SBML Model Report

Model name: "Morris2002_CellCycle_CDK2Cyclin"

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1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Nicolas Le Novre[1] and Sharat Vayttaden[2] at September twelveth 2007 at 8:36 p. m. and last time modified at December first 2010 at 10:10 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	4
events	0	constraints	0
reactions	2	function definitions	0
global parameters	2	unit definitions	0
rules	1	initial assignments	0

Model Notes

Notes from the original DOCQS curator:
In this version of the CDK2/Cyclin A complex activation there is discrepancy in the first curve which plots the binding reaction of CDK2 and Cyclin A expressed in E. coli. With the published

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rate constants the simulation does not match the published graph (Fig.1B) in Morris MC. et al. J Biol Chem. 277(26):23847-53 .

Notes from BioModels DB curator:
Although the parameters are those reported in the table I for CDK2/Cyclin A, the total fluorescence follows exactly the curve reported in the paper for CDK2/Cyclin H in figure 1B. Either the plot legend or the table is wrong.

2 Unit Definitions

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

2.1 Unit `substance`

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

Definition mol

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
`geometry`			3	10^{-12}	l	☑	

3.1 Compartment `geometry`

This is a three dimensional compartment with a constant size of 10^{-12} litre.

4 Species

This model contains four 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
CDK2cycA		geometry	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CyclinA		geometry	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Cdk2		geometry	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CDK2cycA_star_		geometry	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains two global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
basal_fluorescence			1.212		⊟
total_fluorescence			0.139		⊟

6 Rule

This is an overview of one rule.

6.1 Rule total_fluorescence

Rule total_fluorescence is an assignment rule for parameter total_fluorescence:

$$\text{total\_fluorescence} = \frac{[\text{CDK2cycA}] \cdot 599990 \cdot 1000000.0}{43200} + \frac{[\text{CDK2cycA\_star\_}] \cdot 599990 \cdot 1000000.0}{43200} + \text{basal\_fluorescence} \quad (1)$$

7 Reactions

This model contains two 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	`Binding`		$\mathrm{Cdk2} + \mathrm{CyclinA} \rightleftharpoons \mathrm{CDK2cycA}$	
2	`Activation`		$\mathrm{CDK2cycA} \rightleftharpoons \mathrm{CDK2cycA\_star\_}$	

7.1 Reaction Binding

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

Notes kf = 19/sec/uM and kb = 25/sec Morris et al 2002 JBC 277(26): 23847–23853 Table pp.23849

Reaction equation

$$\mathrm{Cdk2} + \mathrm{CyclinA} \rightleftharpoons \mathrm{CDK2cycA} \tag{2}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
Cdk2		
CyclinA		

Product

Table 7: Properties of each product.

Id	Name	SBO
CDK2cycA		

Kinetic Law

Notes kf*Cdk2*CyclinA-kb*CDK2cycA

Derived unit contains undeclared units

$$v_1 = \mathrm{kf} \cdot [\mathrm{Cdk2}] \cdot [\mathrm{CyclinA}] \cdot \mathrm{vol}\,(\mathrm{geometry}) - \mathrm{kb} \cdot [\mathrm{CDK2cycA}] \cdot \mathrm{vol}\,(\mathrm{geometry}) \tag{3}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kf			$1.9 \cdot 10^7$		☑
kb			25.000		☑

7.2 Reaction Activation

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

Notes Morris et al 2002 JBC 277(26): 23847–23853 kf and kb values not published kobs2 = 2.5 +- 0.1 /sec kf=0.813/sec and kb=0.557/sec used simulation

Reaction equation

$$\text{CDK2cycA} \rightleftharpoons \text{CDK2cycA\_star\_} \tag{4}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
CDK2cycA		

Product

Table 10: Properties of each product.

Id	Name	SBO
CDK2cycA_star_		

Kinetic Law

Notes kf*CDK2cycA-kb*CDK2cycA_star_

Derived unit contains undeclared units

$$v_2 = \text{kf} \cdot [\text{CDK2cycA}] \cdot \text{vol}(\text{geometry}) - \text{kb} \cdot [\text{CDK2cycA\_star\_}] \cdot \text{vol}(\text{geometry}) \tag{5}$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kf			0.813		☑
kb			0.557		☑

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.

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.

8.1 Species `CDK2cycA`

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

This species takes part in two reactions (as a reactant in `Activation` and as a product in `Binding`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CDK2cycA} = v_1 - v_2 \tag{6}$$

8.2 Species `CyclinA`

Initial concentration $4\cdot 10^{-7}\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

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

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

8.3 Species `Cdk2`

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cdk2} = -v_1 \tag{8}$$

8.4 Species `CDK2cycA_star_`

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CDK2cycA\_star\_} = v_2 \tag{9}$$

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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