za
To cite JWS Online please refer to: Olivier, B.G. and Snoep, J.L. (2004) Web-based modelling using JWS Online , Bioinformatics, 20:2143-2144

Biomodels Curation The model reproduces the time series depicted in Fig 2 of the paper. Also, by varying the values of Vmax for the second kinase (k5) the time series of X3P as shown in Fig3 can be reproduced. The model was successfully tested on MathSBML and Jarnac.

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

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 dimensionless

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
`compartment`	Cytosol		3	1	litre	☑	

3.1 Compartment `compartment`

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

Name Cytosol

4 Species

This model contains eight 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
R		compartment	item	⊟	⊟
Rin		compartment	item	⊟	⊟
x1		compartment	item	⊟	⊟
x1p		compartment	item	⊟	⊟
x2		compartment	item	⊟	⊟
x2p		compartment	item	⊟	⊟
x3		compartment	item	⊟	⊟
x3p		compartment	item	⊟	⊟

5 Reactions

This model contains eight 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	v1	Receptor inactivation	R $\rightleftharpoons$ Rin	
2	v2	Receptor activation	Rin $\rightleftharpoons$ R	
3	v3	Kinase-1 activation	x1 $\overset{\text{R}}{\rightleftharpoons}$ x1p	
4	v4	Kinase-1 inactivation	x1p $\rightleftharpoons$ x1	
5	v5	Kinase-2 activation	x2 $\overset{\text{x1p}}{\rightleftharpoons}$ x2p	
6	v6	Kinase-2 inactivation	x2p $\rightleftharpoons$ x2	
7	v7	Kinase-3 activation	x3 $\overset{\text{x2p}}{\rightleftharpoons}$ x3p	
8	v8	Kinase-3 inactivation	x3p $\rightleftharpoons$ x3	

5.1 Reaction v1

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

Name Receptor inactivation

Reaction equation

$$\mathrm{R} \rightleftharpoons \mathrm{Rin} \tag{1}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
R		

Product

Table 6: Properties of each product.

Id	Name	SBO
Rin		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{\mathrm{Vm1} \cdot \mathrm{R}}{\mathrm{Km1} + \mathrm{R}} \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm1			1.0		☑
Km1			0.1		☑

5.2 Reaction v2

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

Name Receptor activation

Reaction equation

$$\mathrm{Rin} \rightleftharpoons \mathrm{R} \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
Rin		

Product

Table 9: Properties of each product.

Id	Name	SBO
R		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\mathrm{Vm2} \cdot \mathrm{Rin}}{\mathrm{Km2} + \mathrm{Rin}} \tag{4}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm2			0.01		☑
Km2			0.10		☑

5.3 Reaction v3

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name Kinase-1 activation

Reaction equation

$$\mathrm{x1} \overset{\mathrm{R}}{\rightleftharpoons} \mathrm{x1p} \tag{5}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
x1		

Modifier

Table 12: Properties of each modifier.

Id	Name	SBO
R		

Product

Table 13: Properties of each product.

Id	Name	SBO
x1p		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \frac{\mathrm{k3} \cdot \mathrm{R} \cdot \mathrm{x1}}{\mathrm{Km3} + \mathrm{x1}} \tag{6}$$

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k3			1.0		☑
Km3			0.1		☑

5.4 Reaction v4

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

Name Kinase-1 inactivation

Reaction equation

$$\mathrm{x1p} \rightleftharpoons \mathrm{x1} \tag{7}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
x1p		

Product

Table 16: Properties of each product.

Id	Name	SBO
x1		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \frac{\mathrm{Vm4} \cdot \mathrm{x1p}}{\mathrm{Km4} + \mathrm{x1p}} \tag{8}$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm4			0.3		☑
Km4			1.0		☑

5.5 Reaction v5

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name Kinase-2 activation

Reaction equation

$$\mathrm{x2} \overset{\mathrm{x1p}}{\rightleftharpoons} \mathrm{x2p} \tag{9}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
x2		

Modifier

Table 19: Properties of each modifier.

Id	Name	SBO
x1p		

Product

Table 20: Properties of each product.

Id	Name	SBO
x2p		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \frac{\mathrm{k5} \cdot \mathrm{x1p} \cdot \mathrm{x2}}{\mathrm{Km5} + \mathrm{x2}} \tag{10}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k5			1.0		☑
Km5			0.1		☑

5.6 Reaction v6

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

Name Kinase-2 inactivation

Reaction equation

$$\mathrm{x2p} \rightleftharpoons \mathrm{x2} \tag{11}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
x2p		

Product

Table 23: Properties of each product.

Id	Name	SBO
x2		

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \frac{\mathrm{Vm6} \cdot \mathrm{x2p}}{\mathrm{Km6} + \mathrm{x2p}} \tag{12}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm6			0.3		☑
Km6			1.0		☑

5.7 Reaction v7

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name Kinase-3 activation

Reaction equation

$$\mathrm{x3} \overset{\mathrm{x2p}}{\rightleftharpoons} \mathrm{x3p} \tag{13}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
x3		

Modifier

Table 26: Properties of each modifier.

Id	Name	SBO
x2p		

Product

Table 27: Properties of each product.

Id	Name	SBO
x3p		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \frac{\mathrm{k7} \cdot \mathrm{x2p} \cdot \mathrm{x3}}{\mathrm{Km7} + \mathrm{x3}} \tag{14}$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k7			1.0		☑
Km7			0.1		☑

5.8 Reaction v8

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

Name Kinase-3 inactivation

Reaction equation

$$\mathrm{x3p} \rightleftharpoons \mathrm{x3} \tag{15}$$

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
x3p		

Product

Table 30: Properties of each product.

Id	Name	SBO
x3		

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \frac{\frac{\mathrm{Vm8} \cdot \mathrm{x3p}}{\mathrm{Km8}}}{1 + \frac{\mathrm{x3p}}{\mathrm{Km8}} + \frac{\mathrm{Inh}}{\mathrm{Ki8}}} \tag{16}$$

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm8			0.3		☑
Km8			1.0		☑
Inh			0.0		☑
Ki8			1.0		☑

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 R

Initial amount 0.5 item

This species takes part in three reactions (as a reactant in v1 and as a product in v2 and as a modifier in v3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R} = v_2 - v_1 \tag{17}$$

6.2 Species Rin

Initial amount 0 item

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Rin} = v_1 - v_2 \tag{18}$$

6.3 Species x1

Initial amount 1 item

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x1} = v_4 - v_3 \tag{19}$$

6.4 Species x1p

Initial amount 0 item

This species takes part in three reactions (as a reactant in v4 and as a product in v3 and as a modifier in v5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x1p} = v_3 - v_4 \tag{20}$$

6.5 Species x2

Initial amount 1 item

This species takes part in two reactions (as a reactant in v5 and as a product in v6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x2} = v_6 - v_5 \tag{21}$$

6.6 Species x2p

Initial amount 0 item

This species takes part in three reactions (as a reactant in v6 and as a product in v5 and as a modifier in v7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x2p} = v_5 - v_6 \tag{22}$$

6.7 Species x3

Initial amount 1 item

This species takes part in two reactions (as a reactant in v7 and as a product in v8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x3} = v_8 - v_7 \tag{23}$$

6.8 Species x3p

Initial amount 0 item

This species takes part in two reactions (as a reactant in v8 and as a product in v7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x3p} = v_7 - v_8 \tag{24}$$

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