# **SBML Model Report**

# Model name: "Carbo2013 - Mucosal Immune Response during H.pylori Infection"



May 6, 2016

# 1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah<sup>1</sup> and Adria Carbo<sup>2</sup> at September 17<sup>th</sup> 2013 at 12:08 a.m. and last time modified at April eighth 2016 at 5:37 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	4
species types	0	species	41
events	2	constraints	0
reactions	88	function definitions	13
global parameters	109	unit definitions	3
rules	54	initial assignments	4

#### **Model Notes**

#### 2 Unit Definitions

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

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#### 2.1 Unit volume

Name volume

**Definition** ml

#### 2.2 Unit time

Name time

**Definition** 86400 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<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 Compartments

This model contains four compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
c1	Lumen	0000290	3	1	litre		
c2	Lamina Propia	0000290	3	1	litre	$   \overline{\mathbf{Z}} $	
c4	Epithelium	0000290	3	1	litre		
c3	Gastric Lymph Node	0000290	3	1	litre		

# 3.1 Compartment c1

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

Name Lumen

SBO:0000290 physical compartment

# **3.2 Compartment** c2

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

Name Lamina Propia

SBO:0000290 physical compartment

# 3.3 Compartment c4

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

Name Epithelium

SBO:0000290 physical compartment

# 3.4 Compartment c3

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

Name Gastric Lymph Node

SBO:0000290 physical compartment

# 4 Species

This model contains 41 species. The boundary condition of seven of these species is set to true so that these 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 Condi- tion
s1	HP	c1	item $\cdot$ ml <sup>-1</sup>	$\Box$	
species_7	HP Dose	c1	item $\cdot$ ml <sup>-1</sup>		
species_10	LB	c1	item $\cdot$ ml <sup>-1</sup>		
species_11	LB Dose	c1	item $\cdot$ ml <sup>-1</sup>		
species_12	nTh1	c1	item $\cdot$ ml <sup>-1</sup>		
species_13	nTh1_LP	c1	item $\cdot$ ml <sup>-1</sup>		
species_14	nTh17	c1	item $\cdot$ ml <sup>-1</sup>		
species_15	nTh17_LP	c1	item $\cdot$ ml <sup>-1</sup>		
species_16	nTreg	c1	item $\cdot$ ml <sup>-1</sup>		
species_17	nTreg_LP	c1	item $\cdot$ ml <sup>-1</sup>		
s9	eDC	c2	item $\cdot$ ml <sup>-1</sup>		
s13	Th1	c2	item $\cdot$ ml <sup>-1</sup>		
s15	iTreg	c2	item $\cdot$ ml <sup>-1</sup>		
s16	Th17	c2	item $\cdot$ ml <sup>-1</sup>		
s19	M1	c2	item $\cdot$ ml <sup>-1</sup>		
s21	M2	c2	item $\cdot$ ml <sup>-1</sup>		
s22	M0	c2	item $\cdot$ ml <sup>-1</sup>		
s25	tDC	c2	item $\cdot$ ml <sup>-1</sup>		
s17	emT	c2	item $\cdot$ ml <sup>-1</sup>		
s6	HP	c2	item $\cdot$ ml <sup>-1</sup>		
${ t species\_1}$	iDC	c2	item $\cdot$ ml <sup>-1</sup>	$\Box$	

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
species_2	TotalDC	c2	item $\cdot$ ml <sup>-1</sup>	В	
species_3	TotalM	c2	item $\cdot$ ml <sup>-1</sup>		$\overline{\mathbf{Z}}$
species_4	TotalT	c2	item $\cdot$ ml <sup>-1</sup>	$\Box$	$\overline{\mathbf{Z}}$
species_18	eDCLB	c2	item $\cdot$ ml <sup>-1</sup>		
species_19	pEC	c2	item $\cdot$ ml <sup>-1</sup>		$\Box$
s2	E	c4	item $\cdot$ ml <sup>-1</sup>		
s3	Ep	c4	item $\cdot$ ml <sup>-1</sup>		
species_5	Edead	c4	item $\cdot$ ml <sup>-1</sup>		
s4	iDC	c4	item $\cdot$ ml <sup>-1</sup>		$\Box$
s26	eDC	c3	item $\cdot$ ml <sup>-1</sup>		$\Box$
s27	tDC	c3	item $\cdot$ ml <sup>-1</sup>		
s28	nT	c3	item $\cdot$ ml <sup>-1</sup>		
s29	cmT	c3	item $\cdot$ ml <sup>-1</sup>		
s30	Th17	c3	item $\cdot$ ml <sup>-1</sup>		
s31	Th1	c3	item $\cdot$ ml <sup>-1</sup>		$\Box$
s33	iTreg	c3	item $\cdot$ ml <sup>-1</sup>		
species_6	TotalDC	c3	item $\cdot$ ml <sup>-1</sup>		$\square$
species_8	TotalT	c3	item $\cdot$ ml <sup>-1</sup>		$\overline{\mathbf{Z}}$
species_9	TotalT-s	c3	item $\cdot$ ml <sup>-1</sup>		$\overline{\mathbf{Z}}$
species_20	eDCLB	c3	item $\cdot$ ml <sup>-1</sup>		

# **5 Parameters**

This model contains 109 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
parameter_1	vHP		0.500		
parameter_2	vHP2		0.500		
parameter_3	aTreg		1.000		
parameter_4	aTh17		0.300		$\overline{\mathbf{Z}}$
parameter_5	aTh1		0.700		
$parameter_7$	kEB		$10^{-6}$		
parameter_8	@eIE		0.500		$   \overline{\mathbf{Z}} $
parameter_9	@eEI		1.000		$   \overline{\mathbf{Z}} $
$parameter_10$	atreg		$10^{-6}$		
$parameter_11$	ath1		$7 \cdot 10^{-7}$		
$parameter_12$	ath17		$3 \cdot 10^{-7}$		
$parameter_13$	@uT		0.143		
$parameter_14$	@vT		0.100		
$parameter_{-}15$	toemT		0.006		
$parameter_16$	tcmT		0.009		
$parameter_17$	pt		512.000		
parameter_18	pT		128.000		
$parameter_19$	uHP		1.000		
$parameter_20$	lHP		2.000		
$parameter\_21$	@uE		1.000		
$parameter_22$	Stim_emT_Th17		$3 \cdot 10^{-7}$		
$parameter_23$	Stim_emT_Th1		$7 \cdot 10^{-7}$		$\Box$
parameter_24	Stim_emT_iTreg		$10^{-6}$		
parameter_25	Stim_cmT_Th1		$7 \cdot 10^{-7}$		
parameter_26	Stim_cmT_Th17		$3 \cdot 10^{-7}$		
parameter_27	Stim_cmT_iTreg		$10^{-6}$		$\Box$
parameter_28	Stim_t_Th1		$7 \cdot 10^{-13}$		
parameter_29	Stim_t_Th17		$3 \cdot 10^{-13}$		
$parameter_30$	Stim_t_iTreg		$10^{-12}$		
parameter_31	Bc		1000.000		$\square$
parameter_32	uCE		$10^{-4}$		
parameter_33	@et		100.000		
parameter_34	@ut		1.000		Ø
parameter_35	@lt		$10^{8}$		$\mathbf{Z}_{\underline{a}}$
parameter_36	Bp		1.000		$\mathbf{Z}$
parameter_37	cyto_change		$10^{-6}$		$\Box$
parameter_38	uM1		$10^{-4}$		

Id	Name	SBO Value	Unit	Constant
parameter_39	Bd	1.000		
parameter_40	Br	1000.000		$\overline{Z}$
parameter_41	er	1000.000		$\overline{Z}$
parameter_42	kTD	$10^{-6}$		$\overline{Z}$
$parameter_44$	udi_LP	1.000		$   \overline{\mathbf{Z}} $
$parameter_45$	um	1.000		
$parameter_47$	k_lumen	$10^{-6}$		$\mathbf{Z}$
$parameter_48$	k_LP	$10^{-6}$		
$parameter_49$	@pt_0	512.000		$\mathbf{Z}$
$parameter_50$	$@pT_0$	128.000		
$parameter_51$	m_reg	0.010		$\mathbf{Z}$
$parameter_52$	$m_{-}HP$	0.010		
parameter_53	kGLN	$10^{-6}$		
$parameter_54$	HP_Ep_Lumen	$10^{-6}$		
$parameter_55$	iDCtoeDC_Lumen	0.313		
$parameter_56$	iDCtotDC_Lumen	$5 \cdot 10^{-7}$		
$parameter_57$	iDCtoeDC_LP	0.313		
parameter_58	iDCtotDC_LP	$5 \cdot 10^{-7}$		
parameter_59	M0toM1_LP	$5 \cdot 10^{-7}$		
$parameter\_60$	M0toM2_LP	$5 \cdot 10^{-7}$		
$parameter_61$	vm	1.000		
$parameter_62$	uMA	0.022		
parameter_63	n	2.000		<b>☑</b> ⊟
$parameter\_64$	$T_{-}$ deactivation	0.129		
$parameter_43$	iDC percentage	0.010		
parameter_65	lm	100000.000		
$parameter\_66$	ld	1000000.000		
$parameter_6$	HP Dose Response	$10^{-6}$		
$parameter_67$	iTreg NS (rel)	0.000		<b>☑</b> ⊟ ⊟
$parameter\_68$	Th1 NS (rel)	0.000		
$parameter_69$	Th17 NS (rel)	0.000		
$parameter_{-}70$	Stimulation	10.000		
$parameter_71$	iTreg S (rel)	0.000		
$parameter_72$	Th1 S (rel)	0.000		
parameter_73	Th17 S (rel)	0.000		
$parameter\_46$	@ud	0.500		
$parameter_{-}74$	vLB	0.500		
$parameter_{-}75$	vLB2	0.500		<b>☑</b> ⊟
$parameter_{-}76$	k_LB	1.000		<b>☑</b> ⊟
$parameter_77$	iDCtotDC_LB	0.500		
$parameter_78$	iDCtoeDC_LB	0.313		
$parameter_{-}79$	new_iTreg_GLN	0.000		$\Box$

Id	Name	SBO	Value	Unit	Constant
parameter_80	new_Th1_GLN		14972.236		
$parameter_81$	new_Th17_GLN		6416.673		$\Box$
parameter_82	new_emT_iTreg		0.000		
parameter_83	new_emT_Th1		214.717		
parameter_84	new_emT_Th17		92.022		$\Box$
parameter_85	er_i		10000.000		
parameter_86	et_i		10000.000		$\overline{\mathbf{Z}}$
parameter_87	K_r17		1.000		$\overline{\mathbf{Z}}$
parameter_88	$K_{-}17r$		2.500		$\overline{\mathbf{Z}}$
parameter_89	v21		2.000		$\overline{\mathbf{Z}}$
parameter_90	v12		1.000		$\overline{\mathbf{Z}}$
parameter_91	ri_I	1	000.0000		$\overline{\mathbf{Z}}$
parameter_92	ir_I	1	000.0000		$\overline{\mathbf{Z}}$
parameter_93	phi_HP		0.001		$\overline{\mathbf{Z}}$
parameter_94	uLB		0.071		$\overline{m{arphi}}$
parameter_95	ath17LB		$3 \cdot 10^{-7}$		$\overline{\mathbf{Z}}$
parameter_96	ath1LB		$7 \cdot 10^{-7}$		
parameter_97	aTh17LB		0.300		
parameter_98	aTh1LB		0.700		
parameter_99	Stim_emT- _Th17LB		$3\cdot 10^{-7}$		
parameter- _100	Stim_emT_Th1LB		$7 \cdot 10^{-7}$		
parameter- _101	Stim_cmT_Th1LB		$7 \cdot 10^{-7}$		
parameter- _102	Stim_cmT- _Th17LB		$3\cdot 10^{-7}$		
parameter-	Stim_t_Th1LB		$7\cdot 10^{-13}$		
parameter-	Stim_t_Th17LB		$3\cdot 10^{-13}$		
parameter-	vEC		0.000		
parameter-	Bc2		1.000		$\square$
parameter- _107	k_LP1		0.627		$\square$
ModelValue_3	Initial for aTh17		0.300		$\checkmark$
ModelValue-	Initial for ath17		$3 \cdot 10^{-7}$		$\mathbf{Z}$

# 6 Initialassignments

This is an overview of four initial assignments.

# 6.1 Initialassignment s1

**Derived unit** contains undeclared units

**Math** parameter\_ $6 \cdot [\text{species}\_7]$ 

# **6.2 Initialassignment** species\_10

**Derived unit** item  $\cdot$  ml<sup>-1</sup>

Math [species\_11]

# **6.3 Initialassignment ModelValue\_3**

**Derived unit** contains undeclared units

Math parameter\_4

# **6.4 Initialassignment ModelValue\_10**

**Derived unit** contains undeclared units

**Math** parameter\_12

# 7 Function definitions

This is an overview of 13 function definitions.

# **7.1 Function definition** function\_13

Name Constant flux (irreversible)

Argument v

**Mathematical Expression** 

 $\mathbf{v}$  (1)

# 7.2 Function definition function\_1

Name 1 reactant, 3 activators, KVW

**Arguments** Vf, r1, A1, n1, A2, n2, A3, n3

**Mathematical Expression** 

$$Vf \cdot r1 \cdot (n1 \cdot A1 + n2 \cdot A2 + n3 \cdot A3) \tag{2}$$

#### 7.3 Function definition function\_3

Name 1sub 1 activator 1 parameter

Arguments substrate, a1, k1

**Mathematical Expression** 

substrate 
$$\cdot$$
 a1  $\cdot$  k1 (3)

#### 7.4 Function definition function\_8

Name 1sub 2 activators 2 parameters

**Arguments** substrate, k1, a1, k2, a2

**Mathematical Expression** 

substrate 
$$\cdot (k1 \cdot a1 + k2 \cdot a2)$$
 (4)

#### 7.5 Function definition function\_10

Name Constant Flux, 3 activators

**Arguments** c, k, A, n, kA, B, kB, C, kC

**Mathematical Expression** 

$$c+k\cdot\left(\frac{A^n}{A^n+kA^n}+\frac{B^n}{B^n+kB^n}+\frac{C^n}{C^n+kC^n}\right) \tag{5}$$

#### 7.6 Function definition function\_7

Name Constant Flux, 1 activator

Arguments k, A, n, kA, c

**Mathematical Expression** 

$$c + k \cdot \frac{A^n}{A^n + kA^n} \tag{6}$$

#### 7.7 Function definition function\_2

Name 1 sub 5 activators

**Arguments** k, substrate, A, n, kA, B, kB, C, kC, D, kD, E, kE

#### **Mathematical Expression**

$$k \cdot substrate \cdot \left(\frac{A^n}{A^n + kA^n} + \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n} + \frac{D^n}{D^n + kD^n} + \frac{E^n}{E^n + kE^n}\right) \quad (7)$$

#### 7.8 Function definition function\_4

Name 1 sub 3 activators

**Arguments** k, substrate, A, n, kA, B, kB, C, kC

#### **Mathematical Expression**

$$k \cdot substrate \cdot \left( \frac{A^n}{A^n + kA^n} + \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n} \right) \tag{8}$$

#### 7.9 Function definition function\_11

Name 1 sub 2 activators

**Arguments** k, substrate, A, n, kA, B, kB

#### **Mathematical Expression**

$$k \cdot \text{substrate} \cdot \left( \frac{A^n}{A^n + kA^n} + \frac{B^n}{B^n + kB^n} \right) \tag{9}$$

#### 7.10 Function definition function\_5

Name bact repo

Arguments k, sub, c

#### **Mathematical Expression**

$$\frac{\mathbf{k} \cdot \mathbf{sub}}{\mathbf{c} + \mathbf{sub}} \tag{10}$$

#### **7.11 Function definition** function\_12

Name iDC\_Ep replenishment

Arguments V, s, k, P

#### **Mathematical Expression**

$$V \cdot (s - k \cdot P) \tag{11}$$

#### 7.12 Function definition function\_9

Name 1 sub 2 act 2 params 1 const

Arguments substrate, k, k1, a1, k2, a2

#### **Mathematical Expression**

substrate 
$$\cdot k \cdot (k1 \cdot a1 + k2 \cdot a2)$$
 (12)

#### 7.13 Function definition function\_6

Name 1 sub 3 activators 3 parameters

**Arguments** substrate, k1, a1, k2, a2, k3, a3

#### **Mathematical Expression**

substrate 
$$\cdot$$
 (k1  $\cdot$  a1 + k2  $\cdot$  a2 + k3  $\cdot$  a3) (13)

# 8 Rules

This is an overview of 54 rules.

#### 8.1 Rule parameter\_2

Rule parameter\_2 is an assignment rule for parameter parameter\_2:

$$parameter_2 = 1 - parameter_1$$
 (14)

# 8.2 Rule parameter\_5

Rule parameter\_5 is an assignment rule for parameter parameter\_5:

$$parameter\_5 = 1 - ModelValue\_3$$
 (15)

# **8.3 Rule** parameter\_11

Rule parameter\_11 is an assignment rule for parameter parameter\_11:

$$parameter_11 = 1.0E - 6 - ModelValue_10$$
 (16)

# 8.4 Rule parameter\_16

Rule parameter\_16 is an assignment rule for parameter parameter\_16:

$$parameter_{16} = parameter_{13} \cdot parameter_{14} \cdot 0.6 \tag{17}$$

#### 8.5 Rule parameter\_15

Rule parameter\_15 is an assignment rule for parameter parameter\_15:

$$parameter_{15} = parameter_{13} \cdot 0.4 \cdot parameter_{14}$$
 (18)

# 8.6 Rule species\_2

Rule species\_2 is an assignment rule for species species\_2:

$$species_2 = [s9] + [species_1] + [s25] + [s4]$$
 (19)

**Derived unit** item  $\cdot$  ml<sup>-1</sup>

# 8.7 Rule species\_3

Rule species\_3 is an assignment rule for species species\_3:

$$species_3 = [s22] + [s19] + [s21]$$
 (20)

**Derived unit** item  $\cdot$  ml<sup>-1</sup>

# 8.8 Rule species\_4

Rule species\_4 is an assignment rule for species species\_4:

$$species_4 = [s13] + [s16] + [s15] + [s17]$$
(21)

**Derived unit** item  $\cdot$  ml<sup>-1</sup>

# 8.9 Rule species\_6

Rule species\_6 is an assignment rule for species species\_6:

$$species_6 = [s26] + [s27]$$
 (22)

**Derived unit** item  $\cdot$  ml<sup>-1</sup>

# 8.10 Rule species\_8

Rule species\_8 is an assignment rule for species species\_8:

$$species_8 = [s31] + [s30] + [s33] + [s29] + [s28]$$
 (23)

**Derived unit** item  $\cdot$  ml<sup>-1</sup>

#### 8.11 Rule species\_9

Rule species\_9 is an assignment rule for species species\_9:

species\_9 = 
$$0.01 \cdot \left( [s31] + [s30] + [s33] + \frac{[s28] + [s29]}{parameter_70} \right)$$
 (24)

#### **8.12 Rule** parameter\_17

Rule parameter\_17 is an assignment rule for parameter parameter\_17:

$$parameter_17 = parameter_49 \cdot \frac{1}{1 + parameter_51 \cdot [s33]}$$
 (25)

# 8.13 Rule parameter\_18

Rule parameter\_18 is an assignment rule for parameter parameter\_18:

$$parameter_18 = parameter_50 \cdot \frac{1}{1 + parameter_51 \cdot [s15] + parameter_52 \cdot [s6]}$$
 (26)

#### **8.14 Rule** parameter\_22

Rule parameter\_22 is an assignment rule for parameter parameter\_22:

$$parameter_22 = parameter_4 \cdot parameter_48$$
 (27)

#### 8.15 Rule parameter\_23

Rule parameter\_23 is an assignment rule for parameter parameter\_23:

$$parameter_23 = parameter_48 \cdot parameter_5$$
 (28)

#### 8.16 Rule parameter\_24

Rule parameter\_24 is an assignment rule for parameter parameter\_24:

$$parameter_24 = parameter_3 \cdot parameter_48 \tag{29}$$

#### 8.17 Rule parameter\_25

Rule parameter\_25 is an assignment rule for parameter parameter\_25:

$$parameter_25 = parameter_5 \cdot parameter_53$$
 (30)

#### **8.18 Rule** parameter\_26

Rule parameter\_26 is an assignment rule for parameter parameter\_26:

$$parameter_26 = parameter_4 \cdot parameter_53 \tag{31}$$

#### **8.19 Rule** parameter\_27

Rule parameter\_27 is an assignment rule for parameter parameter\_27:

$$parameter_27 = parameter_3 \cdot parameter_53$$
 (32)

#### 8.20 Rule parameter\_28

Rule parameter\_28 is an assignment rule for parameter parameter\_28:

$$parameter_28 = parameter_11 \cdot parameter_53 \tag{33}$$

#### 8.21 Rule parameter\_29

Rule parameter\_29 is an assignment rule for parameter parameter\_29:

$$parameter_29 = parameter_12 \cdot parameter_53 \tag{34}$$

#### 8.22 Rule parameter\_30

Rule parameter\_30 is an assignment rule for parameter parameter\_30:

$$parameter_30 = parameter_10 \cdot parameter_53 \tag{35}$$

#### **8.23 Rule** parameter\_37

Rule parameter\_37 is an assignment rule for parameter parameter\_37:

$$parameter_37 = parameter_7 \cdot parameter_36$$
 (36)

#### **8.24 Rule** parameter\_54

Rule parameter\_54 is an assignment rule for parameter parameter\_54:

$$parameter_54 = parameter_7 \cdot parameter_39 \tag{37}$$

#### **8.25 Rule** parameter\_55

Rule parameter\_55 is an assignment rule for parameter parameter\_55:

$$parameter_{.}55 = parameter_{.}1 \cdot parameter_{.}107 \tag{38}$$

#### **8.26 Rule** parameter\_56

Rule parameter\_56 is an assignment rule for parameter parameter\_56:

$$parameter_{56} = parameter_{2} \cdot parameter_{47}$$
 (39)

#### **8.27 Rule** parameter\_57

Rule parameter\_57 is an assignment rule for parameter parameter\_57:

$$parameter_57 = parameter_1 \cdot parameter_107 \tag{40}$$

#### 8.28 Rule parameter\_58

Rule parameter\_58 is an assignment rule for parameter parameter\_58:

$$parameter_58 = parameter_2 \cdot parameter_48$$
 (41)

#### 8.29 Rule parameter\_59

Rule parameter\_59 is an assignment rule for parameter parameter\_59:

$$parameter_{-}59 = parameter_{-}1 \cdot parameter_{-}48 \tag{42}$$

#### 8.30 Rule parameter\_60

Rule parameter\_60 is an assignment rule for parameter parameter\_60:

$$parameter_60 = parameter_2 \cdot parameter_48$$
 (43)

#### 8.31 Rule parameter\_79

Rule parameter\_79 is an assignment rule for parameter parameter\_79:

$$parameter_{79} = parameter_{17} \cdot (parameter_{27} \cdot [s29] + parameter_{30} \cdot [s28]) \cdot [s27] \quad (44)$$

#### 8.32 Rule parameter\_64

Rule parameter\_64 is an assignment rule for parameter parameter\_64:

$$parameter_{64} = (1 - parameter_{14}) \cdot parameter_{13}$$
 (45)

#### **8.33 Rule** parameter\_67

Rule parameter\_67 is an assignment rule for parameter parameter\_67:

$$parameter\_67 = \frac{[s33]}{[species\_8]}$$
 (46)

**Derived unit** dimensionless

# **8.34 Rule** parameter\_68

Rule parameter\_68 is an assignment rule for parameter parameter\_68:

$$parameter\_68 = \frac{[s31]}{[species\_8]}$$
 (47)

**Derived unit** dimensionless

# 8.35 Rule parameter\_69

Rule parameter\_69 is an assignment rule for parameter parameter\_69:

$$parameter\_69 = \frac{[s30]}{[species\_8]}$$
 (48)

#### **Derived unit** dimensionless

#### 8.36 Rule parameter\_71

Rule parameter\_71 is an assignment rule for parameter parameter\_71:

$$parameter_{-}71 = \frac{[s33]}{[species_{-}9]}$$
 (49)

#### **Derived unit** dimensionless

#### **8.37 Rule** parameter\_72

Rule parameter\_72 is an assignment rule for parameter parameter\_72:

$$parameter_{72} = \frac{[s31]}{[species_{9}]}$$
 (50)

#### **Derived unit** dimensionless

# 8.38 Rule parameter\_73

Rule parameter\_73 is an assignment rule for parameter parameter\_73:

$$parameter\_73 = \frac{[s30]}{[species\_9]}$$
 (51)

#### **Derived unit** dimensionless

#### **8.39 Rule** parameter\_75

Rule parameter\_75 is an assignment rule for parameter parameter\_75:

$$parameter_{75} = 1 - parameter_{74}$$
 (52)

# 8.40 Rule parameter\_77

Rule parameter\_77 is an assignment rule for parameter parameter\_77:

$$parameter_{77} = parameter_{75} \cdot parameter_{76}$$
 (53)

#### **8.41 Rule** parameter\_78

Rule parameter\_78 is an assignment rule for parameter parameter\_78:

$$parameter_{78} = parameter_{74} \cdot parameter_{107}$$
 (54)

#### **8.42 Rule** parameter\_82

Rule parameter\_82 is an assignment rule for parameter parameter\_82:

$$parameter_82 = parameter_18 \cdot parameter_24 \cdot ([s25] + [s21]) \cdot [s17]$$
 (55)

#### **8.43 Rule** parameter\_96

Rule parameter\_96 is an assignment rule for parameter parameter\_96:

$$parameter_{-}96 = 1.0E - 6 - parameter_{-}95$$
 (56)

#### **8.44 Rule** parameter\_98

Rule parameter\_98 is an assignment rule for parameter parameter\_98:

$$parameter\_98 = 1 - parameter\_97 \tag{57}$$

#### **8.45 Rule** parameter\_100

Rule parameter\_100 is an assignment rule for parameter parameter\_100:

$$parameter_100 = parameter_48 \cdot parameter_98$$
 (58)

#### **8.46 Rule** parameter\_83

Rule parameter\_83 is an assignment rule for parameter parameter\_83:

$$parameter\_83 = parameter\_18$$

$$\cdot (parameter\_23 \cdot ([s19] + [s9]) \cdot [s17] + [s17] \cdot [species\_18] \cdot parameter\_100)$$
(59)

#### 8.47 Rule parameter\_99

Rule parameter\_99 is an assignment rule for parameter parameter\_99:

$$parameter_{99} = parameter_{48} \cdot parameter_{97}$$
 (60)

#### 8.48 Rule parameter\_84

Rule parameter\_84 is an assignment rule for parameter parameter\_84:

$$parameter\_84 = parameter\_18 \\ \cdot (parameter\_22 \cdot ([s19] + [s9]) \cdot [s17] + [s17] \cdot [species\_18] \cdot parameter\_99)$$
(61)

# 8.49 Rule parameter\_101

Rule parameter\_101 is an assignment rule for parameter parameter\_101:

$$parameter_101 = parameter_53 \cdot parameter_98 \tag{62}$$

#### **8.50 Rule** parameter\_102

Rule parameter\_102 is an assignment rule for parameter parameter\_102:

$$parameter_102 = parameter_53 \cdot parameter_97 \tag{63}$$

#### **8.51 Rule** parameter\_103

Rule parameter\_103 is an assignment rule for parameter parameter\_103:

$$parameter_103 = parameter_53 \cdot parameter_96 \tag{64}$$

#### 8.52 Rule parameter\_80

Rule parameter\_80 is an assignment rule for parameter parameter\_80:

parameter\_80 = parameter\_17 
$$\cdot$$
 ((parameter\_25  $\cdot$  [s29] + parameter\_28  $\cdot$  [s28])  $\cdot$  [s26]  
+ ([s29]  $\cdot$  parameter\_101 + [s28]  $\cdot$  parameter\_103)  $\cdot$  [species\_20])

# 8.53 Rule parameter\_104

Rule parameter\_104 is an assignment rule for parameter parameter\_104:

$$parameter_104 = parameter_95 \cdot parameter_53$$
 (66)

#### 8.54 Rule parameter\_81

Rule parameter\_81 is an assignment rule for parameter parameter\_81:

$$\begin{aligned} parameter\_81 &= parameter\_17 \cdot ((parameter\_26 \cdot [s29] + parameter\_29 \cdot [s28]) \cdot [s26] \\ &+ [species\_20] \cdot ([s29] \cdot parameter\_102 + [s28] \cdot parameter\_104)) \end{aligned} \tag{67}$$

# 9 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.

# **9.1 Event** event\_1

Name 2nd Dose

Trigger condition  $time \geq 2 \tag{68}$ 

**Assignments** 

$$s1 = [s1] + [species_7] \cdot parameter_6$$
 (69)

 $species_10 = [species_10] + [species_11]$  (70)

# **9.2 Event** event\_2

Name 3rd Dose

Trigger condition  $time \geq 4 \tag{71}$ 

**Assignments** 

$$s1 = [s1] + [species\_7] \cdot parameter\_6$$
 (72)

 $species_10 = [species_10] + [species_11]$  (73)

# 10 Reactions

This model contains 88 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

$N_{\bar{0}}$	Id	Name	Reaction Equation SBO
1	re2	re055	$s2 \xrightarrow{s1, s2, s1} s3$
2	re3	re066	$s1 \xrightarrow{\text{species}\_5, s1, species}\_5 s6$
3	re4	re059	$s3 \xrightarrow{s13, s16, s19, s3, s13, s16, s19} species_5$
4	re6	re105	$species_1 + s6 \xrightarrow{species_1, s6} s9$
5	re11	re074	$s17 \xrightarrow{s21, s25, s17, s21, s25} s15$
6	re13	re063	$s4 + s1 \xrightarrow{s4, s1} s9$
7	re15	re058	$s2 \xrightarrow{s13, s16, s19, s2, s13, s16, s19} species_5$
8	re16	re070	$s22 \xrightarrow{s19, s9, s13, s16, s3, s22, s19, s9, s13, s16, s3} s19$
9	re17	re073	$s22 \xrightarrow{s21, s15, s25, s22, s21, s15, s25} s21$
10	re18	re072	$s21 \xrightarrow{s13, s19, s9, s16, s3, s21, s13, s19, s9, s16, s3} s19$
11	re20	re077	$species_1 + s6 \xrightarrow{species_1, s6} s25$
12	re21	re078	$s9 \xrightarrow{s9} s26$
13	re22	re079	$s25 \xrightarrow{s25} s27$
14	re23	re080	$s28 \xrightarrow{s26, \text{ species}\_20, s28, s26, \text{ species}\_20} s30$
15	re24	re081	$s28 \xrightarrow{s26, s28, s26} s31$
16	re27	re082	$s28 \xrightarrow{s27, s28, s27} s33$

22	N₀	Id	Name	Reaction Equation	SBO
	17	re28	re083	s29 <u>\$26</u> , species_20, s29, s26, species_20 \$30	
	18	re29	re084	$s29 \xrightarrow{s26, \text{ species}\_20, s29, s26, \text{ species}\_20} s31$	
	19	re31	re085	$s29 \xrightarrow{s27, s29, s27} s33$	
	20	re32	re087	$s30 \xrightarrow{s30} s16$	
	21	re33	re088	$s31 \xrightarrow{s31} s13$	
	22	re35	re089	$s33 \xrightarrow{s33} s15$	
	23	re41	re091	$s33 \xrightarrow{s31, s26, s30, s33, s31, s26, s30} s30$	
Produced by SBML2LATEX	24	re42	re093	s15 s16, s9, s19, s13, s3, s15, s16, s9, s19, s13, s3	s16
ıced	25	re43	re095	$s16 \xrightarrow{s16} s17$	
by	26	re44	re096	$s13 \xrightarrow{s13} s17$	
<u>\$</u>	27	re45	re097	$s15 \xrightarrow{s15} s17$	
	28	re46	re098	$s16 \xrightarrow{s16} s29$	
\ <u>\</u>	29	re47	re099	$s13 \xrightarrow{s13} s29$	
	30	re49	re100	$s15 \xrightarrow{s15} s29$	
	31	${\tt reaction\_1}$	re060	$s3 \xrightarrow{s3} s2$	
	32	${\tt reaction\_2}$	re057	species_5 $\xrightarrow{\text{species}\_5}$ s2	
	33	$reaction_3$	re102	$s6 \xrightarrow{s6} 2 s6$	
	34	${\tt reaction\_4}$	re101	$s6 \xrightarrow{s6} \emptyset$	
	35	${\tt reaction\_5}$	re052	$s1 \xrightarrow{s1} 2 s1$	
	36	${\tt reaction\_6}$	re065	$s1 \xrightarrow{s1} \emptyset$	

No	Id	Name	Reaction Equation	SBO
37	reaction_10	re103	$s17 \xrightarrow{s19, s9, species_18, s17, s19, s9, species_18} s13$	
38	reaction_11	re104	$s17 \xrightarrow{s19, s9, species\_18, s17, s19, s9, species\_18} s16$	
39	${\tt reaction\_12}$	re119	$s16 \xrightarrow{s16} \emptyset$	
40	$reaction_13$	re106	$\emptyset \xrightarrow{s26, s26} s28$	
41	${\tt reaction\_14}$	re107	$s28 \xrightarrow{s28} \emptyset$	
42	${\tt reaction\_16}$	re061	$s1 \xrightarrow{s3, s1, s3} s6$	
43	${\tt reaction\_17}$	re062	$s4 + s1 \xrightarrow{s4, s1} s25$	
44	${\tt reaction\_19}$	re067	$s6 \xrightarrow{s3, s19, s6, s3, s19} \emptyset$	
45	${\tt reaction\_20}$	re053	$s1 \xrightarrow{s3, s1, s3} \emptyset$	
46	${\tt reaction\_24}$	re068	$\emptyset \xrightarrow{s3, s19, s9, s3, s19, s9} \text{species}_1$	
47	reaction_27	re069	$\emptyset \xrightarrow{s19, s3, s9, s19, s3, s9} s22$	
48	reaction_31	re111	$species_{-1} \xrightarrow{species_{-1}} \emptyset$	
49	$reaction_32$	re112	$s22 \xrightarrow{s22} \emptyset$	
50	$reaction_37$	re117	$s19 \xrightarrow{s19} \emptyset$	
51	reaction_38	re118	$s21 \xrightarrow{s21} \emptyset$	
52	reaction_39	re120	$s13 \xrightarrow{s13} \emptyset$	
53	${\tt reaction\_40}$	re121	$s15 \xrightarrow{s15} \emptyset$	
54	${\tt reaction\_7}$	re071	$s19 = \frac{s15, s21, s25, s19, s15, s21, s25}{15, s25, s21, s25} s21$	
55	reaction_8	re094	$s16 \xrightarrow{s15, s25, s21, s16, s15, s25, s21} s15$	
56	reaction_9	re092	$s30 \xrightarrow{s33, s27, s30, s33, s27} s33$	

Nº	Id	Name	Reaction Equation	SBO
57	reaction_15	re122	$s22 + s6 \xrightarrow{s22, s6} s19$	
58	reaction_18	re123	$s22 + s6 \xrightarrow{s22, s6} s21$	
59	reaction_21	re116	$s26 \xrightarrow{s26} \emptyset$	
60	reaction_22	re124	$s27 \xrightarrow{s27} \emptyset$	
61	reaction_23	re127	species_1, $s4$ s4	
62	reaction_25	re128	$s4 \xrightarrow{\text{species}\_10, s4, species}\_10 $	
63	reaction_26	re129	$s4 \xrightarrow{\text{species}\_10, s4, species}\_10 $	
64	reaction_28	re130	$species_10 \xrightarrow{species_10} \emptyset$	
65	reaction_29	re131	$0 \longrightarrow s15$	
66	reaction_30	re132	$\emptyset \longrightarrow s13$	
67	reaction_33	re133	$\emptyset \longrightarrow s16$	
68	reaction_34	re134	$\emptyset \longrightarrow s33$	
69	reaction_35	re135	$\emptyset \longrightarrow s31$	
70	reaction_36	re136	$\emptyset \longrightarrow s30$	
71	reaction_41	re137	species_ $18 \xrightarrow{\text{species}\_18} \text{species}\_20$	
72	reaction_42	re138	species_20 $\xrightarrow{\text{species}\_20} \emptyset$	
73	reaction_43	re139	$s2 \xrightarrow{s13, s16, s9, s19, s3, s2, s13, s16, s9, s19, s3} s3$	
74	reaction_44	re140	species_20 $\xrightarrow{\text{species}\_20} \emptyset$	
75	reaction_45	nTh1 creation	$s28 \xrightarrow{s28} species_12$	
76	reaction_46	nTh1 trans	$species_{12} \xrightarrow{species_{12}} species_{13}$	
77	reaction_47	nTh1_LP deg	species_13 $\xrightarrow{\text{species}\_13} \emptyset$	
78	reaction_48	nTh1_LP expansion	$species_{-13} \xrightarrow{species_{-13}} 2 species_{-13}$	

N⁰	Id	Name	Reaction Equation	SBO
79	reaction_49	nTh1 deg	species_12 $\xrightarrow{\text{species}\_12} \emptyset$	
80	reaction_50	nTh17 creation	$s28 \xrightarrow{s28} species_14$	
81	reaction_51	nTh17 trans	$species_{-14} \xrightarrow{species_{-14}} species_{-15}$	
82	reaction_52	nTh17_LP deg	species_15 $\xrightarrow{\text{species}\_15} \emptyset$	
83	reaction_53	nTh17 deg	species_14 $\xrightarrow{\text{species}\_14} \emptyset$	
84	reaction_54	nTreg creation	$s28 \xrightarrow{s28} species_16$	
85	reaction_55	nTreg trans	$species_{-16} \xrightarrow{species_{-16}} species_{-17}$	
86	reaction_56	nTreg_LP deg	species_17 $\xrightarrow{\text{species}\_17} \emptyset$	
87	reaction_57	nTreg deg	species_ $16 \xrightarrow{\text{species}\_16} \emptyset$	
88	reaction_58	Th17 to Treg	$species_15 \xrightarrow{species_15} species_17$	

# 10.1 Reaction re2

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

Name re055

# **Reaction equation**

$$s2 \xrightarrow{s1, s2, s1} s3$$
 (74)

#### Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
s2	Е	

#### **Modifiers**

Table 7: Properties of each modifier.

Id	Name	SBO
s1	HP	
s2	E	
s1	HP	

# **Product**

Table 8: Properties of each product.

	_	
Id	Name	SBO
s3	Ep	

#### **Kinetic Law**

$$v_1 = \text{vol}(c4) \cdot \text{function}_3([s2], [s1], \text{parameter}_7)$$
 (75)

function\_3 (substrate, 
$$a1, k1$$
) = substrate  $\cdot a1 \cdot k1$  (76)

function\_3 (substrate, 
$$a1, k1$$
) = substrate  $\cdot a1 \cdot k1$  (77)

# 10.2 Reaction re3

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

Name re066

# **Reaction equation**

$$s1 \xrightarrow{\text{species}\_5, s1, species}\_5 s6$$
 (78)

#### Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
s1	HP	

#### **Modifiers**

Table 10: Properties of each modifier.

Id	Name	SBO
species_5	Edead HP	
species_5	Edead	

#### **Product**

Table 11: Properties of each product.

Id	Name	SBO
s6	HP	

#### **Kinetic Law**

$$v_2 = \text{function}_3([s1], [\text{species}_5], \text{parameter}_7)$$
 (79)

function\_3 (substrate, 
$$a1, k1$$
) = substrate  $\cdot a1 \cdot k1$  (80)

# 10.3 Reaction re4

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

Name re059

# **Reaction equation**

$$s3 \xrightarrow{s13, s16, s19, s3, s13, s16, s19} species_5$$
 (81)

#### Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
s3	Ep	

#### **Modifiers**

Table 13: Properties of each modifier.

Id	Name	SBO
s13	Th1	
s16	Th17	
s19	M1	
s3	Ep	
s13	Th1	
s16	Th17	
s19	M1	

#### **Product**

Table 14: Properties of each product.

Id	Name	SBO
species_5	Edead	

#### **Kinetic Law**

$$v_3 = \text{vol}(c4) \cdot \text{function\_1} \text{ (parameter\_48, [s3], [s13], parameter\_32, [s16], parameter\_32, [s19], parameter\_38)}$$
 (82)

function\_1 
$$(Vf, r1, A1, n1, A2, n2, A3, n3) = Vf \cdot r1 \cdot (n1 \cdot A1 + n2 \cdot A2 + n3 \cdot A3)$$
 (83)

#### 10.4 Reaction re6

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

Name re105

# **Reaction equation**

species\_1 + s6 
$$\xrightarrow{\text{species}\_1, \text{ s6}}$$
 s9 (85)

#### **Reactants**

Table 15: Properties of each reactant.

Id	Name	SBO
species_1 s6	iDC HP	

#### **Modifiers**

Table 16: Properties of each modifier.

Id	Name	SBO
species_1 s6	iDC HP	

#### **Product**

Table 17: Properties of each product.

Id	Name	SBO
<b>s</b> 9	eDC	

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_4 = \text{vol}(c2) \cdot \text{parameter\_57} \cdot [\text{species\_1}] \cdot [\text{s6}]$$
 (86)

#### 10.5 Reaction re11

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

Name re074

#### **Reaction equation**

$$s17 \xrightarrow{s21, s25, s17, s21, s25} s15$$
 (87)

#### Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
s17	emT	

#### **Modifiers**

Table 19: Properties of each modifier.

Id	Name	SBO
s21	M2	
s25	tDC	
s17	emT	
s21	M2	
s25	tDC	

#### **Product**

Table 20: Properties of each product.

Id	Name	SBO
s15	iTreg	

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_5 = \text{vol}(c2) \cdot \text{function}_{-8}([s17], \text{parameter}_{-24}, [s21], \text{parameter}_{-24}, [s25])$$
 (88)

$$function_{-8}(substrate, k1, a1, k2, a2) = substrate \cdot (k1 \cdot a1 + k2 \cdot a2)$$
(89)

function\_8 (substrate, 
$$k1$$
,  $a1$ ,  $k2$ ,  $a2$ ) = substrate  $\cdot$  ( $k1 \cdot a1 + k2 \cdot a2$ ) (90)

#### 10.6 Reaction re13

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

Name re063

#### **Reaction equation**

$$s4 + s1 \xrightarrow{s4, s1} s9 \tag{91}$$

#### **Reactants**

Table 21: Properties of each reactant.

Id	Name	SBO
s4	iDC	
s1	HP	

#### **Modifiers**

Table 22: Properties of each modifier.

Id	Name	SBO
s4	iDC	
s1	HP	

# **Product**

Table 23: Properties of each product.

Id	Name	SBO
<b>s</b> 9	eDC	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_6 = \text{parameter\_55} \cdot [\text{s4}] \cdot [\text{s1}] \tag{92}$$

#### 10.7 Reaction re15

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

Name re058

# **Reaction equation**

$$s2 \xrightarrow{s13, s16, s19, s2, s13, s16, s19} species_5$$
 (93)

#### Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
s2	Е	

#### **Modifiers**

Table 25: Properties of each modifier.

Id	Name	SBO
s13	Th1	
s16	Th17	
s19	M1	
s2	E	
s13	Th1	
s16	Th17	
s19	M1	

32

#### **Product**

Table 26: Properties of each product.

Id	Name	SBO
species_5	Edead	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_7 = \text{vol}(c4) \cdot \text{function}_1 \text{ (parameter}_48, [s2], [s13], \text{parameter}_32, [s16], \text{parameter}_32, [s19], \text{parameter}_38)$$
 (94)

# 10.8 Reaction re16

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

Name re070

#### **Reaction equation**

$$s22 \xrightarrow{s19, s9, s13, s16, s3, s22, s19, s9, s13, s16, s3} s19$$
 (97)

#### Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
s22	M0	

#### **Modifiers**

Table 28: Properties of each modifier.

Id	Name	SBO
s19	M1	
s9	eDC	
s13	Th1	
s16	Th17	
s3	Ep	
s22	M0	
s19	M1	
s9	eDC	
s13	Th1	
s16	Th17	
s3	Ep	

#### **Product**

Table 29: Properties of each product.

Id	Name	SBO
s19	M1	

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_8 = \text{vol}(c2) \cdot \text{function}\_2 \text{ (parameter}\_61, [s22], [s19], \text{parameter}\_63, \text{parameter}\_91, [s9], parameter}\_91, [s13], \text{parameter}\_91, [s16], \text{parameter}\_91, [s3], \text{parameter}\_106)$$

$$\begin{aligned} &\text{function\_2}\left(k, \text{substrate}, A, n, kA, B, kB, C, kC, D, kD, E, kE\right) \\ &= k \cdot \text{substrate} \cdot \left(\frac{A^n}{A^n + kA^n} + \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n} + \frac{D^n}{D^n + kD^n} + \frac{E^n}{E^n + kE^n}\right) \end{aligned} \tag{99}$$

$$\begin{aligned} &\text{function\_2}\left(k, substrate, A, n, kA, B, kB, C, kC, D, kD, E, kE\right) \\ &= k \cdot substrate \cdot \left(\frac{A^n}{A^n + kA^n} + \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n} + \frac{D^n}{D^n + kD^n} + \frac{E^n}{E^n + kE^n}\right) \end{aligned} \tag{100}$$

#### 10.9 Reaction re17

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

Name re073

# **Reaction equation**

$$s22 \xrightarrow{s21, s15, s25, s22, s21, s15, s25} s21 \tag{101}$$

#### Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
s22	M0	

#### **Modifiers**

Table 31: Properties of each modifier.

Id	Name	SBO
s21	M2	
s15	iTreg	
s25	tDC	
s22	M0	
s21	M2	
s15	iTreg	
s25	tDC	

#### **Product**

Table 32: Properties of each product.

Id	Name	SBO
s21	M2	

#### **Kinetic Law**

$$v_9 = vol\left(c2\right) \cdot function\_4\left(parameter\_61, [s22], [s21], parameter\_63, parameter\_92, [s15], \right. \\ \left. (102) \right. \\ \left. parameter\_92, [s25], parameter\_92\right)$$

$$\begin{aligned} \text{function\_4}\left(k, \text{substrate}, A, n, kA, B, kB, C, kC\right) &= k \cdot \text{substrate} \cdot \left(\frac{A^n}{A^n + kA^n}\right. \\ &+ \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n}\right) \end{aligned} \tag{103}$$

$$\begin{split} \text{function\_4} \left(k, \text{substrate}, A, n, kA, B, kB, C, kC\right) &= k \cdot \text{substrate} \cdot \left(\frac{A^n}{A^n + kA^n} \right. \\ &+ \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n}\right) \end{split} \tag{104}$$

#### 10.10 Reaction re18

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

Name re072

#### **Reaction equation**

$$s21 \xrightarrow{s13, s19, s9, s16, s3, s21, s13, s19, s9, s16, s3} s19$$
 (105)

#### Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
s21	M2	

#### **Modifiers**

Table 34: Properties of each modifier.

Id	Name	SBO
s13	Th1	
s19	M1	
s9	eDC	
s16	Th17	
s3	Ep	
s21	M2	
s13	Th1	
s19	M1	

Id	Name	SBO
s9	eDC	
s16	Th17	
s3	Ep	

#### **Product**

Table 35: Properties of each product.

Id	Name	SBO
s19	M1	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{10} = vol\left(c2\right) \cdot function\_2\left(parameter\_89, [s21], [s13], parameter\_63, parameter\_91, [s19], parameter\_91, [s9], parameter\_91, [s16], parameter\_91, [s3], parameter\_31\right) \tag{106}$$

$$\begin{aligned} &\text{function\_2}\left(k, \text{substrate}, A, n, kA, B, kB, C, kC, D, kD, E, kE\right) \\ &= k \cdot \text{substrate} \cdot \left(\frac{A^n}{A^n + kA^n} + \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n} + \frac{D^n}{D^n + kD^n} + \frac{E^n}{E^n + kE^n}\right) \end{aligned} \tag{107}$$

$$\begin{aligned} &\text{function\_2}\left(k, substrate, A, n, kA, B, kB, C, kC, D, kD, E, kE\right) \\ &= k \cdot substrate \cdot \left(\frac{A^n}{A^n + kA^n} + \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n} + \frac{D^n}{D^n + kD^n} + \frac{E^n}{E^n + kE^n}\right) \end{aligned} \tag{108}$$

#### **10.11 Reaction** re20

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

Name re077

## **Reaction equation**

species\_1 + s6 
$$\xrightarrow{\text{species}\_1, \text{ s6}}$$
 s25 (109)

Table 36: Properties of each reactant.

Id	Name	SBO
species_1 s6	iDC HP	

Table 37: Properties of each modifier.

Id	Name	SBO
species_1	iDC	
s6	HP	

#### **Product**

Table 38: Properties of each product.

Id	Name	SBO
s25	tDC	

# **Kinetic Law**

Derived unit contains undeclared units

$$v_{11} = \text{vol}(c2) \cdot \text{parameter} \cdot 58 \cdot [\text{species} \cdot 1] \cdot [\text{s6}]$$
 (110)

## **10.12 Reaction** re21

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

Name re078

# **Reaction equation**

$$s9 \xrightarrow{s9} s26 \tag{111}$$

Table 39: Properties of each reactant.

Id	Name	SBO
s9	eDC	

Table 40: Properties of each modifier.

Id	Name	SBO
<b>s</b> 9	eDC	

## **Product**

Table 41: Properties of each product.

Id	Name	SBO
s26	eDC	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{12} = \text{parameter}_{9} \cdot [\text{s9}] \tag{112}$$

## **10.13 Reaction** re22

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

Name re079

# **Reaction equation**

$$s25 \xrightarrow{s25} s27 \tag{113}$$

Table 42: Properties of each reactant.

Id	Name	SBO
s25	tDC	

Table 43: Properties of each modifier.

Id	Name	SBO
s25	tDC	

# **Product**

Table 44: Properties of each product.

Id	Name	SBO
s27	tDC	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{13} = parameter\_9 \cdot [s25] \tag{114}$$

# 10.14 Reaction re23

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

Name re080

# **Reaction equation**

$$s28 \xrightarrow{s26, \text{ species}\_20, s28, s26, \text{ species}\_20} s30$$
 (115)

#### Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
s28	nT	

Table 46: Properties of each modifier.

Id	Name	SBO
s26	eDC	
species_20	eDCLB	
s28	nT	
s26	eDC	
species_20	eDCLB	

#### **Product**

Table 47: Properties of each product.

Id	Name	SBO
s30	Th17	

#### **Kinetic Law**

## **Derived unit** contains undeclared units

$$v_{14} = \text{vol}(c3) \cdot \text{function\_8}([s28], \text{parameter\_29}, [s26], \text{parameter\_104}, [\text{species\_20}])$$
 (116)

function\_8 (substrate, 
$$k1, a1, k2, a2$$
) = substrate  $\cdot (k1 \cdot a1 + k2 \cdot a2)$  (117)

function\_8 (substrate, 
$$k1$$
,  $a1$ ,  $k2$ ,  $a2$ ) = substrate  $\cdot (k1 \cdot a1 + k2 \cdot a2)$  (118)

# **10.15 Reaction** re24

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

Name re081

# **Reaction equation**

$$s28 \xrightarrow{s26, s28, s26} s31$$
 (119)

Table 48: Properties of each reactant.

Id	Name	SBO
s28	nT	

Table 49: Properties of each modifier.

Id	Name	SBO
s26	eDC	
s28	nT	
s26	eDC	

#### **Product**

Table 50: Properties of each product.

Id	Name	SBO
s31	Th1	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{15} = \text{vol}(c3) \cdot \text{function}_{-8}([s28], \text{parameter}_{-28}, [s26], \text{parameter}_{-103}, [s26])$$
 (120)

function\_8 (substrate, 
$$k1$$
,  $a1$ ,  $k2$ ,  $a2$ ) = substrate  $\cdot$  ( $k1 \cdot a1 + k2 \cdot a2$ ) (121)

function\_8 (substrate, 
$$k1$$
,  $a1$ ,  $k2$ ,  $a2$ ) = substrate  $\cdot$  ( $k1 \cdot a1 + k2 \cdot a2$ ) (122)

## **10.16 Reaction** re27

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

Name re082

# **Reaction equation**

$$s28 \xrightarrow{s27, s28, s27} s33$$
 (123)

Table 51: Properties of each reactant.

Id	Name	SBO
s28	nT	

Table 52: Properties of each modifier.

Id	Name	SBO
s27	tDC	
s28	nT	
s27	tDC	

#### **Product**

Table 53: Properties of each product.

Id	Name	SBO
s33	iTreg	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{16} = \text{vol}(c3) \cdot \text{function}_3([s28], [s27], \text{parameter}_30)$$
 (124)

$$function\_3 (substrate, a1, k1) = substrate \cdot a1 \cdot k1$$
 (125)

function\_3 (substrate, 
$$a1, k1$$
) = substrate  $\cdot a1 \cdot k1$  (126)

#### 10.17 Reaction re28

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

Name re083

# **Reaction equation**

$$s29 \xrightarrow{s26, \text{ species}\_20, s29, s26, \text{ species}\_20} s30$$
 (127)

Table 54: Properties of each reactant.

Id	Name	SBO
s29	cmT	

Table 55: Properties of each modifier.

Id	Name	SBO
s26	eDC	
species_20	eDCLB	
s29	cmT	
s26	eDC	
species_20	eDCLB	

#### **Product**

Table 56: Properties of each product.

Id	Name	SBO
s30	Th17	

# **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{17} = \text{vol}(c3) \cdot \text{function}_{-8}([s29], \text{parameter}_{-26}, [s26], \text{parameter}_{-102}, [\text{species}_{-20}])$$
 (128)

function\_8 (substrate, 
$$k1$$
,  $a1$ ,  $k2$ ,  $a2$ ) = substrate  $\cdot (k1 \cdot a1 + k2 \cdot a2)$  (129)

function\_8 (substrate, 
$$k1$$
,  $a1$ ,  $k2$ ,  $a2$ ) = substrate  $\cdot (k1 \cdot a1 + k2 \cdot a2)$  (130)

## 10.18 Reaction re29

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

Name re084

# **Reaction equation**

$$s29 \xrightarrow{s26, \text{ species}\_20, s29, s26, \text{ species}\_20} s31$$
 (131)

#### Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
s29	cmT	

## **Modifiers**

Table 58: Properties of each modifier.

Id	Name	SBO
s26	eDC	
species_20	eDCLB	
s29	cmT	
s26	eDC	
species_20	eDCLB	

#### **Product**

Table 59: Properties of each product.

Id	Name	SBO
s31	Th1	

# **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{18} = vol\left(c3\right) \cdot function\_8\left([s29], parameter\_25, [s26], parameter\_101, [species\_20]\right) \quad (132)$$

$$function\_8 (substrate, k1, a1, k2, a2) = substrate \cdot (k1 \cdot a1 + k2 \cdot a2)$$
 (133)

function\_8 (substrate, 
$$k1$$
,  $a1$ ,  $k2$ ,  $a2$ ) = substrate  $\cdot (k1 \cdot a1 + k2 \cdot a2)$  (134)

## 10.19 Reaction re31

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

Name re085

# **Reaction equation**

$$s29 \xrightarrow{s27, s29, s27} s33$$
 (135)

#### Reactant

Table 60: Properties of each reactant.

Id	Name	SBO
s29	cmT	

#### **Modifiers**

Table 61: Properties of each modifier.

Id	Name	SBO
s27	tDC	
s29	cmT	
s27	tDC	

#### **Product**

Table 62: Properties of each product.

Id	Name	SBO
s33	iTreg	

## **Kinetic Law**

Derived unit contains undeclared units

$$v_{19} = \text{vol}(c3) \cdot \text{function}_3([s29], [s27], \text{parameter}_27)$$
 (136)

function\_3 (substrate, 
$$a1, k1$$
) = substrate  $\cdot a1 \cdot k1$  (137)

function\_3 (substrate, 
$$a1, k1$$
) = substrate  $\cdot a1 \cdot k1$  (138)

# 10.20 Reaction re32

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

Name re087

# **Reaction equation**

$$s30 \xrightarrow{s30} s16 \tag{139}$$

#### Reactant

Table 63: Properties of each reactant.

Id	Name	SBO
s30	Th17	

#### Modifier

Table 64: Properties of each modifier.

Id	Name	SBO
<b>s</b> 30	Th17	

#### **Product**

Table 65: Properties of each product.

Id	Name	SBO
s16	Th17	

## **Kinetic Law**

Derived unit contains undeclared units

$$v_{20} = \text{parameter} \cdot [\text{s}30] \tag{140}$$

## **10.21 Reaction** re33

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

Name re088

# **Reaction equation**

$$s31 \xrightarrow{s31} s13 \tag{141}$$

Table 66: Properties of each reactant.

Id	Name	SBO
s31	Th1	

Table 67: Properties of each modifier.

Id	Name	SBO
s31	Th1	

# **Product**

Table 68: Properties of each product.

Id	Name	SBO
s13	Th1	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{21} = \text{parameter}_{-8} \cdot [\text{s}31] \tag{142}$$

## 10.22 Reaction re35

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

Name re089

# **Reaction equation**

$$s33 \xrightarrow{s33} s15 \tag{143}$$

Table 69: Properties of each reactant.

Id	Name	SBO
s33	iTreg	

Table 70: Properties of each modifier.

Id	Name	SBO
s33	iTreg	

## **Product**

Table 71: Properties of each product.

Id	Name	SBO
s15	iTreg	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{22} = \text{parameter} \cdot [\text{s33}] \tag{144}$$

# 10.23 Reaction re41

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

Name re091

# **Reaction equation**

$$s33 \xrightarrow{s31, s26, s30, s33, s31, s26, s30} s30$$
 (145)

#### Reactant

Table 72: Properties of each reactant.

Id	Name	SBO
s33	iTreg	

Table 73: Properties of each modifier.

Id	Name	SBO
s31	Th1	
s26	eDC	
s30	Th17	
s33	iTreg	
s31	Th1	
s26	eDC	
<b>s</b> 30	Th17	

#### **Product**

Table 74: Properties of each product.

Id	Name	SBO
s30	Th17	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{23} = vol(c3) \cdot function\_4 (parameter\_87, [s33], [s31], parameter\_63, parameter\_91, [s26], parameter\_91, [s30], parameter\_91)$$
 (146)

$$\begin{aligned} \text{function\_4}\left(k, \text{substrate}, A, n, kA, B, kB, C, kC\right) &= k \cdot \text{substrate} \cdot \left(\frac{A^n}{A^n + kA^n} \right. \\ &+ \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n} \right) \end{aligned} \tag{147}$$

$$\begin{aligned} \text{function\_4}\left(k, \text{substrate}, A, n, kA, B, kB, C, kC\right) &= k \cdot \text{substrate} \cdot \left(\frac{A^n}{A^n + kA^n} \right. \\ &+ \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n} \right) \end{aligned} \tag{148}$$

## **10.24 Reaction** re42

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

Name re093

# **Reaction equation**

$$s15 \xrightarrow{s16, s9, s19, s13, s3, s15, s16, s9, s19, s13, s3} s16$$
 (149)

## Reactant

Table 75: Properties of each reactant.

Id	Name	SBO
s15	iTreg	

#### **Modifiers**

Table 76: Properties of each modifier.

Id	Name	SBO
s16	Th17	
s9	eDC	
s19	M1	
s13	Th1	
s3	Ep	
s15	iTreg	
s16	Th17	
s9	eDC	
s19	M1	
s13	Th1	
s3	Ep	

## **Product**

Table 7<u>7</u>: Properties of each product.

Id	Name	SBO
s16	Th17	

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_{24} = vol(c2) \cdot function\_2 (parameter\_87, [s15], [s16], parameter\_63, parameter\_91, [s9], parameter\_91, [s19], parameter\_91, [s13], parameter\_91, [s3], parameter\_31)$$
 (150)

$$\begin{aligned} &\text{function\_2}\left(k, \text{substrate}, A, n, kA, B, kB, C, kC, D, kD, E, kE\right) \\ &= k \cdot \text{substrate} \cdot \left(\frac{A^n}{A^n + kA^n} + \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n} + \frac{D^n}{D^n + kD^n} + \frac{E^n}{E^n + kE^n}\right) \end{aligned} \tag{151}$$

$$\begin{aligned} &\text{function\_2}\left(k, \text{substrate}, A, n, kA, B, kB, C, kC, D, kD, E, kE\right) \\ &= k \cdot \text{substrate} \cdot \left(\frac{A^n}{A^n + kA^n} + \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n} + \frac{D^n}{D^n + kD^n} + \frac{E^n}{E^n + kE^n}\right) \end{aligned} \tag{152}$$

#### **10.25 Reaction** re43

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

Name re095

#### **Reaction equation**

$$s16 \xrightarrow{s16} s17 \tag{153}$$

#### Reactant

Table 78: Properties of each reactant.

Id	Name	SBO
s16	Th17	

#### **Modifier**

Table 79: Properties of each modifier.

Id	Name	SBO
s16	Th17	

## **Product**

Table 80: Properties of each product.

Id	Name	SBO
s17	emT	

**Derived unit** contains undeclared units

$$v_{25} = \text{vol}(c2) \cdot \text{parameter}_{-15} \cdot [\text{s}16] \tag{154}$$

## 10.26 Reaction re44

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

Name re096

# **Reaction equation**

$$s13 \xrightarrow{s13} s17 \tag{155}$$

#### Reactant

Table 81: Properties of each reactant.

Id	Name	SBO
s13	Th1	

#### **Modifier**

Table 82: Properties of each modifier.

Id	Name	SBO
s13	Th1	

#### **Product**

Table 83: Properties of each product.

Id	Name	SBO
s17	emT	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{26} = \text{vol}(c2) \cdot \text{parameter}_{-15} \cdot [\text{s}13] \tag{156}$$

## **10.27 Reaction** re45

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

Name re097

# **Reaction equation**

$$s15 \xrightarrow{s15} s17 \tag{157}$$

#### Reactant

Table 84: Properties of each reactant.

Id	Name	SBO
s15	iTreg	

#### **Modifier**

Table 85: Properties of each modifier.

Id	Name	SBO
s15	iTreg	

#### **Product**

Table 86: Properties of each product.

Id	Name	SBO
s17	emT	

# **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{27} = \text{vol}(c2) \cdot \text{parameter}_{-}15 \cdot [\text{s}15] \tag{158}$$

# **10.28 Reaction** re46

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

Name re098

# **Reaction equation**

$$s16 \xrightarrow{s16} s29 \tag{159}$$

#### Reactant

Table 87: Properties of each reactant.

Id	Name	SBO
s16	Th17	

#### Modifier

Table 88: Properties of each modifier.

Id	Name	SBO
s16	Th17	

#### **Product**

Table 89: Properties of each product.

Id	Name	SBO
s29	cmT	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{28} = \text{parameter}_{-}16 \cdot [\text{s}16] \tag{160}$$

# **10.29 Reaction** re47

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

Name re099

# **Reaction equation**

$$s13 \xrightarrow{s13} s29 \tag{161}$$

Table 90: Properties of each reactant.

Id	Name	SBO
s13	Th1	

Table 91: Properties of each modifier.

Id	Name	SBO
s13	Th1	

# **Product**

Table 92: Properties of each product.

Id	Name	SBO
s29	cmT	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{29} = \text{parameter} \cdot [\text{s}13] \tag{162}$$

## **10.30 Reaction** re49

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

Name re100

# **Reaction equation**

$$s15 \xrightarrow{s15} s29 \tag{163}$$

Table 93: Properties of each reactant.

Id	Name	SBO
s15	iTreg	

Table 94: Properties of each modifier.

Id	Name	SBO
s15	iTreg	

# **Product**

Table 95: Properties of each product.

Id	Name	SBO
s29	cmT	

## **Kinetic Law**

Derived unit contains undeclared units

$$v_{30} = \text{parameter}_{-}16 \cdot [\text{s}15] \tag{164}$$

# 10.31 Reaction reaction\_1

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

Name re060

# **Reaction equation**

$$s3 \xrightarrow{s3} s2$$
 (165)

#### Reactant

Table 96: Properties of each reactant.

Id	Name	SBO
s3	Ep	

Table 97: Properties of each modifier.

Id	Name	SBO
s3	Ep	

## **Product**

Table 98: Properties of each product.

Id	Name	SBO
s2	Е	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{31} = \text{vol}(c4) \cdot \text{parameter} 21 \cdot [s3]$$
 (166)

# 10.32 Reaction reaction\_2

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

Name re057

# **Reaction equation**

species\_5 
$$\xrightarrow{\text{species}\_5}$$
 s2 (167)

#### Reactant

Table 99: Properties of each reactant.

Id	Name	SBO
species_5	Edead	

Table 100: Properties of each modifier.

Id	Name	SBO
species_5	Edead	

# **Product**

Table 101: Properties of each product.

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{32} = \text{vol}(c4) \cdot \text{parameter} \cdot 21 \cdot [\text{species} \cdot 5]$$
 (168)

## 10.33 Reaction reaction\_3

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

Name re102

# **Reaction equation**

$$s6 \xrightarrow{s6} 2 s6$$
 (169)

# Reactant

Table 102: Properties of each reactant.

Id	Name	SBO
s6	HP	

#### **Modifier**

Table 103: Properties of each modifier.

Id	Name	SBO
s6	HP	

#### **Product**

Table 104: Properties of each product.

Id	Name	SBO
s6	HP	

**Derived unit** contains undeclared units

$$v_{33} = \text{vol}(c2) \cdot \text{function}_5 \text{ (parameter}_20, [s6], parameter}_93)$$
 (170)

function\_5 
$$(k, sub, c) = \frac{k \cdot sub}{c + sub}$$
 (171)

function\_5 
$$(k, sub, c) = \frac{k \cdot sub}{c + sub}$$
 (172)

## 10.34 Reaction reaction\_4

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

Name re101

# **Reaction equation**

$$s6 \xrightarrow{s6} \emptyset$$
 (173)

#### Reactant

Table 105: Properties of each reactant.

Id	Name	SBO
s6	HP	

Table 106: Properties of each modifier.

Id	Name	SBO
s6	HP	

**Derived unit** contains undeclared units

$$v_{34} = \text{vol}(c2) \cdot \text{parameter}_{19} \cdot [\text{s6}] \tag{174}$$

# 10.35 Reaction reaction\_5

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

Name re052

#### **Reaction equation**

$$s1 \xrightarrow{s1} 2s1 \tag{175}$$

#### Reactant

Table 107: Properties of each reactant.

Id	Name	SBO
s1	HP	

#### **Modifier**

Table 108: Properties of each modifier.

Id	Name	SBO
s1	HP	

#### **Product**

Table 109: Properties of each product.

Id	Name	SBO
s1	HP	

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_{35} = \text{vol}(c1) \cdot \text{function} \text{\_5} \text{ (parameter} \text{\_20, [s1], parameter} \text{\_93)}$$
 (176)

$$function\_5\left(k,sub,c\right) = \frac{k \cdot sub}{c + sub} \tag{177}$$

$$function\_5\left(k,sub,c\right) = \frac{k \cdot sub}{c + sub} \tag{178}$$

#### 10.36 Reaction reaction\_6

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

Name re065

## **Reaction equation**

$$s1 \xrightarrow{s1} \emptyset$$
 (179)

#### Reactant

Table 110: Properties of each reactant.

Id	Name	SBO
s1	HP	

# **Modifier**

Table 111: Properties of each modifier.

Id	Name	SBO
s1	HP	

## **Kinetic Law**

Derived unit contains undeclared units

$$v_{36} = \text{vol}(c1) \cdot \text{parameter}_{-}19 \cdot [s1] \tag{180}$$

## 10.37 Reaction reaction\_10

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

Name re103

# **Reaction equation**

$$s17 \xrightarrow{s19, s9, species\_18, s17, s19, s9, species\_18} s13$$
 (181)

#### Reactant

Table 112: Properties of each reactant.

Id	Name	SBO
s17	emT	

## **Modifiers**

Table 113: Properties of each modifier.

Id	Name	SBO
s19	M1	
ສ9	eDC	
species_18	eDCLB	
s17	emT	
s19	M1	
<b>s</b> 9	eDC	
species_18	eDCLB	

## **Product**

Table 114: Properties of each product.

Id	Name	SBO
s13	Th1	

#### **Kinetic Law**

#### **Derived unit** contains undeclared units

$$v_{37} = \text{vol}(c2) \cdot \text{function\_6}([s17], \text{parameter\_23}, [s19], \text{parameter\_23}, [s9], \text{parameter\_100}, \\ [\text{species\_18}])$$
 (182)

function\_6 (substrate, 
$$k1$$
,  $a1$ ,  $k2$ ,  $a2$ ,  $k3$ ,  $a3$ ) = substrate  $\cdot (k1 \cdot a1 + k2 \cdot a2 + k3 \cdot a3)$  (183)

function\_6 (substrate, 
$$k1$$
,  $a1$ ,  $k2$ ,  $a2$ ,  $k3$ ,  $a3$ ) = substrate  $\cdot (k1 \cdot a1 + k2 \cdot a2 + k3 \cdot a3)$  (184)

# 10.38 Reaction reaction\_11

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

Name re104

# **Reaction equation**

$$s17 \xrightarrow{s19, s9, species_18, s17, s19, s9, species_18} s16$$
 (185)

# Reactant

Table 115: Properties of each reactant.

Id	Name	SBO
s17	emT	

## **Modifiers**

Table 116: Properties of each modifier.

Id	Name	SBO
s19	M1	
s9	eDC	
species_18	eDCLB	
s17	emT	
s19	M1	
<b>s</b> 9	eDC	
species_18	eDCLB	

## **Product**

Table 117: Properties of each product.

Id	Name	SBO
s16	Th17	

#### **Kinetic Law**

**Derived unit** contains undeclared units

 $v_{38} = \text{vol}(c2) \cdot \text{function}_6([s17], \text{parameter}_22, [s19], \text{parameter}_22, [s9], \text{parameter}_99, [\text{spec(ib86)}8])$ 

function\_6 (substrate, 
$$k1$$
,  $a1$ ,  $k2$ ,  $a2$ ,  $k3$ ,  $a3$ ) = substrate  $\cdot (k1 \cdot a1 + k2 \cdot a2 + k3 \cdot a3)$  (187)

function\_6 (substrate, 
$$k1$$
,  $a1$ ,  $k2$ ,  $a2$ ,  $k3$ ,  $a3$ ) = substrate  $\cdot (k1 \cdot a1 + k2 \cdot a2 + k3 \cdot a3)$  (188)

# 10.39 Reaction reaction\_12

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

Name re119

#### **Reaction equation**

$$s16 \xrightarrow{s16} \emptyset \tag{189}$$

#### Reactant

Table 118: Properties of each reactant.

Id	Name	SBO
s16	Th17	

#### **Modifier**

Table 119: Properties of each modifier.

Id	Name	SBO
s16	Th17	

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_{39} = \text{vol}(c2) \cdot \text{parameter\_64} \cdot [\text{s16}] \tag{190}$$

#### 10.40 Reaction reaction\_13

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

Name re106

# **Reaction equation**

$$\emptyset \xrightarrow{s26, s26} s28 \tag{191}$$

#### **Modifiers**

Table 120: Properties of each modifier.

Id	Name	SBO
s26	eDC	
s26	eDC	

#### **Product**

Table 121: Properties of each product.

Id	Name	SBO
s28	nT	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{40} = \text{vol}(c3) \cdot \text{function}_7 \text{ (parameter}_33, [s26], parameter}_63, parameter}_86, parameter}_35)$$
(192)

$$\text{function\_7}\left(k,A,n,kA,c\right) = c + k \cdot \frac{A^n}{A^n + kA^n} \tag{193} \label{eq:193}$$

$$function\_7\left(k,A,n,kA,c\right) = c + k \cdot \frac{A^n}{A^n + kA^n} \tag{194} \label{eq:194}$$

# 10.41 Reaction reaction\_14

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

Name re107

## **Reaction equation**

$$s28 \xrightarrow{s28} \emptyset \tag{195}$$

Table 122: Properties of each reactant.

Id	Name	SBO
s28	nT	

Table 123: Properties of each modifier.

Id	Name	SBO
s28	nT	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{41} = \text{vol}(c3) \cdot \text{parameter} 34 \cdot [s28] \tag{196}$$

#### 10.42 Reaction reaction\_16

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

Name re061

# **Reaction equation**

$$s1 \xrightarrow{s3, s1, s3} s6$$
 (197)

#### Reactant

Table 124: Properties of each reactant.

Id	Name	SBO
s1	HP	

Table 125: Properties of each modifier.

Id	Name	SBO
s1	HP	
s3	Ep	

## **Product**

Table 126: Properties of each product.

Id	Name	SBO
s6	HP	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{42} = \text{function}_3([s1], [s3], \text{parameter}_37)$$
 (198)

function\_3 (substrate, 
$$a1, k1$$
) = substrate  $\cdot a1 \cdot k1$  (199)

## 10.43 Reaction reaction\_17

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

Name re062

# **Reaction equation**

$$s4 + s1 \xrightarrow{s4, s1} s25$$
 (200)

#### **Reactants**

Table 127: Properties of each reactant.

Id	Name	SBO
s4	iDC	
s1	HP	

Table 128: Properties of each modifier.

Id	Name	SBO
s4	iDC	
s1	HP	

# **Product**

Table 129: Properties of each product.

Id	Name	SBO
s25	tDC	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{43} = \text{parameter} \cdot 56 \cdot [\text{s4}] \cdot [\text{s1}] \tag{201}$$

# 10.44 Reaction reaction\_19

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

Name re067

# **Reaction equation**

$$s6 \xrightarrow{s3, s19, s6, s3, s19} \emptyset$$
 (202)

## Reactant

Table 13<u>0</u>: Properties of each reactant.

Id	Name	SBO
s6	HP	

Table 131: Properties of each modifier.

Id	Name	SBO
s3	Ep	
s19	M1	
s6	HP	
s3	Ep	
s19	M1	

Derived unit contains undeclared units

$$v_{44} = \text{vol}(c2) \cdot \text{function}_{9}([s6], \text{parameter}_{48}, \text{parameter}_{39}, [s3], \text{parameter}_{38}, [s19])$$
 (203)

function\_9 (substrate, k, k1, a1, k2, a2) = substrate 
$$\cdot$$
 k  $\cdot$  (k1  $\cdot$  a1 + k2  $\cdot$  a2) (204)

function\_9 (substrate, k, k1, a1, k2, a2) = substrate 
$$\cdot$$
 k  $\cdot$  (k1  $\cdot$  a1 + k2  $\cdot$  a2) (205)

# 10.45 Reaction reaction\_20

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

Name re053

## **Reaction equation**

$$s1 \xrightarrow{s3, s1, s3} \emptyset \tag{206}$$

#### Reactant

Table 132: Properties of each reactant.

Id	Name	SBO
s1	HP	

Table 133: Properties of each modifier.

Id	Name	SBO
s3	Ep	
s1	HP	
s3	Ep	

**Derived unit** contains undeclared units

$$v_{45} = \text{vol}(c1) \cdot \text{function}_3([s1], [s3], \text{parameter}_54)$$
 (207)

function\_3 (substrate, 
$$a1, k1$$
) = substrate  $\cdot a1 \cdot k1$  (208)

function\_3 (substrate, 
$$a1, k1$$
) = substrate  $\cdot a1 \cdot k1$  (209)

## 10.46 Reaction reaction\_24

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

Name re068

## **Reaction equation**

$$\emptyset \xrightarrow{s3, s19, s9, s3, s19, s9} \text{species}_{1}$$
 (210)

# **Modifiers**

Table 134: Properties of each modifier.

Id	Name	SBO
s3	Ep	
s19	M1	
s9	eDC	
s3	Ep	
s19	M1	
s9	eDC	

## **Product**

Table 135: Properties of each product.

Id	Name	SBO
species_1	iDC	

**Derived unit** contains undeclared units

$$v_{46} = \text{vol}(c2) \cdot \text{function\_10} \text{ (parameter\_66, parameter\_41, [s3], parameter\_63, parameter\_40, [s19], parameter\_85, [s9], parameter\_85)}$$
 (211)

$$function_{-}10\left(c,k,A,n,kA,B,kB,C,kC\right) = c + k \cdot \left(\frac{A^{n}}{A^{n} + kA^{n}} + \frac{B^{n}}{B^{n} + kB^{n}} + \frac{C^{n}}{C^{n} + kC^{n}}\right) \quad (212)$$

$$function\_10 \ (c,k,A,n,kA,B,kB,C,kC) = c + k \cdot \left( \frac{A^n}{A^n + kA^n} + \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n} \right) \quad (213)$$

#### 10.47 Reaction reaction\_27

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

Name re069

## **Reaction equation**

$$\emptyset \xrightarrow{s19, s3, s9, s19, s3, s9} s22$$
 (214)

Table 136: Properties of each modifier.

s19 M1 s3 Ep s9 eDC s19 M1 s3 Ep s9 eDC	Id	Name	SBO
s9 eDC s19 M1 s3 Ep	s19	M1	
s19 M1 s3 Ep	s3	Ep	
s3 Ep	s9	eDC	
•	s19	M1	
s9 eDC	s3	Ep	
	s9	eDC	

### **Product**

Table 137: Properties of each product.

Id	Name	SBO
s22	M0	

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_{47} = vol(c2) \cdot function_10 (parameter_65, parameter_41, [s19], parameter_63, parameter_85, [s3], parameter_40, [s9], parameter_85)$$
 (215)

$$function\_10 \left( c, k, A, n, kA, B, kB, C, kC \right) = c + k \cdot \left( \frac{A^n}{A^n + kA^n} + \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n} \right) \quad (216)$$

$$function\_10 \ (c,k,A,n,kA,B,kB,C,kC) = c + k \cdot \left( \frac{A^n}{A^n + kA^n} + \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n} \right) \quad (217)$$

# 10.48 Reaction reaction\_31

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

### Name re111

#### **Reaction equation**

$$species_{-1} \xrightarrow{species_{-1}} \emptyset$$
 (218)

#### Reactant

Table 138: Properties of each reactant.

Id	Name	SBO
species_1	iDC	

Table 139: Properties of each modifier.

Id	Name	SBO
species_1	iDC	

**Derived unit** contains undeclared units

$$v_{48} = \text{vol}(c2) \cdot \text{parameter\_44} \cdot [\text{species\_1}]$$
 (219)

## 10.49 Reaction reaction\_32

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

Name re112

## **Reaction equation**

$$s22 \xrightarrow{s22} \emptyset \tag{220}$$

#### Reactant

Table 140: Properties of each reactant.

Id	Name	SBO
s22	M0	

## **Modifier**

Table 141: Properties of each modifier.

Id	Name	SBO
s22	M0	

## **Kinetic Law**

$$v_{49} = \text{vol}(c2) \cdot \text{parameter} 45 \cdot [\text{s}22] \tag{221}$$

# 10.50 Reaction reaction\_37

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

Name re117

## **Reaction equation**

$$s19 \xrightarrow{s19} \emptyset \tag{222}$$

#### Reactant

Table 142: Properties of each reactant.

Id	Name	SBO
s19	M1	

#### **Modifier**

Table 143: Properties of each modifier.

Id	Name	SBO
s19	M1	

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_{50} = \text{vol}(c2) \cdot \text{parameter} \underline{-62} \cdot [\text{s}19] \tag{223}$$

## 10.51 Reaction reaction\_38

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

Name re118

## **Reaction equation**

$$s21 \xrightarrow{s21} \emptyset \tag{224}$$

### Reactant

Table 144: Properties of each reactant.

Id	Name	SBO
s21	M2	

## **Modifier**

Table 145: Properties of each modifier.

Id	Name	SBO
s21	M2	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{51} = \text{vol}(c2) \cdot \text{parameter} \cdot 62 \cdot [\text{s}21] \tag{225}$$

## 10.52 Reaction reaction\_39

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

Name re120

## **Reaction equation**

$$s13 \xrightarrow{s13} \emptyset \tag{226}$$

## Reactant

Table 146: Properties of each reactant.

Id	Name	SBO
s13	Th1	

Table 147: Properties of each modifier.

Id	Name	SBO
s13	Th1	

**Derived unit** contains undeclared units

$$v_{52} = \text{vol}(c2) \cdot \text{parameter}_{64} \cdot [\text{s}13] \tag{227}$$

#### 10.53 Reaction reaction\_40

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

Name re121

### **Reaction equation**

$$s15 \xrightarrow{s15} \emptyset \tag{228}$$

#### Reactant

Table 148: Properties of each reactant.

Id	Name	SBO
s15	iTreg	

### **Modifier**

Table 149: Properties of each modifier.

Id	Name	SBO
s15	iTreg	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{53} = \text{vol}(c2) \cdot \text{parameter} \underline{-64} \cdot [\text{s}15] \tag{229}$$

## 10.54 Reaction reaction\_7

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

Name re071

## **Reaction equation**

$$s19 \xrightarrow{s15, s21, s25, s19, s15, s21, s25} s21$$
 (230)

## Reactant

Table 150: Properties of each reactant.

Id	Name	SBO
s19	M1	

#### **Modifiers**

Table 151: Properties of each modifier.

Name	SBO
iTreg	
M2	
tDC	
M1	
iTreg	
M2	
tDC	
	iTreg M2 tDC M1 iTreg M2

## **Product**

Table 152: Properties of each product.

Id	Name	SBO
s21	M2	

#### **Kinetic Law**

$$v_{54} = \text{vol}(c2) \cdot \text{function\_4} \text{ (parameter\_90, [s19], [s15], parameter\_63, parameter\_92, [s21], } parameter\_92, [s25], parameter\_92)$$

$$\begin{aligned} \text{function\_4}\left(k, \text{substrate}, A, n, kA, B, kB, C, kC\right) &= k \cdot \text{substrate} \cdot \left(\frac{A^n}{A^n + kA^n} \right. \\ &+ \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n} \right) \end{aligned} \tag{232}$$

$$\begin{aligned} \text{function\_4}\left(k, \text{substrate}, A, n, kA, B, kB, C, kC\right) &= k \cdot \text{substrate} \cdot \left(\frac{A^n}{A^n + kA^n}\right. \\ &+ \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n}\right) \end{aligned} \tag{233}$$

## 10.55 Reaction reaction\_8

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

Name re094

#### **Reaction equation**

$$s16 \xrightarrow{s15, s25, s21, s16, s15, s25, s21} s15$$
 (234)

#### Reactant

Table 153: Properties of each reactant.

Id	Name	SBO
s16	Th17	

Table 154: Properties of each modifier.

Id	Name	SBO
s15	iTreg	
s25	tDC	
s21	M2	
s16	Th17	
s15	iTreg	
s25	tDC	
s21	M2	

## **Product**

Table 155: Properties of each product.

Id	Name	SBO
s15	iTreg	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{55} = \text{vol}(c2) \cdot \text{function\_4}(\text{parameter\_88}, [\text{s}16], [\text{s}15], \text{parameter\_63}, \text{parameter\_92}, [\text{s}25], \\ \text{parameter\_92}, [\text{s}21], \text{parameter\_92})$$
(235)

$$\begin{aligned} \text{function\_4}\left(k, \text{substrate}, A, n, kA, B, kB, C, kC\right) &= k \cdot \text{substrate} \cdot \left(\frac{A^n}{A^n + kA^n} \right. \\ &+ \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n}\right) \end{aligned} \tag{236}$$

$$\begin{aligned} \text{function\_4}\left(k, \text{substrate}, A, n, kA, B, kB, C, kC\right) &= k \cdot \text{substrate} \cdot \left(\frac{A^n}{A^n + kA^n} \right. \\ &+ \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n}\right) \end{aligned} \tag{237}$$

## 10.56 Reaction reaction\_9

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

Name re092

## **Reaction equation**

$$s30 \xrightarrow{s33, s27, s30, s33, s27} s33$$
 (238)

## Reactant

Table 156: Properties of each reactant.

Id	Name	SBO
s30	Th17	

### **Modifiers**

Table 157: Properties of each modifier.

Id	Name	SBO
s33	iTreg	
s27	tDC	
s30	Th17	
s33	iTreg	
s27	tDC	

#### **Product**

Table 158: Properties of each product.

Id	Name	SBO
s33	iTreg	

#### **Kinetic Law**

#### **Derived unit** contains undeclared units

$$v_{56} = \text{vol}(c3) \cdot \text{function\_11} \text{ (parameter\_88, [s30], [s33], parameter\_63, parameter\_92, [s27], parameter\_92)}$$
 (239)

$$function\_11\left(k, substrate, A, n, kA, B, kB\right) = k \cdot substrate \cdot \left(\frac{A^n}{A^n + kA^n} + \frac{B^n}{B^n + kB^n}\right) \quad (240)$$

$$function\_11\left(k, substrate, A, n, kA, B, kB\right) = k \cdot substrate \cdot \left(\frac{A^n}{A^n + kA^n} + \frac{B^n}{B^n + kB^n}\right) \quad (241)$$

## 10.57 Reaction reaction\_15

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

Name re122

## **Reaction equation**

$$s22 + s6 \xrightarrow{s22, s6} s19$$
 (242)

## **Reactants**

Table 159: Properties of each reactant.

Id	Name	SBO
s22	<b>M</b> 0	
s6	HP	

## **Modifiers**

Table 160: Properties of each modifier.

Id	Name	SBO
s22	M0	
s6	HP	

#### **Product**

Table 161: Properties of each product.

Id	Name	SBO
s19	M1	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{57} = \text{vol}(c2) \cdot \text{parameter} \underline{59} \cdot [\text{s}22] \cdot [\text{s}6]$$
 (243)

## 10.58 Reaction reaction\_18

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

Name re123

# **Reaction equation**

$$s22 + s6 \xrightarrow{s22, s6} s21$$
 (244)

### **Reactants**

Table 162: Properties of each reactant.

Id	Name	SBO
s22	<b>M</b> 0	
s6	HP	

## **Modifiers**

Table 163: Properties of each modifier.

Id	Name	SBO
s22	<b>M</b> 0	
s6	HP	

#### **Product**

Table 164: Properties of each product.

Id	Name	SBO
s21	M2	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{58} = \text{vol}(c2) \cdot \text{parameter} \underline{-60} \cdot [\text{s}22] \cdot [\text{s}6]$$
 (245)

## 10.59 Reaction reaction\_21

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

Name re116

## **Reaction equation**

$$s26 \xrightarrow{s26} \emptyset \tag{246}$$

### Reactant

Table 165: Properties of each reactant.

Id	Name	SBO
s26	eDC	

## **Modifier**

Table 166: Properties of each modifier.

Id	Name	SBO
s26	eDC	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{59} = \text{vol}(c3) \cdot \text{parameter} \cdot [\text{s}26] \tag{247}$$

## 10.60 Reaction reaction\_22

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

Name re124

## **Reaction equation**

$$s27 \xrightarrow{s27} \emptyset \tag{248}$$

## Reactant

Table 167: Properties of each reactant.

Id	Name	SBO
s27	tDC	

Table 168: Properties of each modifier.

Id	Name	SBO
s27	tDC	

**Derived unit** contains undeclared units

$$v_{60} = \text{vol}(c3) \cdot \text{parameter}_{46} \cdot [\text{s}27] \tag{249}$$

## 10.61 Reaction reaction\_23

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name re127

## **Reaction equation**

species\_1 
$$\stackrel{\text{species}_1, \text{ s4}}{=\!=\!=\!=\!=}$$
 s4 (250)

#### Reactant

Table 169: Properties of each reactant.

Id	Name	SBO
species_1	iDC	

#### **Modifiers**

Table 170: Properties of each modifier.

Id	Name	SBO
species_1 s4	iDC iDC	

#### **Product**

Table 171: Properties of each product.

Id	Name	SBO
s4	iDC	

#### **Kinetic Law**

$$v_{61} = \text{function}_{-12}(V, [\text{species}_{-1}], k, [\text{s4}])$$
 (251)

$$function_{12}(V, s, k, P) = V \cdot (s - k \cdot P)$$
(252)

Table 172: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
V	V	94.376	$\overline{Z}$
k	k	1.359	Ø

## 10.62 Reaction reaction\_25

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

Name re128

## **Reaction equation**

$$s4 \xrightarrow{\text{species}\_10, s4, species}\_10$$
  $s25$  (253)

#### Reactant

Table 173: Properties of each reactant.

Id	Name	SBO
s4	iDC	

## **Modifiers**

Table 174: Properties of each modifier.

Id	Name	SBO
species_10	LB	
s4	iDC	
$species_{-}10$	LB	

## **Product**

Table 175: Properties of each product.

Id	Name	SBO
s25	tDC	

**Derived unit** contains undeclared units

$$v_{62} = \text{function}_3([s4], [\text{species}_10], \text{parameter}_77)$$
 (254)

function\_3 (substrate, 
$$a1, k1$$
) = substrate  $\cdot a1 \cdot k1$  (255)

## 10.63 Reaction reaction\_26

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

Name re129

## **Reaction equation**

$$s4 \xrightarrow{\text{species}\_10, s4, species}\_10$$
  $s9$  (256)

## Reactant

Table 176: Properties of each reactant.

Id	Name	SBO
s4	iDC	

#### **Modifiers**

Table 177: Properties of each modifier.

Id	Name	SBO
species_10	LB	
s4	iDC	
${\tt species\_10}$	LB	

## **Product**

Table 178: Properties of each product.

Id	Name	SBO
<b>s</b> 9	eDC	

**Derived unit** contains undeclared units

$$v_{63} = \text{function}_3([s4], [\text{species}_10], \text{parameter}_78)$$
 (257)

function\_3 (substrate, 
$$a1, k1$$
) = substrate  $\cdot a1 \cdot k1$  (258)

## 10.64 Reaction reaction\_28

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

Name re130

## **Reaction equation**

$$species_{10} \xrightarrow{species_{10}} \emptyset$$
 (259)

# Reactant

Table 179: Properties of each reactant.

Id	Name	SBO
species_10	LB	

#### **Modifier**

Table 180: Properties of each modifier.

Id	Name	SBO
species_10	LB	

## **Kinetic Law**

$$v_{64} = \text{vol}(c1) \cdot \text{parameter\_94} \cdot [\text{species\_10}]$$
 (260)

# 10.65 Reaction reaction\_29

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

Name re131

## **Reaction equation**

$$\emptyset \longrightarrow s15$$
 (261)

## **Product**

Table 181: Properties of each product.

Id	Name	SBO
s15	iTreg	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{65} = \text{vol}(c2) \cdot \text{function}_{13} (\text{parameter}_{82})$$
 (262)

$$function_{-}13(v) = v \tag{263}$$

$$function_{-}13(v) = v \tag{264}$$

## 10.66 Reaction reaction\_30

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

Name re132

## **Reaction equation**

$$\emptyset \longrightarrow s13$$
 (265)

### **Product**

Table 182: Properties of each product.

Id	Name	SBO
s13	Th1	

**Derived unit** contains undeclared units

$$v_{66} = \text{vol}(c2) \cdot \text{function}_{13} \text{ (parameter}_{83})$$
 (266)

$$function_{13}(v) = v \tag{267}$$

$$function_{-}13(v) = v \tag{268}$$

## 10.67 Reaction reaction\_33

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

Name re133

## **Reaction equation**

$$\emptyset \longrightarrow s16$$
 (269)

#### **Product**

Table 183: Properties of each product.

Id	Name	SBO
s16	Th17	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{67} = \text{vol}(c2) \cdot \text{function}_{13} (\text{parameter}_{84})$$
 (270)

$$function_{-}13(v) = v \tag{271}$$

$$function_{-}13(v) = v \tag{272}$$

## 10.68 Reaction reaction\_34

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

Name re134

## **Reaction equation**

$$\emptyset \longrightarrow s33$$
 (273)

#### **Product**

Table 184: Properties of each product.

Id	Name	SBO
s33	iTreg	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{68} = \text{vol}(c3) \cdot \text{function}_{13} (\text{parameter}_{79})$$
 (274)

$$function_{-}13(v) = v (275)$$

$$function_{1}3(v) = v (276)$$

## 10.69 Reaction reaction\_35

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

Name re135

## **Reaction equation**

$$\emptyset \longrightarrow s31$$
 (277)

## **Product**

Table 185: Properties of each product.

Id	Name	SBO
s31	Th1	

#### **Kinetic Law**

$$v_{69} = \text{vol}(c3) \cdot \text{function}_{13} \text{ (parameter}_{80})$$
 (278)

$$function_13(v) = v (279)$$

$$function_{-}13(v) = v \tag{280}$$

#### 10.70 Reaction reaction\_36

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

Name re136

## **Reaction equation**

$$\emptyset \longrightarrow s30$$
 (281)

#### **Product**

Table 186: Properties of each product.

Id	Name	SBO
s30	Th17	

## **Kinetic Law**

Derived unit contains undeclared units

$$v_{70} = \text{vol}(c3) \cdot \text{function}_{13} \text{ (parameter}_{81})$$
 (282)

$$function_{13}(v) = v (283)$$

$$function_{-}13(v) = v \tag{284}$$

## 10.71 Reaction reaction\_41

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

Name re137

## **Reaction equation**

$$species_{1}8 \xrightarrow{species_{1}8} species_{2}0$$
 (285)

### Reactant

Table 187: Properties of each reactant.

Id	Name	SBO
species_18	eDCLB	

## **Modifier**

Table 188: Properties of each modifier.

Id	Name	SBO
species_18	eDCLB	

## **Product**

Table 189: Properties of each product.

Id	Name	SBO
species_20	eDCLB	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{71} = \text{parameter} \cdot [\text{species} \cdot 18]$$
 (286)

## 10.72 Reaction reaction\_42

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

Name re138

## **Reaction equation**

$$species_20 \xrightarrow{species_20} \emptyset$$
 (287)

## Reactant

Table 190: Properties of each reactant.

Id	Name	SBO
species_20	eDCLB	

#### **Modifier**

Table 191: Properties of each modifier.

Id	Name	SBO
species_20	eDCLB	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{72} = \text{vol}(c3) \cdot \text{parameter\_46} \cdot [\text{species\_20}]$$
 (288)

## 10.73 Reaction reaction\_43

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

Name re139

## **Reaction equation**

$$s2 \xrightarrow{s13, s16, s9, s19, s3, s2, s13, s16, s9, s19, s3} s3$$
 (289)

#### Reactant

Table 192: Properties of each reactant.

Id	Name	SBO
s2	E	

Table 193: Properties of each modifier.

Id	Name	SBO
s13	Th1	
s16	Th17	
s9	eDC	
s19	M1	
s3	Ep	
s2	E	

Id	Name	SBO
s13	Th1	
s16	Th17	
s9	eDC	
s19	M1	
s3	Ep	

### **Product**

Table 194: Properties of each product.

Id	Name	SBO
s3	Ep	

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_{73} = vol\left(c4\right) \cdot function\_2\left(parameter\_105, [s2], [s13], parameter\_63, parameter\_91, [s16], parameter\_91, [s9], parameter\_91, [s19], parameter\_91, [s3], parameter\_106\right) \tag{290}$$

$$\begin{aligned} &\text{function\_2}\left(k, substrate, A, n, kA, B, kB, C, kC, D, kD, E, kE\right) \\ &= k \cdot substrate \cdot \left(\frac{A^n}{A^n + kA^n} + \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n} + \frac{D^n}{D^n + kD^n} + \frac{E^n}{E^n + kE^n}\right) \end{aligned} \tag{291}$$

$$\begin{aligned} &\text{function\_2}\left(k, substrate, A, n, kA, B, kB, C, kC, D, kD, E, kE\right) \\ &= k \cdot substrate \cdot \left(\frac{A^n}{A^n + kA^n} + \frac{B^n}{B^n + kB^n} + \frac{C^n}{C^n + kC^n} + \frac{D^n}{D^n + kD^n} + \frac{E^n}{E^n + kE^n}\right) \end{aligned} \tag{292}$$

#### 10.74 Reaction reaction\_44

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

Name re140

#### **Reaction equation**

$$species_20 \xrightarrow{species_20} \emptyset$$
 (293)

Reactant

Table 195: Properties of each reactant.

Id	Name	SBO
species_20	eDCLB	

## **Modifier**

Table 196: Properties of each modifier.

Id	Name	SBO
species_20	eDCLB	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{74} = \text{vol}(c3) \cdot \text{parameter} \cdot 46 \cdot [\text{species} \cdot 20]$$
 (294)

#### 10.75 Reaction reaction\_45

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

Name nTh1 creation

# **Reaction equation**

$$s28 \xrightarrow{s28} species_12$$
 (295)

## Reactant

Table 197: Properties of each reactant.

Id	Name	SBO
s28	nT	

Table 198: Properties of each modifier.

Id	Name	SBO
s28	nT	

# **Product**

Table 199: Properties of each product.

Id	Name	SBO
species_12	nTh1	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{75} = k1 \cdot [s28] \tag{296}$$

Table 200: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.003	

## 10.76 Reaction reaction\_46

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

Name nTh1 trans

## **Reaction equation**

$$species_{12} \xrightarrow{species_{12}} species_{13}$$
 (297)

## Reactant

Table 201: Properties of each reactant.

Id	Name	SBO
species_12	nTh1	

Table 202: Properties of each modifier.

Id	Name	SBO
species_12	nTh1	

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## **Product**

Table 203: Properties of each product.

Id	Name	SBO
species_13	nTh1_LP	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{76} = \text{vol}(c1) \cdot k1 \cdot [\text{species}\_12] \tag{298}$$

Table 204: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.106	

## 10.77 Reaction reaction\_47

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

Name nTh1\_LP deg

# **Reaction equation**

$$species_{-}13 \xrightarrow{species_{-}13} \emptyset$$
 (299)

## Reactant

Table 205: Properties of each reactant.

Id	Name	SBO
species_13	nTh1_LP	

Table 206: Properties of each modifier.

Id	Name	SBO
species_13	nTh1_LP	

**Derived unit** contains undeclared units

$$v_{77} = \text{vol}(c1) \cdot k1 \cdot [\text{species}\_13] \tag{300}$$

Table 207: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.158	

## 10.78 Reaction reaction\_48

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

Name nTh1\_LP expansion

## **Reaction equation**

$$species_{13} \xrightarrow{species_{13}} 2 species_{13}$$
 (301)

## Reactant

Table 208: Properties of each reactant.

Id	Name	SBO
species_13	nTh1_LP	

Table 209: Properties of each modifier.

Id	Name	SBO
species_13	nTh1_LP	

## **Product**

Table 210: Properties of each product.

Id	Name	SBO
species_13	nTh1_LP	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{78} = \text{vol}(c1) \cdot k1 \cdot [\text{species}\_13] \tag{302}$$

Table 211: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.1	

## 10.79 Reaction reaction\_49

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

Name nTh1 deg

## **Reaction equation**

$$species_{-12} \xrightarrow{species_{-12}} \emptyset$$
 (303)

## Reactant

Table 212: Properties of each reactant.

Id	Name	SBO
species_12	nTh1	

Table 213: Properties of each modifier.

Id	Name	SBO
species_12	nTh1	

Id	Name	SBO

**Derived unit** contains undeclared units

$$v_{79} = \text{vol}(c1) \cdot k1 \cdot [\text{species}_{-12}] \tag{304}$$

Table 214: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.108	

## 10.80 Reaction reaction\_50

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

Name nTh17 creation

## **Reaction equation**

$$s28 \xrightarrow{s28} species_14$$
 (305)

## Reactant

Table 215: Properties of each reactant.

Id	Name	SBO
s28	nT	

#### **Modifier**

Table 216: Properties of each modifier.

Id	Name	SBO
s28	nT	

## **Product**

Table 217: Properties of each product.

Id	Name	SBO
species_14	nTh17	

**Derived unit** contains undeclared units

$$v_{80} = k1 \cdot [s28] \tag{306}$$

Table 218: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	<b>k</b> 1	0.002	

## 10.81 Reaction reaction\_51

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

Name nTh17 trans

## **Reaction equation**

$$species_{14} \xrightarrow{species_{14}} species_{15}$$
 (307)

## Reactant

Table 219: Properties of each reactant.

Id	Name	SBO
species_14	nTh17	

Table 220: Properties of each modifier.

Id	Name	SBO
species_14	nTh17	

## **Product**

Table 221: Properties of each product.

Id	Name	SBO
species_15	nTh17_LP	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{81} = \text{vol}(c1) \cdot k1 \cdot [\text{species}\_14] \tag{308}$$

Table 222: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.117	

## 10.82 Reaction reaction\_52

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

Name nTh17\_LP deg

## **Reaction equation**

$$species_{-15} \xrightarrow{species_{-15}} \emptyset$$
 (309)

## Reactant

Table 223: Properties of each reactant.

Id	Name	SBO
species_15	nTh17_LP	

Table 224: Properties of each modifier.

Id	Name	SBO
species_15	nTh17_LP	

Id	Name	SBO

**Derived unit** contains undeclared units

$$v_{82} = \text{vol}(c1) \cdot k1 \cdot [\text{species}\_15] \tag{310}$$

Table 225: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.1	

## 10.83 Reaction reaction\_53

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

Name nTh17 deg

## **Reaction equation**

$$species_{-14} \xrightarrow{species_{-14}} \emptyset$$
 (311)

#### Reactant

Table 226: Properties of each reactant.

Id	Name	SBO
species_14	nTh17	

## Modifier

Table 227: Properties of each modifier.

Id	Name	SBO
species_14	nTh17	

#### **Kinetic Law**

$$v_{83} = \text{vol}(c1) \cdot k1 \cdot [\text{species}\_14] \tag{312}$$

Table 228: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.1	$\overline{Z}$

## 10.84 Reaction reaction\_54

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

Name nTreg creation

## **Reaction equation**

$$s28 \xrightarrow{s28} species_16$$
 (313)

#### Reactant

Table 229: Properties of each reactant.

Id	Name	SBO
s28	nT	

## **Modifier**

Table 230: Properties of each modifier.

Id	Name	SBO
s28	nT	

## **Product**

Table 231: Properties of each product.

Id	Name	SBO
species_16	nTreg	

**Derived unit** contains undeclared units

$$v_{84} = k1 \cdot [s28] \tag{314}$$

Table 232: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.003	Ø

## 10.85 Reaction reaction\_55

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

Name nTreg trans

## **Reaction equation**

$$species_{16} \xrightarrow{species_{16}} species_{17}$$
 (315)

## Reactant

Table 233: Properties of each reactant.

Id	Name	SBO
species_16	nTreg	

## **Modifier**

Table 234: Properties of each modifier.

Id	Name	SBO
species_16	nTreg	

## **Product**

Table 235: Properties of each product.

Id	Name	SBO
species_17	nTreg_LP	

Id	Name	SBO

**Derived unit** contains undeclared units

$$v_{85} = \text{vol}(c1) \cdot k1 \cdot [\text{species}\_16] \tag{316}$$

Table 236: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.1	

## 10.86 Reaction reaction\_56

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

Name nTreg\_LP deg

## **Reaction equation**

$$species_{-17} \xrightarrow{species_{-17}} \emptyset$$
 (317)

#### Reactant

Table 237: Properties of each reactant.

Id	Name	SBO
species_17	nTreg_LP	_

# Modifier

Table 238: Properties of each modifier.

Id	Name	SBO
species_17	nTreg_LP	

#### **Kinetic Law**

$$v_{86} = \text{vol}(c1) \cdot k1 \cdot [\text{species}\_17] \tag{318}$$

Table 239: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.1	$\overline{Z}$

## 10.87 Reaction reaction\_57

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

Name nTreg deg

## **Reaction equation**

$$species_{-16} \xrightarrow{species_{-16}} \emptyset$$
 (319)

#### Reactant

Table 240: Properties of each reactant.

Id	Name	SBO
species_16	nTreg	

## **Modifier**

Table 241: Properties of each modifier.

Id	Name	SBO
species_16	nTreg	

## **Kinetic Law**

$$v_{87} = \text{vol}(c1) \cdot k1 \cdot [\text{species}\_16] \tag{320}$$

Table 242: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	0.119	

## 10.88 Reaction reaction\_58

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

Name Th17 to Treg

## **Reaction equation**

$$species_{15} \xrightarrow{species_{15}} species_{17}$$
 (321)

#### Reactant

Table 243: Properties of each reactant.

Id	Name	SBO
species_15	nTh17_LP	-

### **Modifier**

Table 244: Properties of each modifier.

Id	Name	SBO
species_15	nTh17_LP	

### **Product**

Table 245: Properties of each product.

Id	Name	SBO
species_17	nTreg_LP	

### **Kinetic Law**

Derived unit contains undeclared units

$$v_{88} = \text{vol}(c1) \cdot k1 \cdot [\text{species}\_15] \tag{322}$$

Table 246: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	<b>k</b> 1	0.167	

## 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 s1

Name HP

Initial concentration  $5.34 \cdot 10^{-8} \text{ item} \cdot \text{ml}^{-1}$ 

Initial assignment s1

Involved in events event\_1, event\_2

This species takes part in 17 reactions (as a reactant in re3, re13, reaction\_5, reaction\_6, reaction\_16, reaction\_17, reaction\_20 and as a product in reaction\_5 and as a modifier in re2, re2, re3, re13, reaction\_5, reaction\_6, reaction\_16, reaction\_17, reaction\_20).

$$\frac{d}{dt}s1 = 2 v_{35} - v_2 - v_6 - v_{35} - v_{36} - v_{42} - v_{43} - v_{45}$$
 (323)

Furthermore, two events influence this species' rate of change.

## **11.2 Species** species\_7

Name HP Dose

Initial concentration 0.0534 item·ml<sup>-1</sup>

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species}_{-}7 = 0 \tag{324}$$

## 11.3 Species species\_10

Name LB

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

Initial assignment species\_10

Involved in events event\_1, event\_2

This species takes part in six reactions (as a reactant in reaction\_28 and as a modifier in reaction\_25, reaction\_25, reaction\_26, reaction\_26, reaction\_28).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species}_{10} = -v_{64} \tag{325}$$

Furthermore, two events influence this species' rate of change.

## 11.4 Species species\_11

Name LB Dose

Initial concentration 1 item · ml<sup>-1</sup>

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species}_{-}11 = 0 \tag{326}$$

## **11.5 Species** species\_12

Name nTh1

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

This species takes part in five reactions (as a reactant in reaction\_46, reaction\_49 and as a product in reaction\_45 and as a modifier in reaction\_46, reaction\_49).

$$\frac{d}{dt} \text{species}_{-12} = |v_{75}| - |v_{76}| - |v_{79}| \tag{327}$$

## **11.6 Species** species\_13

Name nTh1\_LP

Initial concentration  $150000 \, \mathrm{item} \cdot \mathrm{ml}^{-1}$ 

This species takes part in six reactions (as a reactant in reaction\_47, reaction\_48 and as a product in reaction\_46, reaction\_48 and as a modifier in reaction\_47, reaction\_48).

$$\frac{d}{dt} \text{species}_{13} = |v_{76}| + 2|v_{78}| - |v_{77}| - |v_{78}| \tag{328}$$

## 11.7 Species species\_14

Name nTh17

Initial concentration 1 item  $\cdot$  ml<sup>-1</sup>

This species takes part in five reactions (as a reactant in reaction\_51, reaction\_53 and as a product in reaction\_50 and as a modifier in reaction\_51, reaction\_53).

$$\frac{d}{dt} \text{species}_{14} = |v_{80}| - |v_{81}| - |v_{83}| \tag{329}$$

## **11.8 Species** species\_15

Name nTh17\_LP

Initial concentration  $150000 \text{ item} \cdot \text{ml}^{-1}$ 

This species takes part in five reactions (as a reactant in reaction\_52, reaction\_58 and as a product in reaction\_51 and as a modifier in reaction\_52, reaction\_58).

$$\frac{d}{dt} \text{species}_{-15} = |v_{81}| - |v_{82}| - |v_{88}| \tag{330}$$

## 11.9 Species species\_16

Name nTreg

Initial concentration 1 item · ml<sup>-1</sup>

This species takes part in five reactions (as a reactant in reaction\_55, reaction\_57 and as a product in reaction\_54 and as a modifier in reaction\_55, reaction\_57).

$$\frac{d}{dt} \text{species}_{-16} = |v_{84}| - |v_{85}| - |v_{87}| \tag{331}$$

## 11.10 Species species\_17

Name nTreg\_LP

Initial concentration 150000 item · ml<sup>-1</sup>

This species takes part in four reactions (as a reactant in reaction\_56 and as a product in reaction\_55, reaction\_58 and as a modifier in reaction\_56).

$$\frac{d}{dt} \text{species}_{17} = |v_{85}| + |v_{88}| - |v_{86}| \tag{332}$$

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## **11.11 Species** s9

#### Name eDC

### Initial concentration $1 \text{ item} \cdot \text{ml}^{-1}$

This species takes part in 21 reactions (as a reactant in re21 and as a product in re6, re13, reaction\_26 and as a modifier in re16, re16, re18, re18, re21, re42, re42, reaction\_10, reaction\_11, reaction\_11, reaction\_24, reaction\_24, reaction\_27, reaction\_27, reaction\_43, reaction\_43).

$$\frac{\mathrm{d}}{\mathrm{d}t}s9 = |v_4| + |v_6| + |v_{63}| - |v_{12}| \tag{333}$$

## **11.12 Species** s13

#### Name Th1

## Initial concentration $0 \text{ item} \cdot \text{ml}^{-1}$

This species takes part in 21 reactions (as a reactant in re44, re47, reaction\_39 and as a product in re33, reaction\_10, reaction\_30 and as a modifier in re4, re4, re15, re15, re16, re16, re18, re18, re42, re42, re44, re47, reaction\_39, reaction\_43, reaction\_43).

$$\frac{\mathrm{d}}{\mathrm{d}t}s13 = |v_{21}| + |v_{37}| + |v_{66}| - |v_{26}| - |v_{29}| - |v_{52}| \tag{334}$$

### **11.13 Species** s15

## Name iTreg

## Initial concentration $0 \text{ item} \cdot \text{ml}^{-1}$

This species takes part in 18 reactions (as a reactant in re42, re45, re49, reaction\_40 and as a product in re11, re35, reaction\_8, reaction\_29 and as a modifier in re17, re17, re42, re45, re49, reaction\_40, reaction\_7, reaction\_7, reaction\_8, reaction\_8).

$$\frac{\mathrm{d}}{\mathrm{d}t}s15 = v_5 + v_{22} + v_{55} + v_{65} - v_{24} - v_{27} - v_{30} - v_{53} \tag{335}$$

## **11.14 Species** s16

#### Name Th17

## Initial concentration $0 \text{ item} \cdot \text{ml}^{-1}$

This species takes part in 24 reactions (as a reactant in re43, re46, reaction\_12, reaction\_8 and as a product in re32, re42, reaction\_11, reaction\_33 and as a modifier in re4, re4, re15, re15, re16, re16, re18, re18, re42, re42, re43, re46, reaction\_12, reaction\_8, reaction\_43, reaction\_43).

$$\frac{d}{dt}s16 = v_{20} + v_{24} + v_{38} + v_{67} - v_{25} - v_{28} - v_{39} - v_{55}$$
(336)

## **11.15 Species** s19

#### Name M1

### Initial concentration $0 \text{ item} \cdot \text{ml}^{-1}$

This species takes part in 29 reactions (as a reactant in reaction\_37, reaction\_7 and as a product in re16, re18, reaction\_15 and as a modifier in re4, re4, re15, re15, re16, re16, re18, re18, re42, re42, reaction\_10, reaction\_10, reaction\_11, reaction\_11, reaction\_19, reaction\_24, reaction\_24, reaction\_27, reaction\_27, reaction\_37, reaction\_7, reaction\_43, reaction\_43).

$$\frac{\mathrm{d}}{\mathrm{d}t}s19 = |v_8| + |v_{10}| + |v_{57}| - |v_{50}| - |v_{54}| \tag{337}$$

### **11.16 Species** s21

#### Name M2

## Initial concentration $0 \text{ item} \cdot \text{ml}^{-1}$

This species takes part in 15 reactions (as a reactant in re18, reaction\_38 and as a product in re17, reaction\_7, reaction\_18 and as a modifier in re11, re11, re17, re17, re18, reaction\_38, reaction\_7, reaction\_7, reaction\_8, reaction\_8).

$$\frac{\mathrm{d}}{\mathrm{d}t}s21 = |v_9| + |v_{54}| + |v_{58}| - |v_{10}| - |v_{51}| \tag{338}$$

## **11.17 Species** s22

#### Name M0

### Initial concentration 1000000 item · ml<sup>-1</sup>

This species takes part in eleven reactions (as a reactant in re16, re17, reaction\_32, reaction\_15, reaction\_18 and as a product in reaction\_27 and as a modifier in re16, re17, reaction\_32, reaction\_15, reaction\_18).

$$\frac{\mathrm{d}}{\mathrm{d}t}s22 = |v_{47}| - |v_8| - |v_9| - |v_{49}| - |v_{57}| - |v_{58}| \tag{339}$$

### **11.18 Species** s25

### Name tDC

## Initial concentration $0 \text{ item} \cdot \text{ml}^{-1}$

This species takes part in 13 reactions (as a reactant in re22 and as a product in re20, reaction\_17, reaction\_25 and as a modifier in re11, re11, re17, re17, re22, reaction\_7, reaction\_7, reaction\_8, reaction\_8).

$$\frac{\mathrm{d}}{\mathrm{d}t}s25 = |v_{11}| + |v_{43}| + |v_{62}| - |v_{13}| \tag{340}$$

## **11.19 Species** s17

Name emT

Initial concentration 1198199.01671451 item·ml<sup>-1</sup>

This species takes part in nine reactions (as a reactant in re11, reaction\_10, reaction\_11 and as a product in re43, re44, re45 and as a modifier in re11, reaction\_10, reaction\_11).

$$\frac{\mathrm{d}}{\mathrm{d}t}s17 = |v_{25}| + |v_{26}| + |v_{27}| - |v_{5}| - |v_{37}| - |v_{38}| \tag{341}$$

## **11.20 Species** s6

Name HP

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

This species takes part in 17 reactions (as a reactant in re6, re20, reaction\_3, reaction\_4, reaction\_19, reaction\_15, reaction\_18 and as a product in re3, reaction\_3, reaction\_16 and as a modifier in re6, re20, reaction\_3, reaction\_4, reaction\_19, reaction\_15, reaction\_18).

$$\frac{\mathrm{d}}{\mathrm{d}t}s6 = v_2 + 2v_{33} + v_{42} - v_4 - v_{11} - v_{33} - v_{34} - v_{44} - v_{57} - v_{58}$$
 (342)

## 11.21 Species species\_1

Name iDC

Initial concentration  $1000000 \, \text{item} \cdot \text{ml}^{-1}$ 

This species takes part in nine reactions (as a reactant in re6, re20, reaction\_31, reaction\_23 and as a product in reaction\_24 and as a modifier in re6, re20, reaction\_31, reaction\_23).

$$\frac{d}{dt} \text{species}_{-1} = |v_{46}| - |v_{4}| - |v_{11}| - |v_{48}| - |v_{61}|$$
(343)

## 11.22 Species species\_2

Name TotalDC

Initial concentration 5501140.56260765 item·ml<sup>-1</sup>

Involved in rule species\_2

One rule determines the species' quantity.

## 11.23 Species species\_3

Name TotalM

Initial concentration  $1000000 \, \text{item} \cdot \text{ml}^{-1}$ 

Involved in rule species\_3

One rule determines the species' quantity.

## 11.24 Species species\_4

Name TotalT

Initial concentration 1198199.01671451 item·ml<sup>-1</sup>

Involved in rule species\_4

One rule determines the species' quantity.

## 11.25 Species species\_18

Name eDCLB

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

This species takes part in six reactions (as a reactant in reaction\_41 and as a modifier in reaction\_10, reaction\_10, reaction\_11, reaction\_11, reaction\_41).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species}_{1}18 = -v_{71} \tag{344}$$

### 11.26 Species species\_19

Name pEC

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

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

$$\frac{d}{dt} species_{-}19 = 0 \tag{345}$$

## **11.27 Species** s2

Name E

Initial concentration  $10000 \, \mathrm{item} \cdot \mathrm{ml}^{-1}$ 

This species takes part in eight reactions (as a reactant in re2, re15, reaction\_43 and as a product in reaction\_1, reaction\_2 and as a modifier in re2, re15, reaction\_43).

$$\frac{\mathrm{d}}{\mathrm{d}t}s2 = |v_{31}| + |v_{32}| - |v_{1}| - |v_{7}| - |v_{73}| \tag{346}$$

## **11.28 Species** s3

#### Name Ep

## Initial concentration $0 \text{ item} \cdot \text{ml}^{-1}$

This species takes part in 24 reactions (as a reactant in re4, reaction\_1 and as a product in re2, reaction\_43 and as a modifier in re4, re16, re16, re18, re18, re42, re42, reaction\_1, reaction\_16, reaction\_19, reaction\_19, reaction\_20, reaction\_20, reaction\_24, reaction\_24, reaction\_27, reaction\_27, reaction\_27, reaction\_43, reaction\_43).

$$\frac{\mathrm{d}}{\mathrm{d}t}s3 = |v_1| + |v_{73}| - |v_3| - |v_{31}| \tag{347}$$

## 11.29 Species species\_5

#### Name Edead

### Initial concentration 0 item · ml<sup>-1</sup>

This species takes part in six reactions (as a reactant in reaction\_2 and as a product in re4, re15 and as a modifier in re3, re3, reaction\_2).

$$\frac{d}{dt} \text{species}_{5} = |v_{3}| + |v_{7}| - |v_{32}| \tag{348}$$

### **11.30 Species** s4

### Name iDC

## Initial concentration 4501139.56260765 item·ml<sup>-1</sup>

This species takes part in ten reactions (as a reactant in re13, reaction\_17, reaction\_25, reaction\_26 and as a product in reaction\_23 and as a modifier in re13, reaction\_17, reaction\_23, reaction\_25, reaction\_26).

$$\frac{\mathrm{d}}{\mathrm{d}t}s4 = |v_{61}| - |v_{6}| - |v_{43}| - |v_{62}| - |v_{63}| \tag{349}$$

## **11.31 Species** s26

#### Name eDC

### Initial concentration $0 \text{ item} \cdot \text{ml}^{-1}$

This species takes part in 15 reactions (as a reactant in reaction\_21 and as a product in re21 and as a modifier in re23, re23, re24, re24, re28, re28, re29, re29, re41, re41, reaction\_13, reaction\_13, reaction\_21).

$$\frac{d}{dt}s26 = |v_{12}| - |v_{59}| \tag{350}$$

## **11.32 Species** s27

Name tDC

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

This species takes part in nine reactions (as a reactant in reaction\_22 and as a product in re22 and as a modifier in re27, re31, re31, reaction\_9, reaction\_9, reaction\_22).

$$\frac{\mathrm{d}}{\mathrm{d}t} s27 = |v_{13}| - |v_{60}| \tag{351}$$

## **11.33 Species** s28

Name nT

Initial concentration 10<sup>7</sup> item·ml<sup>-1</sup>

This species takes part in 15 reactions (as a reactant in re23, re24, re27, reaction\_14, reaction\_45, reaction\_50, reaction\_54 and as a product in reaction\_13 and as a modifier in re23, re24, re27, reaction\_14, reaction\_45, reaction\_50, reaction\_54).

$$\frac{\mathrm{d}}{\mathrm{d}t}s28 = |v_{40} - v_{14}| - |v_{15}| - |v_{16}| - |v_{41}| - |v_{75}| - |v_{80}| - |v_{84}| \tag{352}$$

## **11.34 Species** s29

Name cmT

Initial concentration  $4.17752018460542 \cdot 10^7 \text{ item} \cdot \text{ml}^{-1}$ 

This species takes part in nine reactions (as a reactant in re28, re29, re31 and as a product in re46, re47, re49 and as a modifier in re28, re29, re31).

$$\frac{\mathrm{d}}{\mathrm{d}t}s29 = |v_{28}| + |v_{29}| + |v_{30}| - |v_{17}| - |v_{18}| - |v_{19}| \tag{353}$$

## **11.35 Species** s30

Name Th17

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

This species takes part in ten reactions (as a reactant in re32, reaction\_9 and as a product in re23, re28, re41, reaction\_36 and as a modifier in re32, re41, re41, reaction\_9).

$$\frac{\mathrm{d}}{\mathrm{d}t}s30 = |v_{14} + v_{17}| + |v_{23}| + |v_{70}| - |v_{20}| - |v_{56}| \tag{354}$$

## **11.36 Species** s31

Name Th1

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

This species takes part in seven reactions (as a reactant in re33 and as a product in re24, re29, reaction\_35 and as a modifier in re33, re41, re41).

$$\frac{\mathrm{d}}{\mathrm{d}t}s31 = |v_{15}| + |v_{18}| + |v_{69}| - |v_{21}| \tag{355}$$

## **11.37 Species** s33

Name iTreg

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

This species takes part in ten reactions (as a reactant in re35, re41 and as a product in re27, re31, reaction\_9, reaction\_34 and as a modifier in re35, re41, reaction\_9, reaction\_9).

$$\frac{\mathrm{d}}{\mathrm{d}t}s33 = |v_{16} + v_{19}| + |v_{56}| + |v_{68}| - |v_{22}| - |v_{23}| \tag{356}$$

## 11.38 Species species\_6

Name TotalDC

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

Involved in rule species\_6

One rule determines the species' quantity.

## 11.39 Species species\_8

Name TotalT

Initial concentration  $5.17752018460542 \cdot 10^7 \text{ item} \cdot \text{ml}^{-1}$ 

Involved in rule species\_8

One rule determines the species' quantity.

## 11.40 Species species\_9

Name TotalT-s

Notes Multiplied by 0.01 to account for the fact that the data is in percent.

Initial concentration  $51775.2018460542 \text{ item} \cdot \text{ml}^{-1}$ 

Involved in rule species\_9

One rule determines the species' quantity.

### **11.41 Species** species\_20

Name eDCLB

Initial concentration 1 item  $\cdot$  ml<sup>-1</sup>

This species takes part in eleven reactions (as a reactant in reaction\_42, reaction\_44 and as a product in reaction\_41 and as a modifier in re23, re23, re28, re28, re29, re29, reaction\_42, reaction\_44).

$$\frac{d}{dt} \text{species} 20 = |v_{71}| - |v_{72}| - |v_{74}|$$
 (357)

# A Glossary of Systems Biology Ontology Terms

**SBO:0000290 physical compartment:** Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

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