SBML Model Report

Model name: "Fuentes2005_ZymogenActivation"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Jacky L Snoep[1] and Harish Dharuri[2] at March fifth 2007 at 4:37 p. m. and last time modified at February thirteenth 2014 at 3:45 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	4
events	0	constraints	0
reactions	3	function definitions	0
global parameters	0	unit definitions	2
rules	0	initial assignments	0

Model Notes

.

.

.

[1]Stellenbosh University, jls@sun.ac.za
[2]California Institute of Technology, hdharuri@cds.caltech.edu

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

.
.
.
.
.
.

The model reproduces Fig 1A of the paper. The model was successfully tested on MathSBML.

This model originates from BioModels Database: A Database of Annotated Published Models. It is copyright (c) 2005-2006 The BioModels Team.
For more information see the terms of use .

2 Unit Definitions

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

2.1 Unit `M_inv_sec_inv`

Name M_inv_sec_inv

Definition $\mathrm{mol}^{-1} \cdot 1 \cdot \mathrm{s}^{-1}$

2.2 Unit `sec_inv`

Name sec_inv

Definition s^{-1}

2.3 Unit `substance`

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

Definition mol

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

2.7 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	compartment		3	1	litre	☑	

3.1 Compartment compartment

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

Name compartment

4 Species

This model contains four 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
z	Zymogen	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
e	Enzyme	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
w	Peptide	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ez	Enzyme-Substrate complex	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 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 4: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	v1	Intramolecular autoactivation	$z \rightleftharpoons w + e$	
2	v2	Intermolecular autoactivation-Complex formation	$z + e \rightleftharpoons ez$	
3	v3	Intermolecular autoactivation-Enzyme release	$ez \rightleftharpoons w + 2\,e$	

5.1 Reaction v1

This is a reversible reaction of one reactant forming two products.

Name Intramolecular autoactivation

Reaction equation

$$\mathrm{z} \rightleftharpoons \mathrm{w} + \mathrm{e} \tag{1}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
z	Zymogen	

Products

Table 6: Properties of each product.

Id	Name	SBO
w	Peptide	
e	Enzyme	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mol}$

$$v_1 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k1} \cdot [\mathrm{z}] \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.004	s^{-1}	☑

5.2 Reaction v2

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

Name Intermolecular autoactivation-Complex formation

Reaction equation

$$\mathrm{z} + \mathrm{e} \rightleftharpoons \mathrm{ez} \tag{3}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
z	Zymogen	
e	Enzyme	

Product

Table 9: Properties of each product.

Id	Name	SBO
ez	Enzyme-Substrate complex	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mol}$

$$v_2 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k21} \cdot [\mathrm{e}] \cdot [\mathrm{z}] - \mathrm{k22} \cdot [\mathrm{ez}]) \tag{4}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k21			1000.000	$\mathrm{mol}^{-1} \cdot 1 \cdot \mathrm{s}^{-1}$	☑
k22			$2.1 \cdot 10^{-4}$	s^{-1}	☑

5.3 Reaction v3

This is a reversible reaction of one reactant forming two products.

Name Intermolecular autoactivation-Enzyme release

Reaction equation

$$\mathrm{ez} \rightleftharpoons \mathrm{w} + 2\,\mathrm{e} \tag{5}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
ez	Enzyme-Substrate complex	

Products

Table 12: Properties of each product.

Id	Name	SBO
w	Peptide	
e	Enzyme	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mol}$

$$v_3 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k3} \cdot [\mathrm{ez}] \tag{6}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k3			$5.4 \cdot 10^{-4}$	s^{-1}	☑

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.

6.1 Species z

Name Zymogen

Initial concentration $2.4 \cdot 10^{-5}\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{z} = -v_1 - v_2 \tag{7}$$

6.2 Species e

Name Enzyme

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e} = v_1 + 2v_3 - v_2 \tag{8}$$

6.3 Species w

Name Peptide

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

This species takes part in two reactions (as a product in v1, v3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{w} = v_1 + v_3 \tag{9}$$

6.4 Species ez

Name Enzyme-Substrate complex

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ez} = v_2 - v_3 \tag{10}$$

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