SBML Model Report

Model name: "Amara2013 - PCNA ubiquitylation in the activation of PRR pathway"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following four authors: Nick Juty[1], Vijayalakshmi Chelliah[2], Flavio Amara[3] and Marco Muzi Falconi[4] at September sixth 2013 at 4:57 p. m. and last time modified at March fifth 2014 at 4:56 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	23
events	0	constraints	0
reactions	25	function definitions	0
global parameters	1	unit definitions	3
rules	1	initial assignments	0

[1]EMBL-EBI, juty@ebi.ac.uk
[2]EMBL-EBI, viji@ebi.ac.uk
[3]Dipartimento di Bioscienze, Universit degli Studi di Milano, Milano, Italy, flavio.amara@unimi.it
[4]Dipartimento di Bioscienze, Universit degli Studi di Milano, Milano, Italy, marco.muzifalconi@unimi.it

Model Notes

Mechanistic model of the Post-Replication Repair (PRR), the pathway involved in the bypass of DNA lesions induced by sunlight exposure and UV radiation. PRR acts through two different mechanisms, activated by mono- and poly-ubiquitylation of the DNA sliding clamp, called Proliferating Cell Nuclear Antigen (PCNA). This model has been defined according to the stochastic formulation of chemical kinetics [Gillespie DT, J Phys Chem 1977, 81(25):2340-2361], which requires to specify the set of molecular species occurring in the pathway and their respective interactions, formally described as a set of biochemical reactions. The volume considered for this system is 1.666667e-17L; this value can be used to convert the model into the deterministic formulation.

2 Unit Definitions

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

2.1 Unit `volume`

Name volume

Definition dimensionless

2.2 Unit `substance`

Name substance

Definition dimensionless

2.3 Unit `per_second`

Definition s^{-1}

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

2.6 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
compartment_1	compartment		3	1	dimensionless	☑	

3.1 Compartment compartment_1

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

Name compartment

4 Species

This model contains 23 species. 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
species_1	L	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_2	PCNA	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_3	PCNAon	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_4	Rad18:Rad18	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_5	Rad18	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_6	Rad6	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_7	Rad6U	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_8	U	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_9	Rad18:Rad18:PCNAon	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_10	Rad18:Rad18:PCNAon:Rad6U	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_11	Rad18:Rad18:PCNAonU	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
species_12	PCNAonU	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_13	Rad5	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_14	Rad5:PCNAonU	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_15	Ubc13U:Mms2	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_16	Ubc13U:Mms2:Rad5:PCNAonU	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_17	Rad5:PCNAonU:U	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_18	Ubc13:Mms2	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_19	PCNAonU:U	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_20	Ubc13U:Mms2:Rad5:PCNAonU:U	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_21	Rad5:PCNAonU:U:U	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_22	PCNAonU:U:U	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟
species_23	PCNAoff	compartment_1	dimensionless · dimensionless^{-1}	⊟	⊟

5 Parameter

This model contains one global parameter.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
parameter_1	PCNA_sum		0.0		⊟

6 Rule

This is an overview of one rule.

6.1 Rule parameter_1

Rule parameter_1 is an assignment rule for parameter parameter_1:

$$\begin{aligned} \text{parameter\_1} = {} & [\text{species\_12}] + [\text{species\_19}] + [\text{species\_22}] + [\text{species\_11}] + [\text{species\_14}] \\ & + [\text{species\_17}] + [\text{species\_21}] + [\text{species\_20}] + [\text{species\_16}] \end{aligned} \tag{1}$$

Derived unit $\text{dimensionless}^{-1}$

7 Reactions

This model contains 25 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	reaction_1	r01	$\mathrm{species\_2} + \mathrm{species\_1} \xrightarrow{\mathrm{species\_2,\ species\_1}} \mathrm{species\_3}$	
2	reaction_2	r02	$2\,\mathrm{species\_5} \xrightarrow{\mathrm{species\_5}} \mathrm{species\_4}$	
3	reaction_3	r03	$\mathrm{species\_4} \xrightarrow{\mathrm{species\_4}} 2\,\mathrm{species\_5}$	
4	reaction_4	r04	$\mathrm{species\_6} + \mathrm{species\_8} \xrightarrow{\mathrm{species\_6,\ species\_8}} \mathrm{species\_7}$	
5	reaction_5	r05	$\mathrm{species\_3} + \mathrm{species\_4} \xrightarrow{\mathrm{species\_3,\ species\_4}} \mathrm{species\_9}$	
6	reaction_6	r06	$\mathrm{species\_9} \xrightarrow{\mathrm{species\_9}} \mathrm{species\_3} + \mathrm{species\_4}$	
7	reaction_7	r07	$\mathrm{species\_7} + \mathrm{species\_9} \xrightarrow{\mathrm{species\_7,\ species\_9}} \mathrm{species\_10}$	
8	reaction_8	r08	$\mathrm{species\_10} \xrightarrow{\mathrm{species\_10}} \mathrm{species\_7} + \mathrm{species\_9}$	
9	reaction_9	r09	$\mathrm{species\_10} \xrightarrow{\mathrm{species\_10}} \mathrm{species\_6} + \mathrm{species\_11}$	
10	reaction_10	r10	$\mathrm{species\_11} \xrightarrow{\mathrm{species\_11}} \mathrm{species\_4} + \mathrm{species\_12}$	
11	reaction_11	r11	$\mathrm{species\_8} + \mathrm{species\_18} \xrightarrow{\mathrm{species\_8,\ species\_18}} \mathrm{species\_15}$	
12	reaction_12	r12	$\mathrm{species\_12} + \mathrm{species\_13} \xrightarrow{\mathrm{species\_12,\ species\_13}} \mathrm{species\_14}$	
13	reaction_13	r13	$\mathrm{species\_14} \xrightarrow{\mathrm{species\_14}} \mathrm{species\_12} + \mathrm{species\_13}$	
14	reaction_14	r14	$\mathrm{species\_14} + \mathrm{species\_15} \xrightarrow{\mathrm{species\_14,\ species\_15}} \mathrm{species\_16}$	
15	reaction_15	r15	$\mathrm{species\_16} \xrightarrow{\mathrm{species\_16}} \mathrm{species\_14} + \mathrm{species\_15}$	

№	Id	Name	Reaction Equation	SBO
16	reaction_16	r16	$\text{species\_16} \xrightarrow{\text{species\_16}} \text{species\_18} + \text{species\_17}$	
17	reaction_17	r17	$\text{species\_17} \xrightarrow{\text{species\_17}} \text{species\_13} + \text{species\_19}$	
18	reaction_18	r18	$\text{species\_13} + \text{species\_19} \xrightarrow{\text{species\_13, species\_19}} \text{species\_17}$	
19	reaction_19	r19	$\text{species\_15} + \text{species\_17} \xrightarrow{\text{species\_15, species\_17}} \text{species\_20}$	
20	reaction_20	r20	$\text{species\_20} \xrightarrow{\text{species\_20}} \text{species\_15} + \text{species\_17}$	
21	reaction_21	r21	$\text{species\_20} \xrightarrow{\text{species\_20}} \text{species\_18} + \text{species\_21}$	
22	reaction_22	r22	$\text{species\_21} \xrightarrow{\text{species\_21}} \text{species\_13} + \text{species\_22}$	
23	reaction_23	r23	$\text{species\_12} \xrightarrow{\text{species\_12}} \text{species\_8} + \text{species\_23}$	
24	reaction_24	r24	$\text{species\_19} \xrightarrow{\text{species\_19}} 2\,\text{species\_8} + \text{species\_23}$	
25	reaction_25	r25	$\text{species\_22} \xrightarrow{\text{species\_22}} 3\,\text{species\_8} + \text{species\_23}$	

7.1 Reaction `reaction_1`

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

Name r01

Reaction equation

$$\text{species\_2} + \text{species\_1} \xrightarrow{\text{species\_2, species\_1}} \text{species\_3} \tag{2}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
`species_2`	PCNA	
`species_1`	L	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
`species_2`	PCNA	
`species_1`	L	

Product

Table 8: Properties of each product.

Id	Name	SBO
`species_3`	PCNAon	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_2}] \cdot [\text{species\_1}] \tag{3}$$

Table 9: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$1.5 \cdot 10^{-8}$		☑

7.2 Reaction reaction_2

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

Name r02

Reaction equation

$$2\,\text{species\_5} \xrightarrow{\text{species\_5}} \text{species\_4} \tag{4}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
species_5	Rad18	

Modifier

Table 11: Properties of each modifier.

Id	Name	SBO
species_5	Rad18	

Product

Table 12: Properties of each product.

Id	Name	SBO
species_4	Rad18:Rad18	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol}\,(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_5}]^2 \tag{5}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.01		☑

7.3 Reaction reaction_3

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

Name r03

Reaction equation

$$\text{species\_4} \xrightarrow{\text{species\_4}} 2\,\text{species\_5} \tag{6}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
species_4	Rad18:Rad18	

Modifier

Table 15: Properties of each modifier.

Id	Name	SBO
species_4	Rad18:Rad18	

Product

Table 16: Properties of each product.

Id	Name	SBO
species_5	Rad18	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}\,(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_4}] \tag{7}$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		1000.0		☑

7.4 Reaction reaction_4

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

Name r04

Reaction equation

$$\text{species\_6} + \text{species\_8} \xrightarrow{\text{species\_6, species\_8}} \text{species\_7} \tag{8}$$

Reactants

Table 18: Properties of each reactant.

Id	Name	SBO
species_6	Rad6	
species_8	U	

Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
species_6	Rad6	
species_8	U	

Product

Table 20: Properties of each product.

Id	Name	SBO
species_7	Rad6U	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_6}] \cdot [\mathrm{species\_8}] \tag{9}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$2.5 \cdot 10^{-7}$		☑

7.5 Reaction reaction_5

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

Name r05

Reaction equation

$$\mathrm{species\_3} + \mathrm{species\_4} \xrightarrow{\mathrm{species\_3,\ species\_4}} \mathrm{species\_9} \tag{10}$$

Reactants

Table 22: Properties of each reactant.

Id	Name	SBO
species_3	PCNAon	
species_4	Rad18:Rad18	

Modifiers

Table 23: Properties of each modifier.

Id	Name	SBO
species_3	PCNAon	
species_4	Rad18:Rad18	

Product

Table 24: Properties of each product.

Id	Name	SBO
species_9	Rad18:Rad18:PCNAon	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_3}] \cdot [\mathrm{species\_4}] \tag{11}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		100000.0		☑

7.6 Reaction reaction_6

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

Name r06

Reaction equation

$$\mathrm{species\_9} \xrightarrow{\mathrm{species\_9}} \mathrm{species\_3} + \mathrm{species\_4} \tag{12}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
species_9	Rad18:Rad18:PCNAon	

Modifier

Table 27: Properties of each modifier.

Id	Name	SBO
species_9	Rad18:Rad18:PCNAon	

Products

Table 28: Properties of each product.

Id	Name	SBO
species_3	PCNAon	

Id	Name	SBO
species_4	Rad18:Rad18	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_9}] \tag{13}$$

Table 29: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		1000.0		☑

7.7 Reaction reaction_7

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

Name r07

Reaction equation

$$\mathrm{species\_7} + \mathrm{species\_9} \xrightarrow{\mathrm{species\_7,\ species\_9}} \mathrm{species\_10} \tag{14}$$

Reactants

Table 30: Properties of each reactant.

Id	Name	SBO
species_7	Rad6U	
species_9	Rad18:Rad18:PCNAon	

Modifiers

Table 31: Properties of each modifier.

Id	Name	SBO
species_7	Rad6U	
species_9	Rad18:Rad18:PCNAon	

Product

Table 32: Properties of each product.

Id	Name	SBO
species_10	Rad18:Rad18:PCNAon:Rad6U	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_7}] \cdot [\mathrm{species\_9}] \tag{15}$$

Table 33: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.035		☑

7.8 Reaction reaction_8

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

Name r08

Reaction equation

$$\mathrm{species\_10} \xrightarrow{\mathrm{species\_10}} \mathrm{species\_7} + \mathrm{species\_9} \tag{16}$$

Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
species_10	Rad18:Rad18:PCNAon:Rad6U	

Modifier

Table 35: Properties of each modifier.

Id	Name	SBO
species_10	Rad18:Rad18:PCNAon:Rad6U	

Id	Name	SBO

Products

Table 36: Properties of each product.

Id	Name	SBO
species_7	Rad6U	
species_9	Rad18:Rad18:PCNAon	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_10}] \tag{17}$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.01		☑

7.9 Reaction reaction_9

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

Name r09

Reaction equation

$$\mathrm{species\_10} \xrightarrow{\mathrm{species\_10}} \mathrm{species\_6} + \mathrm{species\_11} \tag{18}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
species_10	Rad18:Rad18:PCNAon:Rad6U	

Modifier

Table 39: Properties of each modifier.

Id	Name	SBO
species_10	Rad18:Rad18:PCNAon:Rad6U	

Products

Table 40: Properties of each product.

Id	Name	SBO
species_6	Rad6	
species_11	Rad18:Rad18:PCNAonU	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_10}] \tag{19}$$

Table 41: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.01		☑

7.10 Reaction reaction_10

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

Name r10

Reaction equation

$$\mathrm{species\_11} \xrightarrow{\mathrm{species\_11}} \mathrm{species\_4} + \mathrm{species\_12} \tag{20}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
species_11	Rad18:Rad18:PCNAonU	

Modifier

Table 43: Properties of each modifier.

Id	Name	SBO
species_11	Rad18:Rad18:PCNAonU	

Products

Table 44: Properties of each product.

Id	Name	SBO
species_4	Rad18:Rad18	
species_12	PCNAonU	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_11}] \tag{21}$$

Table 45: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		1.0		☑

7.11 Reaction reaction_11

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

Name r11

Reaction equation

$$\mathrm{species\_8} + \mathrm{species\_18} \xrightarrow{\mathrm{species\_8,\ species\_18}} \mathrm{species\_15} \tag{22}$$

Reactants

Table 46: Properties of each reactant.

Id	Name	SBO
species_8	U	
species_18	Ubc13:Mms2	

Modifiers

Table 47: Properties of each modifier.

Id	Name	SBO
species_8	U	
species_18	Ubc13:Mms2	

Product

Table 48: Properties of each product.

Id	Name	SBO
species_15	Ubc13U:Mms2	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_8}] \cdot [\mathrm{species\_18}] \tag{23}$$

Table 49: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		100000.0		☑

7.12 Reaction reaction_12

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

Name r12

Reaction equation

$$\mathrm{species\_12} + \mathrm{species\_13} \xrightarrow{\mathrm{species\_12,\ species\_13}} \mathrm{species\_14} \tag{24}$$

Reactants

Table 50: Properties of each reactant.

Id	Name	SBO
species_12	PCNAonU	
species_13	Rad5	

Modifiers

Table 51: Properties of each modifier.

Id	Name	SBO
species_12	PCNAonU	
species_13	Rad5	

Product

Table 52: Properties of each product.

Id	Name	SBO
species_14	Rad5:PCNAonU	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_12}] \cdot [\mathrm{species\_13}] \tag{25}$$

Table 53: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$5 \cdot 10^{-6}$		☑

7.13 Reaction reaction_13

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

Name r13

Reaction equation

$$\text{species\_14} \xrightarrow{\text{species\_14}} \text{species\_12} + \text{species\_13} \tag{26}$$

Reactant

Table 54: Properties of each reactant.

Id	Name	SBO
species_14	Rad5:PCNAonU	

Modifier

Table 55: Properties of each modifier.

Id	Name	SBO
species_14	Rad5:PCNAonU	

Products

Table 56: Properties of each product.

Id	Name	SBO
species_12	PCNAonU	
species_13	Rad5	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \text{vol}(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_14}] \tag{27}$$

Table 57: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.005		☑

7.14 Reaction reaction_14

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

Name r14

Reaction equation

$$\text{species\_14} + \text{species\_15} \xrightarrow{\text{species\_14, species\_15}} \text{species\_16} \tag{28}$$

Reactants

Table 58: Properties of each reactant.

Id	Name	SBO
species_14	Rad5:PCNAonU	
species_15	Ubc13U:Mms2	

Modifiers

Table 59: Properties of each modifier.

Id	Name	SBO
species_14	Rad5:PCNAonU	
species_15	Ubc13U:Mms2	

Product

Table 60: Properties of each product.

Id	Name	SBO
species_16	Ubc13U:Mms2:Rad5:PCNAonU	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \text{vol}\left(\text{compartment\_1}\right) \cdot \text{k1} \cdot [\text{species\_14}] \cdot [\text{species\_15}] \tag{29}$$

Table 61: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.078		☑

7.15 Reaction reaction_15

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

Name r15

Reaction equation

$$\text{species\_16} \xrightarrow{\text{species\_16}} \text{species\_14} + \text{species\_15} \tag{30}$$

Reactant

Table 62: Properties of each reactant.

Id	Name	SBO
species_16	Ubc13U:Mms2:Rad5:PCNAonU	

Modifier

Table 63: Properties of each modifier.

Id	Name	SBO
species_16	Ubc13U:Mms2:Rad5:PCNAonU	

Products

Table 64: Properties of each product.

Id	Name	SBO
species_14	Rad5:PCNAonU	
species_15	Ubc13U:Mms2	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_16}] \tag{31}$$

Table 65: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		10^{-10}		☑

7.16 Reaction reaction_16

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

Name r16

Reaction equation

$$\mathrm{species\_16} \xrightarrow{\mathrm{species\_16}} \mathrm{species\_18} + \mathrm{species\_17} \tag{32}$$

Reactant

Table 66: Properties of each reactant.

Id	Name	SBO
species_16	Ubc13U:Mms2:Rad5:PCNAonU	

Modifier

Table 67: Properties of each modifier.

Id	Name	SBO
species_16	Ubc13U:Mms2:Rad5:PCNAonU	

Products

Table 68: Properties of each product.

Id	Name	SBO
species_18	Ubc13:Mms2	
species_17	Rad5:PCNAonU:U	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_16}] \tag{33}$$

Table 69: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.05		☑

7.17 Reaction reaction_17

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

Name r17

Reaction equation

$$\mathrm{species\_17} \xrightarrow{\mathrm{species\_17}} \mathrm{species\_13} + \mathrm{species\_19} \tag{34}$$

Reactant

Table 70: Properties of each reactant.

Id	Name	SBO
species_17	Rad5:PCNAonU:U	

Modifier

Table 71: Properties of each modifier.

Id	Name	SBO
species_17	Rad5:PCNAonU:U	

Products

Table 72: Properties of each product.

Id	Name	SBO
species_13	Rad5	

Id	Name	SBO
species_19	PCNAonU:U	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_17}] \tag{35}$$

Table 73: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$7.5 \cdot 10^{-6}$		☑

7.18 Reaction reaction_18

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

Name r18

Reaction equation

$$\mathrm{species\_13} + \mathrm{species\_19} \xrightarrow{\mathrm{species\_13,\ species\_19}} \mathrm{species\_17} \tag{36}$$

Reactants

Table 74: Properties of each reactant.

Id	Name	SBO
species_13	Rad5	
species_19	PCNAonU:U	

Modifiers

Table 75: Properties of each modifier.

Id	Name	SBO
species_13	Rad5	
species_19	PCNAonU:U	

Product

Table 76: Properties of each product.

Id	Name	SBO
species_17	Rad5:PCNAonU:U	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_13}] \cdot [\mathrm{species\_19}] \tag{37}$$

Table 77: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$5 \cdot 10^{-6}$		☑

7.19 Reaction reaction_19

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

Name r19

Reaction equation

$$\mathrm{species\_15} + \mathrm{species\_17} \xrightarrow{\mathrm{species\_15,\ species\_17}} \mathrm{species\_20} \tag{38}$$

Reactants

Table 78: Properties of each reactant.

Id	Name	SBO
species_15	Ubc13U:Mms2	
species_17	Rad5:PCNAonU:U	

Modifiers

Table 79: Properties of each modifier.

Id	Name	SBO
species_15	Ubc13U:Mms2	
species_17	Rad5:PCNAonU:U	

Product

Table 80: Properties of each product.

Id	Name	SBO
species_20	Ubc13U:Mms2:Rad5:PCNAonU:U	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_15}] \cdot [\mathrm{species\_17}] \tag{39}$$

Table 81: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.078		☑

7.20 Reaction reaction_20

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

Name r20

Reaction equation

$$\mathrm{species\_20} \xrightarrow{\mathrm{species\_20}} \mathrm{species\_15} + \mathrm{species\_17} \tag{40}$$

Reactant

Table 82: Properties of each reactant.

Id	Name	SBO
species_20	Ubc13U:Mms2:Rad5:PCNAonU:U	

Modifier

Table 83: Properties of each modifier.

Id	Name	SBO
species_20	Ubc13U:Mms2:Rad5:PCNAonU:U	

Products

Table 84: Properties of each product.

Id	Name	SBO
species_15	Ubc13U:Mms2	
species_17	Rad5:PCNAonU:U	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{k1} \cdot [\mathrm{species\_20}] \tag{41}$$

Table 85: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		10^{-10}		☑

7.21 Reaction reaction_21

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

Name r21

Reaction equation

$$\mathrm{species\_20} \xrightarrow{\mathrm{species\_20}} \mathrm{species\_18} + \mathrm{species\_21} \tag{42}$$

Reactant

Table 86: Properties of each reactant.

Id	Name	SBO
species_20	Ubc13U:Mms2:Rad5:PCNAonU:U	

Modifier

Table 87: Properties of each modifier.

Id	Name	SBO
species_20	Ubc13U:Mms2:Rad5:PCNAonU:U	

Products

Table 88: Properties of each product.

Id	Name	SBO
species_18	Ubc13:Mms2	
species_21	Rad5:PCNAonU:U:U	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_20}] \tag{43}$$

Table 89: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.005		☑

7.22 Reaction reaction_22

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

Name r22

Reaction equation

$$\mathrm{species\_21} \xrightarrow{\mathrm{species\_21}} \mathrm{species\_13} + \mathrm{species\_22} \tag{44}$$

Reactant

Table 90: Properties of each reactant.

Id	Name	SBO
species_21	Rad5:PCNAonU:U:U	

Modifier

Table 91: Properties of each modifier.

Id	Name	SBO
species_21	Rad5:PCNAonU:U:U	

Products

Table 92: Properties of each product.

Id	Name	SBO
species_13	Rad5	
species_22	PCNAonU:U:U	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{k1} \cdot \left[\mathrm{species\_21}\right] \tag{45}$$

Table 93: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.005		☑

7.23 Reaction reaction_23

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

Name r23

Reaction equation

$$\text{species\_12} \xrightarrow{\text{species\_12}} \text{species\_8} + \text{species\_23} \tag{46}$$

Reactant

Table 94: Properties of each reactant.

Id	Name	SBO
species_12	PCNAonU	

Modifier

Table 95: Properties of each modifier.

Id	Name	SBO
species_12	PCNAonU	

Products

Table 96: Properties of each product.

Id	Name	SBO
species_8	U	
species_23	PCNAoff	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \text{vol}(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_12}] \tag{47}$$

Table 97: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$3 \cdot 10^{-8}$		☑

7.24 Reaction reaction_24

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

Name r24

Reaction equation

$$\text{species\_19} \xrightarrow{\text{species\_19}} 2\,\text{species\_8} + \text{species\_23} \tag{48}$$

Reactant

Table 98: Properties of each reactant.

Id	Name	SBO
species_19	PCNAonU:U	

Modifier

Table 99: Properties of each modifier.

Id	Name	SBO
species_19	PCNAonU:U	

Products

Table 100: Properties of each product.

Id	Name	SBO
species_8	U	
species_23	PCNAoff	

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \text{vol}\,(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_19}] \tag{49}$$

Table 101: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$8 \cdot 10^{-4}$		☑

7.25 Reaction reaction_25

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

Name r25

Reaction equation

$$\text{species\_22} \xrightarrow{\text{species\_22}} 3\,\text{species\_8} + \text{species\_23} \tag{50}$$

Reactant

Table 102: Properties of each reactant.

Id	Name	SBO
species_22	PCNAonU:U:U	

Modifier

Table 103: Properties of each modifier.

Id	Name	SBO
species_22	PCNAonU:U:U	

Products

Table 104: Properties of each product.

Id	Name	SBO
species_8	U	
species_23	PCNAoff	

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_22}] \tag{51}$$

Table 105: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.005		☑

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.

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.

8.1 Species species_1

Name L

Initial concentration 1001 dimensionless $\cdot$ dimensionless^{-1}

This species takes part in two reactions (as a reactant in reaction_1 and as a modifier in reaction_1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_1} = -v_1 \tag{52}$$

8.2 Species species_2

Name PCNA

Initial concentration 7480 dimensionless $\cdot$ dimensionless^{-1}

This species takes part in two reactions (as a reactant in reaction_1 and as a modifier in reaction_1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_2} = -v_1 \tag{53}$$

8.3 Species species_3

Name PCNAon

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

This species takes part in four reactions (as a reactant in reaction_5 and as a product in reaction_1, reaction_6 and as a modifier in reaction_5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_3} = v_1 + v_6 - v_5 \tag{54}$$

8.4 Species species_4

Name Rad18:Rad18

SBO:0000286 multimer

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

This species takes part in seven reactions (as a reactant in reaction_3, reaction_5 and as a product in reaction_2, reaction_6, reaction_10 and as a modifier in reaction_3, reaction_5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_4} = v_2 + v_6 + v_{10} - v_3 - v_5 \tag{55}$$

8.5 Species species_5

Name Rad18

Initial concentration $206\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in three reactions (as a reactant in reaction_2 and as a product in reaction_3 and as a modifier in reaction_2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_5} = 2\,v_3 - 2\,v_2 \tag{56}$$

8.6 Species species_6

Name Rad6

Initial concentration $194\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in three reactions (as a reactant in reaction_4 and as a product in reaction_9 and as a modifier in reaction_4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_6} = v_9 - v_4 \tag{57}$$

8.7 Species species_7

Name Rad6U

Initial concentration 0 dimensionless · dimensionless^{-1}

This species takes part in four reactions (as a reactant in reaction_7 and as a product in reaction_4, reaction_8 and as a modifier in reaction_7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_7} = v_4 + v_8 - v_7 \tag{58}$$

8.8 Species species_8

Name U

Initial concentration 8698 dimensionless · dimensionless^{-1}

This species takes part in seven reactions (as a reactant in reaction_4, reaction_11 and as a product in reaction_23, reaction_24, reaction_25 and as a modifier in reaction_4, reaction_11).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_8} = v_{23} + 2\,v_{24} + 3\,v_{25} - v_4 - v_{11} \tag{59}$$

8.9 Species species_9

Name Rad18:Rad18:PCNAon

SBO:0000297 protein complex

Initial concentration 0 dimensionless · dimensionless^{-1}

This species takes part in six reactions (as a reactant in reaction_6, reaction_7 and as a product in reaction_5, reaction_8 and as a modifier in reaction_6, reaction_7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_9} = v_5 + v_8 - v_6 - v_7 \tag{60}$$

8.10 Species species_10

Name Rad18:Rad18:PCNAon:Rad6U

SBO:0000297 protein complex

Initial concentration 0 dimensionless · dimensionless^{-1}

This species takes part in five reactions (as a reactant in reaction_8, reaction_9 and as a product in reaction_7 and as a modifier in reaction_8, reaction_9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_10} = v_7 - v_8 - v_9 \tag{61}$$

8.11 Species species_11

Name Rad18:Rad18:PCNAonU

SBO:0000297 protein complex

Initial concentration 0 dimensionless · dimensionless^{-1}

This species takes part in three reactions (as a reactant in reaction_10 and as a product in reaction_9 and as a modifier in reaction_10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_11} = v_9 - v_{10} \tag{62}$$

8.12 Species species_12

Name PCNAonU

Initial concentration 0 dimensionless · dimensionless^{-1}

This species takes part in six reactions (as a reactant in reaction_12, reaction_23 and as a product in reaction_10, reaction_13 and as a modifier in reaction_12, reaction_23).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_12} = v_{10} + v_{13} - v_{12} - v_{23} \tag{63}$$

8.13 Species species_13

Name Rad5

Initial concentration 1520 dimensionless · dimensionless^{-1}

This species takes part in seven reactions (as a reactant in reaction_12, reaction_18 and as a product in reaction_13, reaction_17, reaction_22 and as a modifier in reaction_12, reaction_18).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_13} = v_{13} + v_{17} + v_{22} - v_{12} - v_{18} \tag{64}$$

8.14 Species species_14

Name Rad5:PCNAonU

SBO:0000297 protein complex

Initial concentration 0 dimensionless · dimensionless^{-1}

This species takes part in six reactions (as a reactant in reaction_13, reaction_14 and as a product in reaction_12, reaction_15 and as a modifier in reaction_13, reaction_14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_14} = v_{12} + v_{15} - v_{13} - v_{14} \tag{65}$$

8.15 Species species_15

Name Ubc13U:Mms2

SBO:0000297 protein complex

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

This species takes part in seven reactions (as a reactant in reaction_14, reaction_19 and as a product in reaction_11, reaction_15, reaction_20 and as a modifier in reaction_14, reaction_19).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_15} = v_{11} + v_{15} + v_{20} - v_{14} - v_{19} \tag{66}$$

8.16 Species species_16

Name Ubc13U:Mms2:Rad5:PCNAonU

SBO:0000297 protein complex

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

This species takes part in five reactions (as a reactant in reaction_15, reaction_16 and as a product in reaction_14 and as a modifier in reaction_15, reaction_16).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_16} = v_{14} - v_{15} - v_{16} \tag{67}$$

8.17 Species species_17

Name Rad5:PCNAonU:U

SBO:0000297 protein complex

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

This species takes part in seven reactions (as a reactant in reaction_17, reaction_19 and as a product in reaction_16, reaction_18, reaction_20 and as a modifier in reaction_17, reaction_19).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_17} = v_{16} + v_{18} + v_{20} - v_{17} - v_{19} \tag{68}$$

8.18 Species species_18

Name Ubc13:Mms2

SBO:0000297 protein complex

Initial concentration 193 dimensionless · dimensionless^{-1}

This species takes part in four reactions (as a reactant in reaction_11 and as a product in reaction_16, reaction_21 and as a modifier in reaction_11).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_18} = v_{16} + v_{21} - v_{11} \tag{69}$$

8.19 Species species_19

Name PCNAonU:U

Initial concentration 0 dimensionless · dimensionless^{-1}

This species takes part in five reactions (as a reactant in reaction_18, reaction_24 and as a product in reaction_17 and as a modifier in reaction_18, reaction_24).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_19} = v_{17} - v_{18} - v_{24} \tag{70}$$

8.20 Species species_20

Name Ubc13U:Mms2:Rad5:PCNAonU:U

SBO:0000297 protein complex

Initial concentration 0 dimensionless · dimensionless^{-1}

This species takes part in five reactions (as a reactant in reaction_20, reaction_21 and as a product in reaction_19 and as a modifier in reaction_20, reaction_21).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_20} = v_{19} - v_{20} - v_{21} \tag{71}$$

8.21 Species species_21

Name Rad5:PCNAonU:U:U

SBO:0000297 protein complex

Initial concentration 0 dimensionless · dimensionless^{-1}

This species takes part in three reactions (as a reactant in reaction_22 and as a product in reaction_21 and as a modifier in reaction_22).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_21} = v_{21} - v_{22} \tag{72}$$

8.22 Species species_22

Name PCNAonU:U:U

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

This species takes part in three reactions (as a reactant in reaction_25 and as a product in reaction_22 and as a modifier in reaction_25).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_22} = v_{22} - v_{25} \tag{73}$$

8.23 Species species_23

Name PCNAoff

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

This species takes part in three reactions (as a product in reaction_23, reaction_24, reaction_25).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_23} = v_{23} + v_{24} + v_{25} \tag{74}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000286 multimer: Non-covalent association of identical, or pseudo-identical, entities. By pseudo-identical entities, we mean biochemical elements that differ chemically, although remaining globally identical in structure and/or function. Examples are homologous subunits in an hetero-oligomeric receptor

SBO:0000297 protein complex: Macromolecular complex containing one or more polypeptide chains possibly associated with simple chemicals. CHEBI:3608

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.

[a]Center for Bioinformatics Tübingen (ZBIT), Germany
[b]California Institute of Technology, Beckman Institute BNMC, Pasadena, United States
[c]European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom
[d]EML Research gGmbH, Heidelberg, Germany