SBML Model Report

Model name: "Bhartiya2003_Tryptophan_operon"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Jacky L Snoep[1] and Harish Dharuri[2] at February fourth 2010 at 5:43 p. m. and last time modified at February twelveth 2014 at 3:48 p. 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	4
events	0	constraints	0
reactions	5	function definitions	0
global parameters	8	unit definitions	5
rules	6	initial assignments	0

Model Notes

SBML level 2 code originaly generated for the JWS Online project by Jacky Snoep using PySCeS
Run this model online at http://jjj.biochem.sun.ac.za

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BioModels Curation : The model reproduces Fig 3 of the publication. By substituting a value of 1.4 for Tex it is possible to reproduce Fig 3C and 3D(iii), Fig 3A and 3D(i), are obtained by setting Tex=0. Also, note that the tryptophan concentrations have been normalized by 82 micromolar in the figures; the normalized concetrations can be obtained via the parameters To/s/t_norm. The model was successfully tested on MathSBML and Copasi.

2 Unit Definitions

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

2.1 Unit `substance`

Name micromole

Definition μmol

2.2 Unit `time`

Name minutes

Definition 60 s

2.3 Unit `concentration`

Name microM

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

2.4 Unit `Concentration_per_time`

Name microM_per_min

Definition $\mu\text{mol} \cdot 1^{-1} \cdot (60\ \text{s})^{-1}$

2.5 Unit time_inverse

Name per_min

Definition $(60\ \mathrm{s})^{-1}$

2.6 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

2.7 Unit area

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

Definition m^2

2.8 Unit length

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

Definition m

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
compartment	cell		3	1	litre	☑	

3.1 Compartment compartment

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

Name cell

4 Species

This model contains four species. The boundary condition of one of these species is set to `true` so that this species' amount cannot be changed by any reaction. 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
`Enz`	Anthranilate synthase	`compartment`	$\mu mol \cdot l^{-1}$	☐	☐
`Ts`	Synthesized tryptophan	`compartment`	$\mu mol \cdot l^{-1}$	☐	☐
`Tt`	Total tryptophan	`compartment`	$\mu mol \cdot l^{-1}$	☐	☐
`To`	exog. Trp	`compartment`	$\mu mol \cdot l^{-1}$	☐	☑

5 Parameters

This model contains eight global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Tomax			100.00	$\mu mol \cdot l^{-1}$	☑
Tex			0.14	$\mu mol \cdot l^{-1}$	☑
e_val			0.90	$\mu mol \cdot l^{-1}$	☑
f_val			380.00	$\mu mol \cdot l^{-1}$	☑
Ts_norm	Ts_norm		0.00	dimensionless	⊟
To_norm	To_norm		0.00	dimensionless	⊟
Tt_norm	Tt_norm		0.00	dimensionless	⊟
Enz_norm	Enz_norm		0.00	dimensionless	⊟

6 Rules

This is an overview of six rules.

6.1 Rule To

Rule To is an assignment rule for species To:

$$\mathrm{To} = \frac{\mathrm{Tomax} \cdot \mathrm{Tex}}{\mathrm{Tex} \cdot \left(1 + \frac{[\mathrm{Ts}]}{\mathrm{f\_val}}\right) + \mathrm{e\_val}} \tag{1}$$

6.2 Rule Tt

Rule Tt is an assignment rule for species Tt:

$$\mathrm{Tt} = [\mathrm{To}] + [\mathrm{Ts}] \tag{2}$$

Derived unit $\mu mol \cdot l^{-1}$

6.3 Rule Enz_norm

Rule Enz_norm is an assignment rule for parameter Enz_norm:

$$\mathrm{Enz\_norm} = \frac{[\mathrm{Enz}]}{1} \tag{3}$$

6.4 Rule `Ts_norm`

Rule `Ts_norm` is an assignment rule for parameter `Ts_norm`:

$$\mathrm{Ts\_norm} = \frac{[\mathrm{Ts}]}{82} \tag{4}$$

6.5 Rule `Tt_norm`

Rule `Tt_norm` is an assignment rule for parameter `Tt_norm`:

$$\mathrm{Tt\_norm} = \frac{[\mathrm{Tt}]}{82} \tag{5}$$

6.6 Rule `To_norm`

Rule `To_norm` is an assignment rule for parameter `To_norm`:

$$\mathrm{To\_norm} = \frac{[\mathrm{To}]}{82} \tag{6}$$

7 Reactions

This model contains five 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	`Enzyme_synthesis`	Anthranilate synthase synthesis	$\emptyset \overset{\text{Tt}}{\rightleftharpoons} \text{Enz}$	
2	`Enzyme_dilution`	Enzyme dilution due to cell growth	$\text{Enz} \rightleftharpoons \emptyset$	
3	`tryptophan_synthesis`	Tryptophan synthesis	$\emptyset \overset{\text{Enz, Tt}}{\rightleftharpoons} \text{Ts}$	
4	`tryptophan_consumption`	Tryptophan consumption for protein synthesis	$\text{Ts} \rightleftharpoons \emptyset$	
5	`tryptophan_dilution`	Tryptophan dilution due to cell growth	$\text{Ts} \rightleftharpoons \emptyset$	

7.1 Reaction Enzyme_synthesis

This is a reversible reaction of no reactant forming one product influenced by one modifier.

Name Anthranilate synthase synthesis

Reaction equation

$$\emptyset \overset{\text{Tt}}{\rightleftharpoons} \text{Enz} \tag{7}$$

Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
Tt	Total tryptophan	

Product

Table 7: Properties of each product.

Id	Name	SBO
Enz	Anthranilate synthase	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{\text{vol}\,(\text{compartment}) \cdot \text{k1} \cdot \text{ki1}^{\text{nH}} \cdot \text{Ot}}{\text{ki1}^{\text{nH}} + [\text{Tt}]^{\text{nH}}} \tag{8}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			65.000	$(60\ \text{s})^{-1}$	☑
ki1			3.530	$\mu\text{mol} \cdot \text{l}^{-1}$	☑
nH			1.920	dimensionless	☑
Ot			0.003	$\mu\text{mol} \cdot \text{l}^{-1}$	☑

7.2 Reaction Enzyme_dilution

This is a reversible reaction of one reactant forming no product.

Name Enzyme dilution due to cell growth

Reaction equation

$$\mathrm{Enz} \rightleftharpoons \emptyset \tag{9}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
Enz	Anthranilate synthase	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_2 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{mu} \cdot [\mathrm{Enz}] \tag{10}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			0.01	$(60\ \mathrm{s})^{-1}$	☑

7.3 Reaction tryptophan_synthesis

This is a reversible reaction of no reactant forming one product influenced by two modifiers.

Name Tryptophan synthesis

Reaction equation

$$\emptyset \xrightleftharpoons{\mathrm{Enz,\ Tt}} \mathrm{Ts} \tag{11}$$

Modifiers

Table 11: Properties of each modifier.

Id	Name	SBO
Enz	Anthranilate synthase	
Tt	Total tryptophan	

Product

Table 12: Properties of each product.

Id	Name	SBO
Ts	Synthesized tryptophan	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot 10^{-6}\ \mathrm{mol}$

$$v_3 = \frac{\mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k2} \cdot [\mathrm{Enz}] \cdot \mathrm{Ki2}}{\mathrm{Ki2} + [\mathrm{Tt}]} \tag{12}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k2			25.0	$(60\ \mathrm{s})^{-1}$	☑
Ki2			810.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑

7.4 Reaction tryptophan_consumption

This is a reversible reaction of one reactant forming no product.

Name Tryptophan consumption for protein synthesis

Reaction equation

$$\mathrm{Ts} \rightleftharpoons \emptyset \tag{13}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
Ts	Synthesized tryptophan	

Kinetic Law

Derived unit $10^{-6}\,\mathrm{mol}\cdot(60\,\mathrm{s})^{-1}$

$$v_4 = \frac{\mathrm{vol}\,(\mathrm{compartment})\cdot \mathrm{g}\cdot[\mathrm{Ts}]}{\mathrm{Kg}+[\mathrm{Ts}]} \tag{14}$$

Table 15: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
g			25.0	$\mu\mathrm{mol}\cdot\mathrm{l}^{-1}\cdot(60\,\mathrm{s})^{-1}$	☑
Kg			0.2	$\mu\mathrm{mol}\cdot\mathrm{l}^{-1}$	☑

7.5 Reaction tryptophan_dilution

This is a reversible reaction of one reactant forming no product.

Name Tryptophan dilution due to cell growth

Reaction equation

$$\mathrm{Ts} \rightleftharpoons \emptyset \tag{15}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
Ts	Synthesized tryptophan	

Kinetic Law

Derived unit $(60\,\mathrm{s})^{-1}\cdot\mu\mathrm{mol}$

$$v_5 = \mathrm{vol}\,(\mathrm{compartment})\cdot \mathrm{mu}\cdot[\mathrm{Ts}] \tag{16}$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mu			0.01	$(60\ \mathrm{s})^{-1}$	☑

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 Enz

Name Anthranilate synthase

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

This species takes part in three reactions (as a reactant in Enzyme_dilution and as a product in Enzyme_synthesis and as a modifier in tryptophan_synthesis).

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

8.2 Species Ts

Name Synthesized tryptophan

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

This species takes part in three reactions (as a reactant in tryptophan_consumption, tryptophan_dilution and as a product in tryptophan_synthesis).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ts} = v_3 - v_4 - v_5 \tag{18}$$

8.3 Species Tt

Name Total tryptophan

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

Involved in rule Tt

This species takes part in two reactions (as a modifier in Enzyme_synthesis, tryptophan_synthesis) and is also involved in one rule which determines this species' quantity.

8.4 Species To

Name exog. Trp

Involved in rule To

One rule determines the species' quantity.

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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