# **SBML Model Report**

# Model name: "Mandlik2015 - Tristable genetic circuit of Leishmania"



May 6, 2016

### 1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Shailza Singh<sup>1</sup> and Vijayalakshmi Chelliah<sup>2</sup> at October 26<sup>th</sup> 2015 at 12:57 a.m. and last time modified at February twelveth 2016 at 3:21 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	35
events	0	constraints	0
reactions	14	function definitions	0
global parameters	34	unit definitions	0
rules	14	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.

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## 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** 1

#### 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
DefaultCompartment	DefaultCompartment		3	1	litre	Z	

## 3.1 Compartment DefaultCompartment

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

Name DefaultCompartment

# 4 Species

This model contains 35 species. The boundary condition of 14 of these species is set to true so that these 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 Condi-
					tion
AUR1	AUR1	DefaultCompartment	$\text{mol} \cdot l^{-1}$		$\overline{\hspace{1cm}}$
IPTG	IPTG	DefaultCompartment	$\text{mol} \cdot l^{-1}$		
LACI	LACI	DefaultCompartment	$\text{mol} \cdot l^{-1}$		
LAMDAR	LAMDAR	DefaultCompartment	$\text{mol} \cdot 1^{-1}$		
SLS1	SLS1	DefaultCompartment	$\text{mol} \cdot 1^{-1}$		
SLS4	SLS4	DefaultCompartment	$\text{mol} \cdot l^{-1}$		
TETR	TETR	DefaultCompartment	$\text{mol} \cdot l^{-1}$		
as1	as1	DefaultCompartment	$\text{mol} \cdot l^{-1}$		
ia1_ActiveTF	ia1_ActiveTF	DefaultCompartment	$\text{mol} \cdot l^{-1}$		
$ia1\_InactiveTF$	ia1_InactiveTF	DefaultCompartment	$\text{mol} \cdot l^{-1}$		$\Box$
ope1	ope1	DefaultCompartment	$\text{mol} \cdot l^{-1}$		
p1	p1	DefaultCompartment	$\text{mol} \cdot l^{-1}$		
p2	p2	DefaultCompartment	$\text{mol} \cdot l^{-1}$		$\Box$
р3	p3	DefaultCompartment	$\text{mol} \cdot l^{-1}$		$\Box$
pAUR1	pAUR1	DefaultCompartment	$\text{mol} \cdot l^{-1}$		$\Box$
pSLS1	pSLS1	DefaultCompartment	$\text{mol} \cdot l^{-1}$		$\Box$
pSLS4	pSLS4	DefaultCompartment	$\text{mol} \cdot l^{-1}$		$\Box$
proAUR1	proAUR1	DefaultCompartment	$\text{mol} \cdot l^{-1}$		$\Box$
proLACI	proLACI	DefaultCompartment	$\text{mol} \cdot l^{-1}$		$\Box$
proLAMDAR	proLAMDAR	DefaultCompartment	$\text{mol} \cdot l^{-1}$		$\Box$
proSLS1	proSLS1	DefaultCompartment	$\text{mol} \cdot l^{-1}$		

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
proSLS4	proSLS4	DefaultCompartment	$\text{mol} \cdot l^{-1}$		
proTETR	proTETR	${\tt DefaultCompartment}$	$\text{mol} \cdot 1^{-1}$		
rs1	rs1	${\tt DefaultCompartment}$	$\text{mol} \cdot 1^{-1}$		$\square$
rs2	rs2	${\tt DefaultCompartment}$	$\text{mol} \cdot 1^{-1}$	$\Box$	$\square$
rs3	rs3	${\tt DefaultCompartment}$	$\text{mol} \cdot 1^{-1}$	$\Box$	$\square$
rs4	rs4	${\tt DefaultCompartment}$	$\text{mol} \cdot 1^{-1}$		$\square$
rs5	rs5	${\tt DefaultCompartment}$	$\text{mol} \cdot 1^{-1}$		$\square$
rs6	rs6	${\tt DefaultCompartment}$	$\text{mol} \cdot 1^{-1}$		$\square$
ter1	ter1	${\tt DefaultCompartment}$	$\text{mol} \cdot 1^{-1}$		
ter2	ter2	${\tt DefaultCompartment}$	$\text{mol} \cdot 1^{-1}$		
ter3	ter3	${\tt DefaultCompartment}$	$\text{mol} \cdot 1^{-1}$		
ter4	ter4	${\tt DefaultCompartment}$	$\text{mol} \cdot 1^{-1}$		
ter5	ter5	DefaultCompartment	$\text{mol} \cdot 1^{-1}$	$\Box$	
ter6	ter6	DefaultCompartment	$\text{mol} \cdot 1^{-1}$	$\Box$	$\Box$

# **5 Parameters**

This model contains 34 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
tr3_Kd	tr3_Kd		1.000		$\checkmark$
tr3_h	tr3_h		2.000		$\overline{\mathbf{Z}}$
tr4_Kd	tr4_Kd		1.000		$\overline{\mathbf{Z}}$
$\mathtt{tr4}\_\mathtt{h}$	tr4_h		2.000		$\overline{\mathbf{Z}}$
pSLS4-	pSLS4_strength		2.570		
$_{ t strength}$					
tr5_Kd	tr5_Kd		1.000		
$\mathtt{tr}5\_\mathtt{h}$	tr5_h		2.000		
tr6_Kd	tr6_Kd		1.000		$\square$
tr6_h	tr6_h		2.000		$\square$
$\mathtt{p1\_strength}$	p1_strength		2.500		
$p2\_strength$	p2_strength		2.400		
proLACI-	proLACI-		0.070		
_degradation- _rate	_degradation_rate				
$p3\_strength$	p3_strength		2.500		$\square$
proSLS1-	proSLS1-		0.070		
_degradation- _rate	_degradation_rate				
proSLS4-	proSLS4-		0.040		
_degradation- _rate	_degradation_rate				
proLAMDAR-	proLAMDAR-		0.042		
_degradation- _rate	_degradation_rate				
proAUR1-	proAUR1-		0.100		
_degradation- _rate	_degradation_rate				
ia1_Kd	ia1_Kd		0.001		
ia1-	ia1_repression_Kd		1.000		
_repression- _Kd					
ia1-	ia1_repression_h		2.000		
$\_$ repression $\_$ h					
pAUR1- _strength	pAUR1_strength		2.014		

Id	Name	SBO	Value	Unit	Constant
proTETR-	proTETR-		0.080		Ø
_degradation- _rate	_degradation_rate				
ta1_Kd	ta1_Kd		1.000		
ta1_h	ta1_h		2.000		
pp2-	pp2_translation-		1.000		
$_{ extsf{ iny translation-}}$	_rate				
_rate					
pp3-	pp3_translation-		1.000		
$_{ extstyle }$ translation-	_rate				
_rate					
pp4-	pp4_translation-		1.000		
_translation-	_rate				
_rate					
pp5-	pp5_translation-		1.000		
$_{ extstyle }$ translation-	_rate				
_rate					
pp6-	pp6_translation-		1.000		
$_{ t translation-}$	_rate				
_rate					
tr1_Kd	tr1_Kd		1.000		$\square$
tr1_h	tr1_h		2.000		$   \overline{\mathbf{Z}} $
pSLS1-	pSLS1_strength		2.500		
$\_\mathtt{strength}$					
tr2_Kd	tr2_Kd		1.000		
tr2_h	tr2_h		2.000		$\square$

# 6 Rules

This is an overview of 14 rules.

## **6.1 Rule** rs6

Rule rs6 is an assignment rule for species rs6:

$$rs6 = \frac{1}{1 + \left(\frac{[proTETR]}{tr4\_Kd}\right)^{tr4\_h}}$$
 (1)

#### **6.2 Rule** rs3

Rule rs3 is an assignment rule for species rs3:

$$rs3 = \frac{1}{1 + \left(\frac{[proLACI]}{tr6\_Kd}\right)^{tr6\_h}}$$
 (2)

#### **6.3 Rule** rs4

Rule rs4 is an assignment rule for species rs4:

$$rs4 = \frac{1}{1 + \left(\frac{[proLAMDAR]}{tr5\_Kd}\right)^{tr5\_h}}$$
(3)

#### **6.4 Rule** rs5

Rule rs5 is an assignment rule for species rs5:

$$rs5 = \frac{1}{1 + \left(\frac{[proLACI]}{tr3\_Kd}\right)^{tr3\_h}}$$
(4)

#### 6.5 Rule LAMDAR

Rule LAMDAR is an assignment rule for species LAMDAR:

$$LAMDAR = p1\_strength \cdot [rs6]$$
 (5)

#### 6.6 Rule LACI

Rule LACI is an assignment rule for species LACI:

$$LACI = p2\_strength \cdot [rs4]$$
 (6)

## 6.7 Rule TETR

Rule TETR is an assignment rule for species TETR:

$$TETR = p3\_strength \cdot [rs5]$$
 (7)

#### **6.8 Rule** rs1

Rule rs1 is an assignment rule for species rs1:

$$rs1 = \frac{1}{1 + \left(\frac{[proSLS1]}{tr1\_Kd}\right)^{tr1\_h}}$$
(8)

#### **6.9 Rule** rs2

Rule rs2 is an assignment rule for species rs2:

$$rs2 = \frac{1}{1 + \left(\frac{[proAUR1]}{tr2\_Kd}\right)^{tr2\_h}}$$
(9)

## **6.10 Rule** ope1

Rule ope1 is an assignment rule for species ope1:

$$ope1 = \frac{1}{1 + \left(\frac{[ia1\_ActiveTF]}{ia1\_repression\_Kd}\right)^{ia1\_repression\_h}}$$
(10)

#### **6.11 Rule** as1

Rule as1 is an assignment rule for species as1:

$$as1 = \frac{1 + \left(\frac{[proSLS4]}{ta1\_Kd}\right)^{ta1\_h} - 1}{1 + \left(\frac{[proSLS4]}{ta1\_Kd}\right)^{ta1\_h}}$$
(11)

#### **6.12 Rule SLS1**

Rule SLS1 is an assignment rule for species SLS1:

$$SLS1 = pSLS1\_strength \cdot [as1] \cdot [ope1] \cdot [rs3]$$
 (12)

#### **6.13 Rule SLS4**

Rule SLS4 is an assignment rule for species SLS4:

$$SLS4 = pSLS4\_strength \cdot [rs2]$$
 (13)

#### **6.14 Rule AUR1**

Rule AUR1 is an assignment rule for species AUR1:

$$AUR1 = pAUR1\_strength \cdot [rs1]$$
 (14)

# **7 Reactions**

This model contains 14 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

N⁰	Id	Name	Reaction Equation SBO
1	pp1_v1	pp1_v1	$\emptyset \longrightarrow proSLS1$
2	pp1_v2	pp1_v2	$\operatorname{proSLS1} \xrightarrow{\operatorname{proSLS1}} \emptyset$
3	pp5_v1	pp5_v1	$\emptyset \xrightarrow{\text{LAMDAR}, \text{LAMDAR}} \text{proLAMDAR}$
4	pp5_v2	pp5_v2	$\operatorname{proLAMDAR} \xrightarrow{\operatorname{proLAMDAR}} \emptyset$
5	ia1_bind- _forward	ia1_bind_forward	IPTG+ia1_ActiveTF   IPTG, ia1_ActiveTF ia1_InactiveTF
6	ia1_bind- _reverse	ia1_bind_reverse	ia1_InactiveTF ia1_InactiveTF IPTG + ia1_ActiveTF
7	pp2_v1	pp2_v1	$\emptyset \xrightarrow{\text{AUR1, AUR1}} \text{proAUR1}$
8	pp2_v2	pp2_v2	$proAUR1 \xrightarrow{proAUR1} \emptyset$
9	pp6_v1	pp6_v1	$\emptyset \xrightarrow{\text{TETR}, \text{TETR}} \text{proTETR}$
10	pp6_v2	pp6_v2	$\operatorname{proTETR} \xrightarrow{\operatorname{proTETR}} \emptyset$
11	pp3_v1	pp3_v1	$\emptyset \xrightarrow{\text{SLS4, SLS4}} \text{proSLS4}$
12	pp3_v2	pp3_v2	$proSLS4 \xrightarrow{proSLS4} \emptyset$
13	pp4_v1	pp4_v1	$\emptyset \xrightarrow{\text{LACI, LACI}} \text{proLACI}$
14	pp4_v2	pp4_v2	$\operatorname{proLACI} \xrightarrow{\operatorname{proLACI}} \emptyset$

# 7.1 Reaction pp1\_v1

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

Name  $pp1_v1$ 

## **Reaction equation**

$$\emptyset \longrightarrow proSLS1$$
 (15)

#### **Product**

Table 6: Properties of each product.

Id	Name	SBO
proSLS1	proSLS1	

#### **Kinetic Law**

Derived unit not available

$$v_1 = 1 \tag{16}$$

## **7.2 Reaction** pp1\_v2

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

Name  $pp1_v2$ 

## **Reaction equation**

$$proSLS1 \xrightarrow{proSLS1} \emptyset$$
 (17)

#### Reactant

Table 7: Properties of each reactant.

Id	Name	SBO
proSLS1	proSLS1	

#### **Modifier**

Table 8: Properties of each modifier.

Id	Name	SBO
proSLS1	proSLS1	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_2 = \text{proSLS1\_degradation\_rate} \cdot [\text{proSLS1}]$$
 (18)

## 7.3 Reaction pp5\_v1

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

Name pp5\_v1

#### **Reaction equation**

$$\emptyset \xrightarrow{LAMDAR, LAMDAR} proLAMDAR$$
 (19)

#### **Modifiers**

Table 9: Properties of each modifier.

Id	Name	SBO
LAMDAR	LAMDAR	
LAMDAR	LAMDAR	

#### **Product**

Table 10: Properties of each product.

Id	Name	SBO
proLAMDAR	proLAMDAR	

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_3 = pp5\_translation\_rate \cdot p1\_strength \cdot [LAMDAR]$$
 (20)

## **7.4 Reaction** pp5\_v2

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

Name pp5\_v2

## **Reaction equation**

$$proLAMDAR \xrightarrow{proLAMDAR} \emptyset$$
 (21)

#### Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
proLAMDAR	proLAMDAR	

#### **Modifier**

Table 12: Properties of each modifier.

Id	Name	SBO
proLAMDAR	proLAMDAR	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_4 = \text{proLAMDAR\_degradation\_rate} \cdot [\text{proLAMDAR}]$$
 (22)

#### 7.5 Reaction ia1\_bind\_forward

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

Name ial\_bind\_forward

## **Reaction equation**

#### **Reactants**

Table 13: Properties of each reactant.

Table 13. I Toperties of each reactant.		
Id	Name	SBO
IPTG	IPTG	
$ia1\_ActiveTF$	ia1_ActiveTF	

#### **Modifiers**

Table 14: Properties of each modifier.

Id	Name	SBO
IPTG	IPTG	
$ia1\_ActiveTF$	ia1_ActiveTF	

#### **Product**

Table 15: Properties of each product.

Id	Name	SBO
ia1_InactiveTF	ia1_InactiveTF	

## **Kinetic Law**

Derived unit  $mol^2 \cdot l^{-2}$ 

$$v_5 = [IPTG] \cdot [ia1\_ActiveTF]$$
 (24)

## 7.6 Reaction ial\_bind\_reverse

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

Name ia1\_bind\_reverse

## **Reaction equation**

$$ia1\_InactiveTF \xrightarrow{ia1\_InactiveTF} IPTG + ia1\_ActiveTF$$
 (25)

#### Reactant

Table 16: Properties of each reactant.

Id Name SBC		SBO
ia1_InactiveTF	ia1_InactiveTF	

## **Modifier**

Table 17: Properties of each modifier.

Id Name		SBO
ia1_InactiveTF	ia1_InactiveTF	

## **Products**

Table 18: Properties of each product.

Id	Name	SBO
IPTG	IPTG	
$ia1\_ActiveTF$	ia1_ActiveTF	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_6 = ia1 \text{ Kd} \cdot [ia1 \text{ InactiveTF}]$$
 (26)

## 7.7 Reaction pp2\_v1

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

Name  $pp2_v1$ 

## **Reaction equation**

$$\emptyset \xrightarrow{AUR1, AUR1} proAUR1$$
 (27)

## **Modifiers**

Table 19: Properties of each modifier.

Id	Name	SBO
AUR1	AUR1	
AUR1	AUR1	

#### **Product**

Table 20: Properties of each product.

Id	Name	SBO
proAUR1	proAUR1	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_7 = pp2\_translation\_rate \cdot pAUR1\_strength \cdot [AUR1]$$
 (28)

# 7.8 Reaction pp2\_v2

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

Name  $pp2_v2$ 

## **Reaction equation**

$$proAUR1 \xrightarrow{proAUR1} \emptyset$$
 (29)

#### Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
proAUR1	proAUR1	

#### **Modifier**

Table 22: Properties of each modifier.

Id	Name	SBO
proAUR1	proAUR1	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_8 = \text{proAUR1\_degradation\_rate} \cdot [\text{proAUR1}]$$
 (30)

## 7.9 Reaction pp6\_v1

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

Name pp6\_v1

#### **Reaction equation**

$$\emptyset \xrightarrow{\text{TETR, TETR}} \text{proTETR}$$
 (31)

#### **Modifiers**

Table 23: Properties of each modifier.

Id	Name	SBO
TETR	TETR	
TETR	TETR	

#### **Product**

Table 24: Properties of each product.

Id	Name	SBO
proTETR	proTETR	_

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_9 = pp6\_translation\_rate \cdot p3\_strength \cdot [TETR]$$
 (32)

# **7.10 Reaction** pp6\_v2

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

Name pp6\_v2

## **Reaction equation**

$$proTETR \xrightarrow{proTETR} \emptyset$$
 (33)

#### Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
proTETR	proTETR	

#### **Modifier**

Table 26: Properties of each modifier.

Id	Name	SBO
proTETR	proTETR	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{10} = \text{proTETR\_degradation\_rate} \cdot [\text{proTETR}]$$
 (34)

## 7.11 Reaction pp3\_v1

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

Name  $pp3_v1$ 

#### **Reaction equation**

$$\emptyset \xrightarrow{\text{SLS4, SLS4}} \text{proSLS4}$$
 (35)

#### **Modifiers**

Table 27: Properties of each modifier.

Name	SBO
SLS4 SLS4	
	SLS4

#### **Product**

Table 28: Properties of each product.

Id	Name	SBO
proSLS4	proSLS4	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{11} = pp3\_translation\_rate \cdot pSLS4\_strength \cdot [SLS4]$$
 (36)

# 7.12 Reaction pp3\_v2

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

Name  $pp3_v2$ 

## **Reaction equation**

$$proSLS4 \xrightarrow{proSLS4} \emptyset$$
 (37)

#### Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
proSLS4	proSLS4	

#### **Modifier**

Table 30: Properties of each modifier.

Id	Name	SBO
proSLS4	proSLS4	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{12} = \text{proSLS4\_degradation\_rate} \cdot [\text{proSLS4}]$$
 (38)

## 7.13 Reaction pp4\_v1

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

Name  $pp4_v1$ 

#### **Reaction equation**

$$\emptyset \xrightarrow{\text{LACI, LACI}} \text{proLACI}$$
 (39)

#### **Modifiers**

Table 31: Properties of each modifier.

Id	Name	SBO
LACI	LACI	
LACI	LACI	

#### **Product**

Table 32: Properties of each product.

Id	Name	SBO
proLACI	proLACI	

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_{13} = pp4\_translation\_rate \cdot p2\_strength \cdot [LACI]$$
 (40)

#### **7.14 Reaction** pp4\_v2

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

Name pp4\_v2

#### **Reaction equation**

$$proLACI \xrightarrow{proLACI} \emptyset$$
 (41)

#### Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
proLACI	proLACI	

#### **Modifier**

Table 34: Properties of each modifier.

Id	Name	SBO
proLACI	proLACI	

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_{14} = \text{proLACI\_degradation\_rate} \cdot [\text{proLACI}]$$
 (42)

# 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 AUR1

Name AUR1

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

Involved in rule AUR1

This species takes part in two reactions (as a modifier in pp2\_v1, pp2\_v1). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

## 8.2 Species IPTG

Name IPTG

Initial concentration  $10000 \text{ mol} \cdot l^{-1}$ 

This species takes part in three reactions (as a reactant in ial\_bind\_forward and as a product in ial\_bind\_reverse and as a modifier in ial\_bind\_forward).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IPTG} = v_6 - v_5 \tag{43}$$

## 8.3 Species LACI

Name LACI

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

Involved in rule LACI

This species takes part in two reactions (as a modifier in pp4\_v1, pp4\_v1). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

#### 8.4 Species LAMDAR

Name LAMDAR

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

Involved in rule LAMDAR

This species takes part in two reactions (as a modifier in pp5\_v1, pp5\_v1). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

#### 8.5 Species SLS1

Name SLS1

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

Involved in rule SLS1

One rule determines the species' quantity.

#### 8.6 Species SLS4

Name SLS4

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

Involved in rule SLS4

This species takes part in two reactions (as a modifier in pp3\_v1, pp3\_v1). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

## 8.7 Species TETR

Name TETR

Initial concentration  $10 \text{ mol} \cdot 1^{-1}$ 

Involved in rule TETR

This species takes part in two reactions (as a modifier in pp6\_v1, pp6\_v1). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

#### 8.8 Species as1

Name as1

Initial concentration  $10 \text{ mol} \cdot 1^{-1}$ 

Involved in rule as1

One rule determines the species' quantity.

## 8.9 Species ia1\_ActiveTF

Name ia1\_ActiveTF

Initial concentration  $100 \text{ mol} \cdot l^{-1}$ 

This species takes part in three reactions (as a reactant in ial\_bind\_forward and as a product in ial\_bind\_reverse and as a modifier in ial\_bind\_forward).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ial}\,\Delta\mathrm{ctiveTF} = v_6 - v_5 \tag{44}$$

#### 8.10 Species ia1\_InactiveTF

Name ia1\_InactiveTF

Initial concentration  $100 \text{ mol} \cdot l^{-1}$ 

This species takes part in three reactions (as a reactant in ial\_bind\_reverse and as a product in ial\_bind\_forward and as a modifier in ial\_bind\_reverse).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ial}\,\mathrm{InactiveTF} = v_5 - v_6 \tag{45}$$

## 8.11 Species ope1

Name ope1

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

Involved in rule ope1

One rule determines the species' quantity.

#### 8.12 Species p1

Name p1

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

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{p}\mathbf{1} = 0\tag{46}$$

## 8.13 Species p2

Name p2

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

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{p}2 = 0\tag{47}$$

## 8.14 Species p3

Name p3

Initial concentration  $10 \text{ mol} \cdot 1^{-1}$ 

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{p}3 = 0\tag{48}$$

## 8.15 Species pAUR1

Name pAUR1

Initial concentration  $10 \text{ mol} \cdot 1^{-1}$ 

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{pAUR1} = 0\tag{49}$$

## 8.16 Species pSLS1

Name pSLS1

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

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{pSLS1} = 0\tag{50}$$

## 8.17 Species pSLS4

Name pSLS4

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

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{pSLS4} = 0\tag{51}$$

#### 8.18 Species proAUR1

Name proAUR1

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

This species takes part in three reactions (as a reactant in pp2\_v2 and as a product in pp2\_v1 and as a modifier in pp2\_v2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{proAUR1} = v_7 - v_8 \tag{52}$$

## 8.19 Species proLACI

#### Name proLACI

#### Initial concentration $0 \text{ mol} \cdot l^{-1}$

This species takes part in three reactions (as a reactant in pp4\_v2 and as a product in pp4\_v1 and as a modifier in pp4\_v2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{proLACI} = v_{13} - v_{14} \tag{53}$$

#### 8.20 Species proLAMDAR

#### Name proLAMDAR

### Initial concentration $0 \text{ mol} \cdot l^{-1}$

This species takes part in three reactions (as a reactant in pp5\_v2 and as a product in pp5\_v1 and as a modifier in pp5\_v2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{proLAMDAR} = |v_3| - |v_4| \tag{54}$$

### 8.21 Species proSLS1

#### Name proSLS1

#### Initial concentration $0 \text{ mol} \cdot l^{-1}$

This species takes part in three reactions (as a reactant in pp1\_v2 and as a product in pp1\_v1 and as a modifier in pp1\_v2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{proSLS1} = |v_1| - |v_2| \tag{55}$$

#### 8.22 Species proSLS4

## Name proSLS4

## Initial concentration $0 \text{ mol} \cdot l^{-1}$

This species takes part in three reactions (as a reactant in pp3\_v2 and as a product in pp3\_v1 and as a modifier in pp3\_v2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{proSLS4} = v_{11} - v_{12} \tag{56}$$

## 8.23 Species proTETR

Name proTETR

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

This species takes part in three reactions (as a reactant in pp6\_v2 and as a product in pp6\_v1 and as a modifier in pp6\_v2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{proTETR} = |v_9| - |v_{10}| \tag{57}$$

#### 8.24 Species rs1

Name rs1

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

Involved in rule rs1

One rule determines the species' quantity.

## 8.25 Species rs2

Name rs2

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

Involved in rule rs2

One rule determines the species' quantity.

#### 8.26 Species rs3

Name rs3

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

Involved in rule rs3

One rule determines the species' quantity.

## 8.27 Species rs4

Name rs4

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

Involved in rule rs4

One rule determines the species' quantity.

## 8.28 Species rs5

Name rs5

Initial concentration  $10 \text{ mol} \cdot 1^{-1}$ 

Involved in rule rs5

One rule determines the species' quantity.

## 8.29 Species rs6

Name rs6

Initial concentration  $10 \text{ mol} \cdot 1^{-1}$ 

Involved in rule rs6

One rule determines the species' quantity.

## 8.30 Species ter1

Name ter1

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

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ter1} = 0\tag{58}$$

## 8.31 Species ter2

Name ter2

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

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ter}2 = 0\tag{59}$$

## 8.32 Species ter3

Name ter3

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

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ter3} = 0\tag{60}$$

## 8.33 Species ter4

Name ter4

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

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ter4} = 0\tag{61}$$

#### 8.34 Species ter5

Name ter5

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

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ter}5 = 0\tag{62}$$

## 8.35 Species ter6

Name ter6

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

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ter6} = 0\tag{63}$$

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