# **SBML Model Report**

# Model name: "Zatorsky2006\_p53\_Model2"



May 5, 2016

### 1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Harish Dharuri<sup>1</sup> and Vijayalakshmi Chelliah<sup>2</sup> at January tenth 2008 at 5:38 p.m. and last time modified at March 20<sup>th</sup> 2014 at 4:30 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	3
events	2	constraints	0
reactions	6	function definitions	0
global parameters	14	unit definitions	2
rules	1	initial assignments	0

#### **Model Notes**

The model reproduces time profile of p53 and Mdm2 as depicted in Fig 6B of the paper for Model 2. Results obtained using MathSBML.

To the extent possible under law, all copyright and related or neighbouring rights to this encoded model have been dedicated to the public domain worldwide. Please refer to CCO Public Domain Dedication for more information.

<sup>&</sup>lt;sup>1</sup>California Institute of Technology, hdharuri@cds.caltech.edu

<sup>&</sup>lt;sup>2</sup>EMBL-EBI, viji@ebi.ac.uk

In summary, you are entitled to use this encoded model in absolutely any manner you deem suitable, verbatim, or with modification, alone or embedded it in a larger context, redistribute it, commercially or not, in a restricted way or not.

To cite BioModels Database, please use: Li C, Donizelli M, Rodriguez N, Dharuri H, Endler L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novre N, Laibe C (2010) BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models. BMC Syst Biol., 4:92.

#### 2 Unit Definitions

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

#### 2.1 Unit substance

Name dimensionless

**Definition** item

#### 2.2 Unit time

Name hours

**Definition** 3600 s

#### 2.3 Unit volume

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

**Definition** 1

#### 2.4 Unit area

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

**Definition** m<sup>2</sup>

#### 2.5 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	Ø	

# 3.1 Compartment compartment

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

Name cell

# 4 Species

This model contains three species. Section 9 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 Condi- tion
x	p53	compartment	item $\cdot 1^{-1}$	$\Box$	$\Box$
У	Mdm2	compartment	item $\cdot 1^{-1}$		$\Box$
yO	precursor Mdm2	compartment	item $\cdot 1^{-1}$		

#### **5 Parameters**

This model contains 14 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO Valu		Constant
beta_x		2.5	5	<u> </u>
psi		1.0	0	
${\tt alpha\_x}$		0.0	0	
${\tt alpha\_xy}$		3.1	5	
$beta_y$		0.8	5	
${\tt alpha\_y}$		0.6	0	
${\tt alpha\_0}$		55.0	0	
fx		0.0	0	
flag1		0.0	0	$\Box$
flag2		0.0	0	$\Box$
flag3		1.0	0	$\Box$
М		34.0	0	
xmax		0.9	2	
xmin		0.1	2	

## 6 Rule

This is an overview of one rule.

#### 6.1 Rule fx

Rule fx is an assignment rule for parameter fx:

$$fx = beta\_x \cdot flag1 + \frac{beta\_x}{M} \cdot flag2 + \frac{flag3 \cdot beta\_x}{M} \cdot \left(1 + (M-1) \cdot \frac{[x] - xmin}{xmax - xmin}\right) \quad (1)$$

## 7 Events

This is an overview of two events. 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.

#### **7.1 Event** event\_0000001

**Trigger condition** 

$$[x] \ge x max$$
 (2)

# **Assignments**

$$flag 1 = 1 (3)$$

$$flag 2 = 0 (4)$$

$$flag3 = 0 (5)$$

# **7.2 Event** event\_0000002

# **Trigger condition**

$$[x] < xmax (6)$$

# **Assignments**

$$flag1 = 0 (7)$$

$$flag 2 = 0 (8)$$

$$flag3 = 1$$
 (9)

# 8 Reactions

This model contains six 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

Nº	Id	Name	Reaction Equation	SBO
1	R1	p53 production	$\emptyset \longrightarrow x$	
2	R2	Mdm2 independent p53 degradation	$x \longrightarrow \emptyset$	
3	R3	Mdm2 dependent p53 degradation	$x \xrightarrow{y} \emptyset$	
4	R4	p53 dependent Mdm2 precursor production	$\emptyset \xrightarrow{X} y0$	
5	R5	Mdm2 synthesis from precursor	$y0 \longrightarrow y$	
6	R6	Mdm2 degradation	y <del>====`</del> ∅	

#### 8.1 Reaction R1

This is an irreversible reaction of no reactant forming one product.

Name p53 production

# **Reaction equation**

$$\emptyset \longrightarrow x$$
 (10)

#### **Product**

Table 6: Properties of each product.

Id	Name	SBO
х	p53	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_1 = \text{vol}\left(\text{compartment}\right) \cdot \text{fx} \cdot \text{psi}$$
 (11)

#### 8.2 Reaction R2

This is an irreversible reaction of one reactant forming no product.

Name Mdm2 independent p53 degradation

#### **Reaction equation**

$$x \longrightarrow \emptyset$$
 (12)

#### Reactant

Table 7: Properties of each reactant.

Id	Name	SBO
х	p53	

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_2 = \text{vol}\left(\text{compartment}\right) \cdot \text{alpha\_x} \cdot [x]$$
 (13)

#### 8.3 Reaction R3

This is an irreversible reaction of one reactant forming no product influenced by one modifier.

Name Mdm2 dependent p53 degradation

## **Reaction equation**

$$x \xrightarrow{y} \emptyset \tag{14}$$

#### Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
х	p53	

#### **Modifier**

Table 9: Properties of each modifier.

Id	Name	SBO
У	Mdm2	

### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_3 = \text{vol} (\text{compartment}) \cdot \text{alpha}_x y \cdot [y] \cdot [x]$$
 (15)

#### 8.4 Reaction R4

This is an irreversible reaction of no reactant forming one product influenced by one modifier.

Name p53 dependent Mdm2 precursor production

#### **Reaction equation**

$$\emptyset \xrightarrow{X} y0 \tag{16}$$

### **Modifier**

Table 10: Properties of each modifier.

Id	Name	SBO
х	p53	

## **Product**

Table 11: Properties of each product.

Id	Name	SBO
уO	precursor Mdm2	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_4 = \text{vol} (\text{compartment}) \cdot \text{beta\_y} \cdot [x] \cdot \text{psi}$$
 (17)

#### 8.5 Reaction R5

This is an irreversible reaction of one reactant forming one product.

Name Mdm2 synthesis from precursor

# **Reaction equation**

$$y0 \longrightarrow y$$
 (18)

#### Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
yО	precursor Mdm2	

#### **Product**

Table 13: Properties of each product.

Id	Name	SBO
у	Mdm2	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_5 = \text{vol} (\text{compartment}) \cdot \text{alpha}_0 \cdot [y_0]$$
 (19)

#### 8.6 Reaction R6

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

Name Mdm2 degradation

#### **Reaction equation**

$$y \rightleftharpoons \emptyset$$
 (20)

#### Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
У	Mdm2	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_6 = \text{vol}\left(\text{compartment}\right) \cdot \text{alpha\_y} \cdot [y]$$
 (21)

# 9 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.

#### 9.1 Species x

Name p53

Initial concentration  $0.28 \text{ item} \cdot l^{-1}$ 

This species takes part in four reactions (as a reactant in R2, R3 and as a product in R1 and as a modifier in R4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x} = |v_1| - |v_2| - |v_3| \tag{22}$$

#### 9.2 Species y

Name Mdm2

Initial concentration  $0.73 \text{ item} \cdot l^{-1}$ 

This species takes part in three reactions (as a reactant in R6 and as a product in R5 and as a modifier in R3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{y} = |v_5| - |v_6| \tag{23}$$

### 9.3 Species y0

Name precursor Mdm2

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

This species takes part in two reactions (as a reactant in R5 and as a product in R4).

$$\frac{\mathrm{d}}{\mathrm{d}t}y0 = v_4 - v_5 \tag{24}$$

SML2ATEX was developed by Andreas Dräger<sup>a</sup>, Hannes Planatscher<sup>a</sup>, Dieudonné M Wouamba<sup>a</sup>, Adrian Schröder<sup>a</sup>, Michael Hucka<sup>b</sup>, Lukas Endler<sup>c</sup>, Martin Golebiewski<sup>d</sup> and Andreas Zell<sup>a</sup>. Please see http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX for more information.

<sup>&</sup>lt;sup>a</sup>Center for Bioinformatics Tübingen (ZBIT), Germany

<sup>&</sup>lt;sup>b</sup>California Institute of Technology, Beckman Institute BNMC, Pasadena, United States

<sup>&</sup>lt;sup>c</sup>European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom

<sup>&</sup>lt;sup>d</sup>EML Research gGmbH, Heidelberg, Germany