SBML Model Report

Model name: "Ibrahim2008_Cdc20-_Sequestring_Template_Model"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by the following five authors: Lukas Endler[1], Eberhard Schmitt[2], Peter Dittrich[3], Stephan Diekmann[4] and Bashar Ibrahim[5] at September eleventh 2008 at 8:58 p. m. and last time modified at September 23rd 2009 at 5:09 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	5
events	1	constraints	0
reactions	3	function definitions	0
global parameters	7	unit definitions	2
rules	0	initial assignments	0

Model Notes

Biophysical Chemistry 134 (2008) 93-100

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Mad2 binding is not sufficient for complete Cdc20 sequestering in mitotic transition control (an *in silico* study)

Bashar Ibrahim, Peter Dittrich, Stephan Diekmann, Eberhard Schmitt

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 `ps`

Name per second

Definition s^{-1}

2.2 Unit `pMps`

Name liter per mole per second

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

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
`Cytoplasm`	Cytoplasm		3	1	litre	☑	

3.1 Compartment `Cytoplasm`

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

Name Cytoplasm

4 Species

This model contains five 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
Mad1_CMad2	Mad1:C-Mad2	Cytoplasm	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
OMad2	O-Mad2	Cytoplasm	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Mad1_CMad2_OMad2	Mad1:C-Mad2:O-Mad2*	Cytoplasm	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Cdc20	Cdc20	Cytoplasm	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Cdc20_CMad2	Cdc20:C-Mad2	Cytoplasm	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains seven global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
eta_T		0000338	0.010	s^{-1}	☑
gamma_T		0000036	10^9	$l \cdot mol^{-1} \cdot s^{-1}$	☑
alpha_T		0000339	200000.000	$l \cdot mol^{-1} \cdot s^{-1}$	☑
beta_T		0000338	0.200	s^{-1}	☑
u			1.000	dimensionless	☐
const_val_0			0.000	dimensionless	☑
const_val_1			1.000	dimensionless	☑

6 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.

6.1 Event mt_attachment

Name Microtubule attachment

Trigger condition

$$\text{time} > 2000 \tag{1}$$

Assignment

$$\text{u} = \text{const\_val\_0} \tag{2}$$

7 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	R6		$\mathrm{Mad1\_CMad2} + \mathrm{OMad2} \rightleftharpoons \mathrm{Mad1\_CMad2\_OMad2}$	
2	R7		$\mathrm{Mad1\_CMad2\_OMad2} + \mathrm{Cdc20} \longrightarrow \mathrm{Mad1\_CMad2} + \mathrm{Cdc20\_CMad2}$	
3	R8		$\mathrm{Cdc20\_CMad2} \longrightarrow \mathrm{Cdc20} + \mathrm{OMad2}$	

7.1 Reaction R6

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

Reaction equation

$$\text{Mad1\_CMad2} + \text{OMad2} \rightleftharpoons \text{Mad1\_CMad2\_OMad2} \tag{3}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
Mad1_CMad2	Mad1:C-Mad2	
OMad2	O-Mad2	

Product

Table 7: Properties of each product.

Id	Name	SBO
Mad1_CMad2_OMad2	Mad1:C-Mad2:O-Mad2*	

Kinetic Law

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, continuous scheme

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

$$v_1 = \mathrm{vol}\,(\mathrm{Cytoplasm}) \cdot (\mathrm{u} \cdot \mathrm{alpha\_T} \cdot [\mathrm{Mad1\_CMad2}] \cdot [\mathrm{OMad2}] - \mathrm{beta\_T} \cdot [\mathrm{Mad1\_CMad2\_OMad2}]) \tag{4}$$

7.2 Reaction R7

This is an irreversible reaction of two reactants forming two products.

Reaction equation

$$\text{Mad1\_CMad2\_OMad2} + \text{Cdc20} \longrightarrow \text{Mad1\_CMad2} + \text{Cdc20\_CMad2} \tag{5}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
Mad1_CMad2_OMad2	Mad1:C-Mad2:O-Mad2*	
Cdc20	Cdc20	

Products

Table 9: Properties of each product.

Id	Name	SBO
Mad1_CMad2	Mad1:C-Mad2	
Cdc20_CMad2	Cdc20:C-Mad2	

Kinetic Law

SBO:0000054 mass action rate law for second order irreversible reactions, two reactants, continuous scheme

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

$$v_2 = \mathrm{vol}\,(\mathrm{Cytoplasm}) \cdot \mathrm{u} \cdot \mathrm{gamma\_T} \cdot [\mathrm{Mad1\_CMad2\_OMad2}] \cdot [\mathrm{Cdc20}] \tag{6}$$

7.3 Reaction R8

This is an irreversible reaction of one reactant forming two products.

Reaction equation

$$\mathrm{Cdc20\_CMad2} \longrightarrow \mathrm{Cdc20} + \mathrm{OMad2} \tag{7}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
Cdc20_CMad2	Cdc20:C-Mad2	

Products

Table 11: Properties of each product.

Id	Name	SBO
Cdc20	Cdc20	
OMad2	O-Mad2	

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

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

$$v_3 = \mathrm{vol}\,(\mathrm{Cytoplasm}) \cdot \mathrm{eta\_T} \cdot [\mathrm{Cdc20\_CMad2}] \tag{8}$$

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.

8.1 Species Mad1_CMad2

Name Mad1:C-Mad2

SBO:0000297 protein complex

Initial concentration $5 \cdot 10^{-8}\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in R6 and as a product in R7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Mad1\_CMad2} = v_2 - v_1 \tag{9}$$

8.2 Species OMad2

Name O-Mad2

Notes Open conformation of Mad2

Initial concentration $1.5 \cdot 10^{-7}\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in R6 and as a product in R8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{OMad2} = v_3 - v_1 \tag{10}$$

8.3 Species Mad1_CMad2_OMad2

Name Mad1:C-Mad2:O-Mad2*

SBO:0000297 protein complex

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

This species takes part in two reactions (as a reactant in R7 and as a product in R6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Mad1\_CMad2\_OMad2} = v_1 - v_2 \tag{11}$$

8.4 Species Cdc20

Name Cdc20

Initial concentration $2.2\cdot 10^{-7}\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in R7 and as a product in R8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cdc20} = v_3 - v_2 \tag{12}$$

8.5 Species Cdc20_CMad2

Name Cdc20:C-Mad2

SBO:0000297 protein complex

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

This species takes part in two reactions (as a reactant in R8 and as a product in R7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cdc20\_CMad2} = v_2 - v_3 \tag{13}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000036 forward bimolecular rate constant, continuous case: Numerical parameter that quantifies the forward velocity of a chemical reaction involving two reactants. This parameter encompasses all the contributions to the velocity except the quantity of the reactants. It is to be used in a reaction modelled using a continuous framework

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme: Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does not include any reverse process that creates the reactants from the products. The change of a product quantity is proportional to the quantity of one reactant. It is to be used in a reaction modelled using a continuous framework.

SBO:0000054 mass action rate law for second order irreversible reactions, two reactants, continuous scheme: Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does not include any reverse process that creates the reactants from the products. The change of a product quantity is proportional to the product of two reactant quantities. It is to be used in a reaction modelled using a continuous framework.

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, continuous scheme: Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does include a reverse process that creates the reactants from the products. The rate of the forward process is proportional to the product of two reactant quantities. The rate of the reverse process is proportional to the quantity of one product. It is to be used in a reaction modelled using a continuous framework.

SBO:0000297 protein complex: Macromolecular complex containing one or more polypeptide chains possibly associated with simple chemicals. CHEBI:3608

SBO:0000338 dissociation rate constant: Rate with which a complex dissociates into its components

SBO:0000339 bimolecular association rate constant: Rate with which two components associate into a complex

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