SBML Model Report

Model name: "Talemi2015 - Persistent telomere-associated DNA damage foci (TAF), a measure to predict cancer risks"

February 11, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Soheil Rastgou Talemi[1] and Joerg Schaber[2] at December 20th 2014 at 2:53 p. m. and last time modified at December 20th 2014 at 2:53 p. m. 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	6
events	1	constraints	0
reactions	6	function definitions	1
global parameters	15	unit definitions	3
rules	5	initial assignments	4

Model Notes

A Robust Model of DNA Damage Dynamics.
Rasgou Talemi and Schaber, 12.20.2014.

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[1]OVGU University of Magdeburg, soheil.rastgou@med.ovgu.de
[2]OVGU University of Magdeburg, joerg.schaber@med.ovgu.de

2 Unit Definitions

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

2.1 Unit `volume`

Name volume

Definition dimensionless

2.2 Unit `time`

Name time

Definition 3600 s

2.3 Unit `substance`

Name substance

Definition item

2.4 Unit `area`

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

Definition m^2

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	compartment		3	1	dimensionless	✓	

3.1 Compartment `compartment`

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

Name compartment

4 Species

This model contains six 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 11 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
TAF	TAF	compartment	item $\cdot$ dimensionless^{-1}	⊟	☑
FAST	FAST	compartment	item $\cdot$ dimensionless^{-1}	⊟	⊟
FASTi	FASTi	compartment	item $\cdot$ dimensionless^{-1}	⊟	⊟
SLOWi	SLOWi	compartment	item $\cdot$ dimensionless^{-1}	⊟	⊟
SLOW	SLOW	compartment	item $\cdot$ dimensionless^{-1}	⊟	⊟
RP	RP	compartment	item $\cdot$ dimensionless^{-1}	⊟	⊟

5 Parameters

This model contains 15 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Tot	Tot		1.879		⊟
DNAdamagefoci_0	DNAdamagefoci_0		750.500		⊟
Gy	Gy		20.000		☑
FociperGy	FociperGy		167.817		☑
prop_C	prop_C		0.023		☑
TAF0	TAF0		0.890		☑
k_TAF	k_TAF		0.791		☑
BaseDNAdamage	BaseDNAdamage		0.989		☑
percentTAF	percentTAF		47.358		⊟
kcross	kcross		$1.51844699335433 \cdot 10^{-4}$		☑
TotalRP	TotalRP		20.000		⊟
Toti	Toti		0.000		⊟
Metabolite_1	Initial for TAF		0.890		☑
ModelValue_3	Initial for FociperGy		167.817		☑
ModelValue_2	Initial for Gy		20.000		☑

6 Initialassignments

This is an overview of four initialassignments.

6.1 Initialassignment `TAF`

Derived unit contains undeclared units

Math TAF0

6.2 Initialassignment `Metabolite_1`

Derived unit item

Math [TAF]

6.3 Initialassignment `ModelValue_3`

Derived unit contains undeclared units

Math FociperGy

6.4 Initialassignment `ModelValue_2`

Derived unit contains undeclared units

Math Gy

7 Function definition

This is an overview of one function definition.

7.1 Function definition `comb_2dn_order_MA`

Name comb 2dn order MA

Arguments S1, S2, k, Tot

Mathematical Expression

$$\text{S1} \cdot \text{k} \cdot \text{S2} \cdot \text{Tot} \tag{1}$$

8 Rules

This is an overview of five rules.

8.1 Rule `Tot`

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

$$\text{Tot} = \text{BaseDNAdamage} + [\text{FAST}] + [\text{FASTi}] + [\text{SLOW}] + [\text{SLOWi}] + [\text{TAF}] \tag{2}$$

8.2 Rule `DNAdamagefoci_0`

Rule `DNAdamagefoci_0` is an assignment rule for parameter `DNAdamagefoci_0`:

$$\text{DNAdamagefoci\_0} = \sqrt{2} \cdot \text{ModelValue\_3} \tag{3}$$

8.3 Rule `percentTAF`

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

$$\text{percentTAF} = \frac{100 \cdot [\text{TAF}]}{\text{Tot}} \tag{4}$$

8.4 Rule `TotalRP`

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

$$\text{TotalRP} = [\text{FAST}] + [\text{RP}] + [\text{SLOW}] \tag{5}$$

Derived unit item

8.5 Rule `Toti`

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

$$\text{Toti} = [\text{FASTi}] + [\text{SLOWi}] \tag{6}$$

Derived unit item

9 Event

This is an overview of one event. 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.

9.1 Event `DNAdamage`

Name DNAdamage

Trigger condition

$$\text{time} > 0 \tag{7}$$

Assignments

$$\text{TAF} = \text{Metabolite\_1} + \text{k\_TAF} \cdot \sqrt{2} \tag{8}$$
$$\text{SLOWi} = \text{prop\_C} \cdot \text{DNAdamagefoci\_0} \tag{9}$$
$$\text{FASTi} = (1 - \text{prop\_C}) \cdot \text{DNAdamagefoci\_0} \tag{10}$$

10 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

№	Id	Name	Reaction Equation	SBO
1	rf	rf	$FAST \xrightarrow{FAST} RP$	
2	rs	rs	$SLOW \xrightarrow{SLOW} RP$	
3	v1	v1	$FASTi + RP \xrightarrow{FASTi,\ RP} FAST$	
4	v3	v3	$SLOWi + RP \xrightarrow{SLOWi,\ RP} SLOW$	
5	vcross1	vcross1	$FASTi + RP \xrightarrow{FASTi,\ RP} FAST$	
6	vcross2	vcross2	$SLOWi + RP \xrightarrow{SLOWi,\ RP} SLOW$	

10.1 Reaction `rf`

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

Name rf

Reaction equation

$$\text{FAST} \xrightarrow{\text{FAST}} \text{RP} \tag{11}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
FAST	FAST	

Modifier

Table 7: Properties of each modifier.

Id	Name	SBO
FAST	FAST	

Product

Table 8: Properties of each product.

Id	Name	SBO
RP	RP	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}\,(\text{compartment}) \cdot \text{k1} \cdot [\text{FAST}] \tag{12}$$

Table 9: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		2000.0		☑

10.2 Reaction `rs`

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

Name rs

Reaction equation

$$SLOW \xrightarrow{\text{SLOW}} RP \tag{13}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
SLOW	SLOW	

Modifier

Table 11: Properties of each modifier.

Id	Name	SBO
SLOW	SLOW	

Product

Table 12: Properties of each product.

Id	Name	SBO
RP	RP	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol}\,(\text{compartment}) \cdot \text{k1} \cdot [\text{SLOW}] \tag{14}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.005		✓

Produced by SBML2LATEX

10.3 Reaction v1

This is an irreversible reaction of two reactants forming one product influenced by two modifiers.

Name v1

Reaction equation

$$\text{FASTi} + \text{RP} \xrightarrow{\text{FASTi, RP}} \text{FAST} \tag{15}$$

Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
FASTi	FASTi	
RP	RP	

Modifiers

Table 15: Properties of each modifier.

Id	Name	SBO
FASTi	FASTi	
RP	RP	

Product

Table 16: Properties of each product.

Id	Name	SBO
FAST	FAST	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}\,(\text{compartment}) \cdot \text{k1} \cdot [\text{FASTi}] \cdot [\text{RP}] \tag{16}$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.005		☑

10.4 Reaction v3

This is an irreversible reaction of two reactants forming one product influenced by two modifiers.

Name v3

Reaction equation

$$SLOWi + RP \xrightarrow{SLOWi, RP} SLOW \tag{17}$$

Reactants

Table 18: Properties of each reactant.

Id	Name	SBO
SLOWi	SLOWi	
RP	RP	

Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
SLOWi	SLOWi	
RP	RP	

Product

Table 20: Properties of each product.

Id	Name	SBO
SLOW	SLOW	

Kinetic Law

Derived unit contains undeclared units

Produced by SBML2LATEX

$$v_4 = \text{vol}\,(\text{compartment}) \cdot \text{k1} \cdot [\text{SLOWi}] \cdot [\text{RP}] \tag{18}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$4.67362 \cdot 10^{-4}$		☑

10.5 Reaction `vcross1`

This is an irreversible reaction of two reactants forming one product influenced by two modifiers.

Name vcross1

Reaction equation

$$\text{FASTi} + \text{RP} \xrightarrow{\text{FASTi, RP}} \text{FAST} \tag{19}$$

Reactants

Table 22: Properties of each reactant.

Id	Name	SBO
FASTi	FASTi	
RP	RP	

Modifiers

Table 23: Properties of each modifier.

Id	Name	SBO
FASTi	FASTi	
RP	RP	

Product

Table 24: Properties of each product.

Id	Name	SBO
FAST	FAST	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{vol}\,(\text{compartment}) \cdot \text{comb\_2dn\_order\_MA}\,([\text{FASTi}], [\text{RP}], \text{kcross}, \text{Toti}) \tag{20}$$

$$\text{comb\_2dn\_order\_MA}\,(\text{S1}, \text{S2}, \text{k}, \text{Tot}) = \text{S1} \cdot \text{k} \cdot \text{S2} \cdot \text{Tot} \tag{21}$$

$$\text{comb\_2dn\_order\_MA}\,(\text{S1}, \text{S2}, \text{k}, \text{Tot}) = \text{S1} \cdot \text{k} \cdot \text{S2} \cdot \text{Tot} \tag{22}$$

10.6 Reaction `vcross2`

This is an irreversible reaction of two reactants forming one product influenced by two modifiers.

Name vcross2

Reaction equation

$$\text{SLOWi} + \text{RP} \xrightarrow{\text{SLOWi, RP}} \text{SLOW} \tag{23}$$

Reactants

Table 25: Properties of each reactant.

Id	Name	SBO
SLOWi	SLOWi	
RP	RP	

Modifiers

Table 26: Properties of each modifier.

Id	Name	SBO
SLOWi	SLOWi	
RP	RP	

Product

Table 27: Properties of each product.

Id	Name	SBO
SLOW	SLOW	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{vol}\,(\text{compartment}) \cdot \text{comb\_2dn\_order\_MA}\,([\text{SLOWi}], [\text{RP}], \text{kcross}, \text{Toti}) \qquad (24)$$

$$\text{comb\_2dn\_order\_MA}\,(\text{S1}, \text{S2}, \text{k}, \text{Tot}) = \text{S1} \cdot \text{k} \cdot \text{S2} \cdot \text{Tot} \qquad (25)$$

$$\text{comb\_2dn\_order\_MA}\,(\text{S1}, \text{S2}, \text{k}, \text{Tot}) = \text{S1} \cdot \text{k} \cdot \text{S2} \cdot \text{Tot} \qquad (26)$$

11 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.

11.1 Species TAF

Name TAF

Initial concentration 0.889883170980968 item $\cdot$ dimensionless^{-1}

Initial assignment TAF

Involved in event DNAdamage

one event influences the species' quantity.

11.2 Species `FAST`

Name FAST

Initial concentration $0 \, \text{item} \cdot \text{dimensionless}^{-1}$

This species takes part in four reactions (as a reactant in `rf` and as a product in `v1`, `vcross1` and as a modifier in `rf`).

$$\frac{\text{d}}{\text{d}t}\text{FAST} = v_3 + v_5 - v_1 \tag{27}$$

11.3 Species `FASTi`

Name FASTi

Initial concentration $0 \, \text{item} \cdot \text{dimensionless}^{-1}$

Involved in event `DNAdamage`

This species takes part in four reactions (as a reactant in `v1`, `vcross1` and as a modifier in `v1`, `vcross1`).

$$\frac{\text{d}}{\text{d}t}\text{FASTi} = -v_3 - v_5 \tag{28}$$

Furthermore, one event influences this species' rate of change.

11.4 Species `SLOWi`

Name SLOWi

Initial concentration $0 \, \text{item} \cdot \text{dimensionless}^{-1}$

Involved in event `DNAdamage`

This species takes part in four reactions (as a reactant in `v3`, `vcross2` and as a modifier in `v3`, `vcross2`).

$$\frac{\text{d}}{\text{d}t}\text{SLOWi} = -v_4 - v_6 \tag{29}$$

Furthermore, one event influences this species' rate of change.

11.5 Species `SLOW`

Name SLOW

Initial concentration $0 \, \text{item} \cdot \text{dimensionless}^{-1}$

This species takes part in four reactions (as a reactant in `rs` and as a product in `v3`, `vcross2` and as a modifier in `rs`).

$$\frac{\text{d}}{\text{d}t}\text{SLOW} = v_4 + v_6 - v_2 \tag{30}$$

11.6 Species RP

Name RP

Initial concentration $20\,\text{item}\cdot\text{dimensionless}^{-1}$

This species takes part in ten reactions (as a reactant in `v1`, `v3`, `vcross1`, `vcross2` and as a product in `rf`, `rs` and as a modifier in `v1`, `v3`, `vcross1`, `vcross2`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{RP} = v_1 + v_2 - v_3 - v_4 - v_5 - v_6 \tag{31}$$