SBML Model Report

Model name: “S”

February 4, 2009

1. General Overview

This is a document in SBML Level 2 Version 3 format. Table 1 shows an overview of the quantities of all components of this model.

Table 1: The SBML components in this model.
All components are described in more detail in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	6
events	0	constraints	0
reactions	1	function definitions	1
global parameters	0	unit definitions	3
rules	0	initial assignments	0

Model Notes

This model has been created with the help of the SABIO-RK Database(http://sabio.villa-bosch.de/SABIORK)

2. Unit Definitions

This is an overview of eight unit definitions. The units `substance`, `volume`, `area`, `length`, and `time` are predefined by SBML and not mentioned in the model.

2.1. Unit `onedivsec`

Name onedivsec

Definition s^{-1}

2.2. Unit `microM`

Name microM

Definition $\mu mol \cdot l^{-1}$

2.3. Unit `onedivMsec`

Name onedivMsec

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

2.4. Unit `substance`

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

Definition mol

2.5. Unit `volume`

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

Definition l

2.6. Unit `area`

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

Definition m^2

2.7. Unit `length`

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

Definition m

2.8. 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
compart_1	Cell		3	1	litre	☑	

3.1. Compartment compart_1

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

Name Cell

4. Species

This model contains six species. Section 7 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
SPC_1334	dUMP	compart_1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
SPC_1308	5,10-Methylenetetrahydrofolate	compart_1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
SPC_1336	Dihydrofolate	compart_1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
SPC_65	dTMP	compart_1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
SPC_21324	E-5-(2-Bromovinyl)-2'-deoxyuridine monophosphate	compart_1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ENZ_26405	Thymidylate synthase(Enzyme) wildtype	compart_1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5. Function definition

This is an overview of one function definition.

5.1. Function definition KL_5046

SBO:0000260 enzymatic rate law for simple competitive inhibition of irreversible unireactant enzymes by one inhibitor

Arguments kcat, Km_A, E, B, kcatKm_A, Ki, I, A

Mathematical Expression

$$\frac{\mathtt{E} \cdot \mathtt{kcat} \cdot \mathtt{A}}{\mathtt{Km\_A} \cdot \left(1 + \frac{\mathtt{I}}{\mathtt{Ki}}\right) + \mathtt{A}} \tag{1}$$

6. Reaction

This model contains one reaction. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by one or more modifiers, the identifiers of the modifier species are written above the reaction arrow.

Table 4: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	REAC_0		SPC_1334 + SPC_1308 $\xrightleftharpoons{\text{SPC\_21324, ENZ\_26405}}$ SPC_1336 + SPC_65	

6.1. Reaction REAC_0

This is a reversible reaction of two reactants forming two products influenced by two modifiers.

Reaction equation

$$\mathtt{SPC\_1334} + \mathtt{SPC\_1308} \xrightleftharpoons{\mathtt{SPC\_21324},\ \mathtt{ENZ\_26405}} \mathtt{SPC\_1336} + \mathtt{SPC\_65} \tag{2}$$

Reactants

Table 5: Properties of each reactant.

Id	Name	SBO
SPC_1334	dUMP	
SPC_1308	5,10-Methylenetetrahydrofolate	

Modifiers

Table 6: Properties of each modifier.

Id	Name	SBO
SPC_21324	E-5-(2-Bromovinyl)-2'-deoxyuridine monophosphate	
ENZ_26405	Thymidylate synthase(Enzyme) wildtype	

Products

Table 7: Properties of each product.

Id	Name	SBO
SPC_1336	Dihydrofolate	
SPC_65	dTMP	

Kinetic Law

SBO:0000260 enzymatic rate law for simple competitive inhibition of irreversible unireactant enzymes by one inhibitor

Derived unit contains undeclared units

$$v_1 = \mathtt{KL\_5046}\,(\mathtt{kcat}, \mathtt{Km\_A\_SPC\_1334}, [\mathtt{ENZ\_26405}], [\mathtt{SPC\_1308}], \mathtt{kcatKm\_A\_SPC\_1334}, \mathtt{Ki\_SPC\_21324}, [\mathtt{SPC\_21324}], [\mathtt{SPC\_1334}]) \tag{3}$$

$$\mathtt{KL\_5046}\left(\mathtt{kcat}, \mathtt{Km\_A}, \mathtt{E}, \mathtt{B}, \mathtt{kcatKm\_A}, \mathtt{Ki}, \mathtt{I}, \mathtt{A}\right) = \frac{\mathtt{E} \cdot \mathtt{kcat} \cdot \mathtt{A}}{\mathtt{Km\_A} \cdot \left(1 + \frac{\mathtt{I}}{\mathtt{Ki}}\right) + \mathtt{A}} \tag{4}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcat		0000025	0.213	s^{-1}	☑
Km_A_SPC_1334		0000027	2.700	$\mu mol \cdot l^{-1}$	☑
kcatKm_A-_SPC_1334		0000302	79000.000	$s^{-1} \cdot l \cdot mol^{-1}$	☑
Ki_SPC_21324		0000261	4.170	$\mu mol \cdot l^{-1}$	☑

7. Derived Rate Equations

When interpreted as an ordinary differential equation framework, this model implies the following equation 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 a unit definition are involved or
- volume correction is necessary because the hasOnlySubstanceUnits flag may be set to false and spacialDimensions> 0 for certain species.

7.1. Species SPC_1334

Name dUMP

This species takes part in one reaction (as a reactant in REAC_0).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathtt{SPC\_1334} = -v_1 \tag{5}$$

7.2. Species SPC_1308

Name 5,10-Methylenetetrahydrofolate

This species takes part in one reaction (as a reactant in REAC_0).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathtt{SPC\_1308} = -v_1 \tag{6}$$

7.3. Species SPC_1336

Name Dihydrofolate

This species takes part in one reaction (as a product in REAC_0).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathtt{SPC\_1336} = v_1 \tag{7}$$

7.4. Species SPC_65

Name dTMP

This species takes part in one reaction (as a product in REAC_0).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathtt{SPC\_65} = v_1 \tag{8}$$

7.5. Species SPC_21324

Name E-5-(2-Bromovinyl)-2'-deoxyuridine monophosphate

This species takes part in one reaction (as a modifier in REAC_0).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathtt{SPC\_21324} = 0 \tag{9}$$

7.6. Species ENZ_26405

Name Thymidylate synthase(Enzyme) wildtype

This species takes part in one reaction (as a modifier in REAC_0).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathtt{ENZ\_26405} = 0 \tag{10}$$

A. Glossary of Systems Biology Ontology Terms

SBO:0000025 catalytic rate constant: Numerical parameter that quantifies the velocity of an enzymatic reaction

SBO:0000027 Michaelis constant: Substrate concentration at which the velocity of reaction is half its maximum. Michaelis constant is an experimental parameter. According to the underlying molecular mechanism it can be interpreted differently in terms of microscopic constants

SBO:0000260 enzymatic rate law for simple competitive inhibition of irreversible unireactant enzymes by one inhibitor: Inhibition of a unireactant enzyme by one inhibitor that binds once to the free enzyme and prevents the binding of the substrate. The enzymes do not catalyse the reactions in both directions.

SBO:0000261 inhibitory constant: Dissociation constant of a compound from a target of which it inhibits the function.

SBO:0000302 catalytic efficiency: Constant representing the actual efficiency of an enzyme, taking into account its microscopic catalytic activity and the rates of substrate binding and dissociation.

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