SBML Model Report

Model name: “Mufudza2012 - Estrogen effect on the dynamics of breast cancer”

April 19, 2013

1 General Overview

This is a document in SBML Level 2 Version 4 format. 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	0	function definitions	0
global parameters	18	unit definitions	0
rules	4	initial assignments	0

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
Tissue	Tissue		3	1	litre	☑	

3.1 Compartment Tissue

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

Name Tissue

4 Species

This model contains four 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
H	normal cells	Tissue	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
T	Tumour cells	Tissue	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
I	Immune cells	Tissue	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
E	17-beta estradiol	Tissue	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 18 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
alpha1	alpha1		0.700		☑
alpha2	alpha2		0.980		☑
beta1	beta1		0.300		☑
beta2	beta2		0.400		☑
delta1	delta1		1.000		☑
gamma2	gamma2		0.900		☑
s	s		0.400		☑
rho	rho		0.200		☑
omega	omega		0.300		☑
mu	mu		0.290		☑
alpha3	alpha3		1.000		☑
gamma3	gamma3		0.085		☑
sigma1	sigma1		1.200		☑
sigma2	sigma2		0.940		☑
sigma3	sigma3		0.300		☑
v	v		0.400		☑
theta	theta		0.800		☑
pi	pi		0.300		☑

6 Rules

This is an overview of four rules.

6.1 Rule H

Rule H is a rate rule for species H:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{H} = [\mathrm{H}] \cdot (\mathrm{alpha1} - \mathrm{beta1} \cdot [\mathrm{H}] - \mathrm{delta1} \cdot [\mathrm{T}]) - \mathrm{sigma1} \cdot [\mathrm{H}] \cdot [\mathrm{E}] \tag{1}$$

6.2 Rule T

Rule T is a rate rule for species T:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{T} = [\mathrm{T}] \cdot (\mathrm{alpha3} - \mathrm{beta2} \cdot [\mathrm{T}]) - \mathrm{gamma2} \cdot [\mathrm{I}] \cdot [\mathrm{T}] + \mathrm{sigma2} \cdot [\mathrm{H}] \cdot [\mathrm{E}] \tag{2}$$

6.3 Rule I

Rule I is a rate rule for species I:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{I} = \mathrm{s} + \frac{\mathrm{rho} \cdot [\mathrm{I}] \cdot [\mathrm{T}]}{\mathrm{omega} + [\mathrm{T}]} - \mathrm{gamma3} \cdot [\mathrm{I}] \cdot [\mathrm{T}] - \mathrm{mu} \cdot [\mathrm{I}] - \frac{\mathrm{sigma3} \cdot [\mathrm{I}] \cdot [\mathrm{E}]}{\mathrm{v} + [\mathrm{E}]} \tag{3}$$

6.4 Rule E

Rule E is a rate rule for species E:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E} = \pi - \mathrm{theta} \cdot [\mathrm{E}] \tag{4}$$

7 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.

7.1 Species H

Name normal cells

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

Involved in rule H

One rule which determines this species' quantity.

7.2 Species T

Name Tumour cells

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

Involved in rule T

One rule which determines this species' quantity.

7.3 Species I

Name Immune cells

Initial concentration $1.379310345\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

Involved in rule I

One rule which determines this species' quantity.

7.4 Species E

Name 17-beta estradiol

Initial concentration $2\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

Involved in rule E

One rule which determines this species' quantity.

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