SBML Model Report

Model name: "Sharp2013 - Lipopolysaccharide induced NFkB activation"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following three authors: Nick Juty[1], Vijayalakshmi Chelliah[2] and Gemma Sharp[3] at September 24th 2013 at 3:42 p. m. and last time modified at March eighth 2014 at 8:25 p. m. Table 1 provides an overview of the quantities of all components of this model.

Table 1: Number of components in this model, which are described in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	53
events	0	constraints	0
reactions	59	function definitions	2
global parameters	0	unit definitions	2
rules	0	initial assignments	0

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2 Unit Definitions

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

2.1 Unit `volume`

Name volume

Definition ml

2.2 Unit `substance`

Name substance

Definition µmol

2.3 Unit `area`

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

Definition m^2

2.4 Unit `length`

Notes Metre is the predefined SBML unit for `length` since SBML Level 2 Version 1.

Definition m

2.5 Unit `time`

Notes Second is the predefined SBML unit for `time`.

Definition s

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
`compartment_1`	compartment	0000290	3	1	litre	☑	

3.1 Compartment compartment_1

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

Name compartment

SBO:0000290 physical compartment

4 Species

This model contains 53 species. The boundary condition of 18 of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 7 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
species_1	CD14	compartment_1	$\mu mol \cdot ml^{-1}$	☑	☑
species_2	IRAK4	compartment_1	$\mu mol \cdot ml^{-1}$	☑	☑
species_3	LBP	compartment_1	$\mu mol \cdot ml^{-1}$	☑	☑
species_4	LPS	compartment_1	$\mu mol \cdot ml^{-1}$	☑	☑
species_5	LPS:LBP:CD14:TLR4:TIRAP:MyD88:IRAK4	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_6	MyD88	compartment_1	$\mu mol \cdot ml^{-1}$	☑	☑
species_7	TIRAP	compartment_1	$\mu mol \cdot ml^{-1}$	☑	☑
species_8	TLR4	compartment_1	$\mu mol \cdot ml^{-1}$	☑	☑
species_9	IRAK1	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_10	TRAF6	compartment_1	$\mu mol \cdot ml^{-1}$	☑	☑
species_11	TRAF6:IRAK1[P]	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_12	TAK1:TAB1:TAB2	compartment_1	$\mu mol \cdot ml^{-1}$	☑	☑
species_13	TAK1:TAB1:TAB2:TRAF6	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_14	IKK	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_15	IKK[P]	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_16	RIP1	compartment_1	$\mu mol \cdot ml^{-1}$	☑	☑
species_17	TRAM	compartment_1	$\mu mol \cdot ml^{-1}$	☑	☑
species_18	TRIF	compartment_1	$\mu mol \cdot ml^{-1}$	☑	☑
species_19	IRF3	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_20	IRF3[P]	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_21	IRF3[P](nuc)	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
species_22	source	compartment_1	$\mu mol \cdot ml^{-1}$	☑	☑
species_23	sink	compartment_1	$\mu mol \cdot ml^{-1}$	☑	☑
species_24	TNFa	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_25	TNFR1	compartment_1	$\mu mol \cdot ml^{-1}$	☑	☑
species_26	TRADD	compartment_1	$\mu mol \cdot ml^{-1}$	☑	☑
species_27	TRAF2	compartment_1	$\mu mol \cdot ml^{-1}$	☑	☑
species_28	TNFa:TNFR1:TRAF2:TRADD:RIP1	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_29	IkBa	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_30	IkBa:NFkB	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_31	NFkB	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_32	IKK[P]:IkBa:NFkB	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_33	IkBb	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_34	IkBb:NFkB	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_35	IKK[P]:IkBb:NFkB	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_36	IkBe	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_37	IkBe:NFkB	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_38	IKK[P]:IkBe:NFkB	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_39	NFkB(nuc)	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_40	IkBa(nuc)	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_41	IkBa:NFkB(nuc)	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_42	IkBb(nuc)	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_43	IkBb:NFkB(nuc)	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_44	IkBe(nuc)	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_45	IkBe:NFkB(nuc)	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_46	IkBa_mRNA	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_47	IkBb_mRNA	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐
species_48	IkBe_mRNA	compartment_1	$\mu mol \cdot ml^{-1}$	☐	☐

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
species_49	IKK[P]:IkBa	compartment_1	$\mu mol \cdot ml^{-1}$	⊟	⊟
species_50	IKK[P]:IkBb	compartment_1	$\mu mol \cdot ml^{-1}$	⊟	⊟
species_51	IKK[P]:IkBe	compartment_1	$\mu mol \cdot ml^{-1}$	⊟	⊟
species_52	LPS:LBP:CD14:TLR4:RIP1:TRAM:TRIF:TBK1/IKKe	compartment_1	$\mu mol \cdot ml^{-1}$	⊟	⊟
species_53	TBK1/IKKe	compartment_1	$\mu mol \cdot ml^{-1}$	☑	☑

5 Function definitions

This is an overview of two function definitions.

5.1 Function definition `function_2`

Name Modified Michaelis Menten

Arguments k, Enzyme, Substrate, Km

Mathematical Expression

$$\frac{\mathrm{k} \cdot \mathrm{Enzyme} \cdot \mathrm{Substrate}}{\mathrm{Km} + \mathrm{Substrate}} \tag{1}$$

5.2 Function definition `function_1`

Name Modified Mass Action

Arguments k1, Enzyme, Substrate1, Substrate2, k2, Product

Mathematical Expression

$$\mathrm{k1} \cdot \mathrm{Enzyme} \cdot \mathrm{Substrate1} \cdot \mathrm{Substrate2} - \mathrm{k2} \cdot \mathrm{Product} \tag{2}$$

6 Reactions

This model contains 59 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 4: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	reaction_1	MYD881) Receptor Complex Formation	$\text{species\_4} + \text{species\_3} + \text{species\_1} + \text{species\_8} + \text{species\_6} + \text{species\_2} + \text{species\_7} \xleftarrow{\text{species\_4, species\_3, species\_1, species\_8, species\_6, species\_2, species\_7, sp}}$	
2	reaction_2	MYD882) IRAK1 and TRAF6 Phosphorylation	$\text{species\_9} + \text{species\_10} \xleftrightarrows{\text{species\_5, species\_5, species\_9, species\_10, species\_11}} \text{species\_}$	
3	reaction_3	MYD883) TAK/TAB Binds to TRAF6	$\text{species\_11} + \text{species\_12} \xleftrightarrows{\text{species\_11, species\_12, species\_13}} \text{species\_13}$	
4	reaction_4	MYD884) IKK Phosphorylation by TAK1	$\text{species\_14} \xrightarrow{\text{species\_13, species\_13, species\_14}} \text{species\_15}$	
5	reaction_5	MYD885) IKK[P] Dephosphorylation	$\text{species\_15} \xrightarrow{\text{species\_15}} \text{species\_14}$	
6	reaction_6	TRIF01) Receptor Complex Formation	$\text{species\_4} + \text{species\_3} + \text{species\_1} + \text{species\_8} + \text{species\_18} + \text{species\_17} + \text{species\_16} + \text{species\_53} \xleftarrow{\text{species\_4, species\_3, species\_1, species\_8, species\_18, species\_17, species\_1}}$	
7	reaction_7	TRIF02) IRF3 Phosphorylation	$\text{species\_19} \xrightarrow{\text{species\_52, species\_52, species\_19}} \text{species\_20}$	
8	reaction_8	TRIF03) IRF3 Dephosphorylation	$\text{species\_20} \xrightarrow{\text{species\_20}} \text{species\_19}$	
9	reaction_9	TRIF04) IRF3 Nuclear Import/Export	$\text{species\_20} \xleftrightarrows{\text{species\_20, species\_21}} \text{species\_21}$	
10	reaction_10	TRIF05) Inducible TNFa Synthesis	$2\,\text{species\_21} \xrightarrow{\text{species\_21}} \text{species\_24} + 2\,\text{species\_21}$	
11	reaction_11	TRIF06) Constitutive TNFa Synthesis	$\text{species\_22} \xrightarrow{\text{species\_22}} \text{species\_24}$	
12	reaction_12	TRIF09) TNFa Degradation	$\text{species\_24} \xrightarrow{\text{species\_24}} \text{species\_23}$	

№	Id	Name	Reaction Equation	SBO
13	reaction_13	TRIF10) TNFa Receptor Complex Formation	species_24 + species_25 + species_27 + species_26 + species_16 $\xrightleftharpoons{\text{species\_24, species\_25, species\_27, species\_26, species\_16, species\_28}}$ spec	
14	reaction_14	TRIF11) IKK Phosphorylation by RIP1	species_14 $\xrightarrow{\text{species\_28, species\_28, species\_14}}$ species_15	
15	reaction_15	NFkB01) IkBa:NFkB Binding	species_29 + species_31 $\xrightleftharpoons{\text{species\_29, species\_31, species\_30}}$ species_30	
16	reaction_16	NFkB02) IKK:IkBa:NFkB Binding (1)	species_15 + species_30 $\xrightleftharpoons{\text{species\_15, species\_30, species\_32}}$ species_32	
17	reaction_17	NFkB03) IkBb:NFkB Binding	species_33 + species_31 $\xrightleftharpoons{\text{species\_33, species\_31, species\_34}}$ species_34	
18	reaction_18	NFkB04) IKK:IkBb:NFkB Binding (1)	species_15 + species_34 $\xrightleftharpoons{\text{species\_15, species\_34, species\_35}}$ species_35	
19	reaction_19	NFkB05) IkBe:NFkB Binding	species_36 + species_31 $\xrightleftharpoons{\text{species\_36, species\_31, species\_37}}$ species_37	
20	reaction_20	NFkB06) IKK:IkBe:NFkB Binding (1)	species_15 + species_37 $\xrightleftharpoons{\text{species\_15, species\_37, species\_38}}$ species_38	
21	reaction_21	NFkB07) IKK:IkBa:NFkB Catalysis	species_32 $\xrightarrow{\text{species\_32}}$ species_15 + species_31	
22	reaction_22	NFkB08) IKK:IkBb:NFkB Catalysis	species_35 $\xrightarrow{\text{species\_35}}$ species_15 + species_31	
23	reaction_23	NFkB09) IKK:IkBe:NFkB Catalysis	species_38 $\xrightarrow{\text{species\_38}}$ species_15 + species_31	
24	reaction_24	NFkB10) IkBa:NFkB Constitutive Degradation	species_30 $\xrightarrow{\text{species\_30}}$ species_31	
25	reaction_25	NFkB11) IkBb:NFkB Constitutive Degradation	species_34 $\xrightarrow{\text{species\_34}}$ species_31	
26	reaction_26	NFkB12) IkBe:NFkB Constitutive Degradation	species_37 $\xrightarrow{\text{species\_37}}$ species_31	
27	reaction_27	NFkB13) NFkB Nuclear Import/Export	species_31 $\xrightleftharpoons{\text{species\_31, species\_39}}$ species_39	
28	reaction_28	NFkB14) Nuclear IkBa:NFkB Binding	species_40 + species_39 $\xrightleftharpoons{\text{species\_40, species\_39, species\_41}}$ species_41	

№	Id	Name	Reaction Equation	SBO
29	reaction_29	NFkB15) Nuclear IkBb:NFkB Binding	$\text{species\_42} + \text{species\_39} \xrightleftharpoons{\text{species\_42, species\_39, species\_43}} \text{species\_43}$	
30	reaction_30	NFkB16) Nuclear IkBe:NFkB Binding	$\text{species\_44} + \text{species\_39} \xrightleftharpoons{\text{species\_44, species\_39, species\_45}} \text{species\_45}$	
31	reaction_31	NFkB17) Constitutive IkBa mRNA Synthesis	$\text{species\_22} \xrightarrow{\text{species\_22}} \text{species\_46}$	
32	reaction_32	NFkB18) Inducible IkBa mRNA Synthesis	$2\,\text{species\_39} \xrightarrow{\text{species\_39}} \text{species\_46} + 2\,\text{species\_39}$	
33	reaction_33	NFkB19) IkBa mRNA degradation	$\text{species\_46} \xrightarrow{\text{species\_46}} \text{species\_23}$	
34	reaction_34	NFkB20) Constitutive IkBb mRNA Synthesis	$\text{species\_22} \xrightarrow{\text{species\_22}} \text{species\_47}$	
35	reaction_35	NFkB21) IkBb mRNA degradation	$\text{species\_47} \xrightarrow{\text{species\_47}} \text{species\_23}$	
36	reaction_36	NFkB22) Constitutive IkBe mRNA Synthesis	$\text{species\_22} \xrightarrow{\text{species\_22}} \text{species\_48}$	
37	reaction_37	NFkB23) IkBe mRNA degradation	$\text{species\_48} \xrightarrow{\text{species\_48}} \text{species\_23}$	
38	reaction_38	NFkB24) IKK:IkBa Binding	$\text{species\_15} + \text{species\_29} \xrightleftharpoons{\text{species\_15, species\_29, species\_49}} \text{species\_49}$	
39	reaction_39	NFkB25) IkBa Translation	$\text{species\_46} \xrightarrow{\text{species\_46}} \text{species\_29} + \text{species\_46}$	
40	reaction_40	NFkB26) IkBa Degradation	$\text{species\_29} \xrightarrow{\text{species\_29}} \text{species\_23}$	
41	reaction_41	NFkB27) IkBa Nuclear Import/Export	$\text{species\_29} \xrightleftharpoons{\text{species\_29, species\_40}} \text{species\_40}$	
42	reaction_42	NFkB28) IKK:IkBb Binding	$\text{species\_15} + \text{species\_33} \xrightleftharpoons{\text{species\_15, species\_33, species\_50}} \text{species\_50}$	
43	reaction_43	NFkB29) IkBb Translation	$\text{species\_47} \xrightarrow{\text{species\_47}} \text{species\_33} + \text{species\_47}$	
44	reaction_44	NFkB30) IkBb Degradation	$\text{species\_33} \xrightarrow{\text{species\_33}} \text{species\_23}$	
45	reaction_45	NFkB31) IkBb Nuclear Import/Export	$\text{species\_33} \xrightleftharpoons{\text{species\_33, species\_42}} \text{species\_42}$	
46	reaction_46	NFkB32) IKK:IkBe Binding	$\text{species\_15} + \text{species\_36} \xrightleftharpoons{\text{species\_15, species\_36, species\_51}} \text{species\_51}$	
47	reaction_47	NFkB33) IkBe Translation	$\text{species\_48} \xrightarrow{\text{species\_48}} \text{species\_36} + \text{species\_48}$	

№	Id	Name	Reaction Equation	SBO
48	reaction_48	NFkB34) IkBe Degradation	$\text{species\_36} \xrightarrow{\text{species\_36}} \text{species\_23}$	
49	reaction_49	NFkB35) IkBe Nuclear Import/Export	$\text{species\_36} \xrightleftharpoons{\text{species\_36, species\_44}} \text{species\_44}$	
50	reaction_50	NFkB36) IKK:IkBa:NFkB Binding (2)	$\text{species\_49} + \text{species\_31} \xrightleftharpoons{\text{species\_49, species\_31, species\_32}} \text{species\_32}$	
51	reaction_51	NFkB37) IkBa:NFkB Nuclear Export	$\text{species\_41} \xrightarrow{\text{species\_41}} \text{species\_30}$	
52	reaction_52	NFkB38) IKK:IkBb:NFkB Binding (2)	$\text{species\_50} + \text{species\_31} \xrightleftharpoons{\text{species\_50, species\_31, species\_35}} \text{species\_35}$	
53	reaction_53	NFkB39) IkBb:NFkB Nuclear Export	$\text{species\_43} \xrightarrow{\text{species\_43}} \text{species\_34}$	
54	reaction_54	NFkB40) IKK:IkBe:NFkB Binding (2)	$\text{species\_51} + \text{species\_31} \xrightleftharpoons{\text{species\_51, species\_31, species\_38}} \text{species\_38}$	
55	reaction_55	NFkB41) IkBe:NFkB Nuclear Export	$\text{species\_45} \xrightarrow{\text{species\_45}} \text{species\_37}$	
56	reaction_56	NFkB42) IKK:IkBa Catalysis	$\text{species\_49} \xrightarrow{\text{species\_49}} \text{species\_15}$	
57	reaction_57	NFkB43) IKK:IkBb Catalysis	$\text{species\_50} \xrightarrow{\text{species\_50}} \text{species\_15}$	
58	reaction_58	NFkB44) IKK:IkBe Catalysis	$\text{species\_51} \xrightarrow{\text{species\_51}} \text{species\_15}$	
59	reaction_59	TRIF06a)Inducible TNFa Synthesis by NFkB	$2\,\text{species\_39} \xrightarrow{\text{species\_39}} \text{species\_24} + 2\,\text{species\_39}$	

6.1 Reaction `reaction_1`

This is a reversible reaction of seven reactants forming one product influenced by eight modifiers.

Name MYD881) Receptor Complex Formation

Reaction equation

$$\text{species\_4} + \text{species\_3} + \text{species\_1} + \text{species\_8} + \text{species\_6} + \text{species\_2} + \text{species\_7} \xrightleftharpoons{\text{species\_4, species\_3, species\_1, sp}} \tag{3}$$

Reactants

Table 5: Properties of each reactant.

Id	Name	SBO
`species_4`	LPS	
`species_3`	LBP	
`species_1`	CD14	
`species_8`	TLR4	
`species_6`	MyD88	
`species_2`	IRAK4	
`species_7`	TIRAP	

Modifiers

Table 6: Properties of each modifier.

Id	Name	SBO
`species_4`	LPS	
`species_3`	LBP	
`species_1`	CD14	
`species_8`	TLR4	
`species_6`	MyD88	
`species_2`	IRAK4	
`species_7`	TIRAP	
`species_5`	LPS:LBP:CD14:TLR4:TIRAP:MyD88:IRAK4	

Product

Table 7: Properties of each product.

Id	Name	SBO
species_5	LPS:LBP:CD14:TLR4:TIRAP:MyD88:IRAK4	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot (\mathrm{k1} \cdot [\mathrm{species\_4}] \cdot [\mathrm{species\_3}] \cdot [\mathrm{species\_1}] \cdot [\mathrm{species\_8}] \cdot [\mathrm{species\_6}] \cdot [\mathrm{species\_2}] \cdot [\mathrm{species\_7}] - \mathrm{k2} \cdot [\mathrm{species\_5}]) \quad (4)$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		10^{-4}		☑
k2	k2		10^{-4}		☑

6.2 Reaction reaction_2

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

Name MYD882) IRAK1 and TRAF6 Phosphorylation

Reaction equation

$$\mathrm{species\_9} + \mathrm{species\_10} \xrightleftharpoons{\mathrm{species\_5,\ species\_5,\ species\_9,\ species\_10,\ species\_11}} \mathrm{species\_11} \quad (5)$$

Reactants

Table 9: Properties of each reactant.

Id	Name	SBO
species_9	IRAK1	
species_10	TRAF6	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
species_5	LPS:LBP:CD14:TLR4:TIRAP:MyD88:IRAK4	
species_5	LPS:LBP:CD14:TLR4:TIRAP:MyD88:IRAK4	
species_9	IRAK1	
species_10	TRAF6	
species_11	TRAF6:IRAK1[P]	

Product

Table 11: Properties of each product.

Id	Name	SBO
species_11	TRAF6:IRAK1[P]	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_1}\left(\mathrm{k1}, [\mathrm{species\_5}], [\mathrm{species\_9}], [\mathrm{species\_10}], \mathrm{k2}, [\mathrm{species\_11}]\right) \tag{6}$$

$$\begin{aligned} &\mathrm{function\_1}\left(\mathrm{k1}, \mathrm{Enzyme}, \mathrm{Substrate1}, \mathrm{Substrate2}, \mathrm{k2}, \mathrm{Product}\right) \\ &\quad = \mathrm{k1} \cdot \mathrm{Enzyme} \cdot \mathrm{Substrate1} \cdot \mathrm{Substrate2} - \mathrm{k2} \cdot \mathrm{Product} \end{aligned} \tag{7}$$

$$\begin{aligned} &\mathrm{function\_1}\left(\mathrm{k1}, \mathrm{Enzyme}, \mathrm{Substrate1}, \mathrm{Substrate2}, \mathrm{k2}, \mathrm{Product}\right) \\ &\quad = \mathrm{k1} \cdot \mathrm{Enzyme} \cdot \mathrm{Substrate1} \cdot \mathrm{Substrate2} - \mathrm{k2} \cdot \mathrm{Product} \end{aligned} \tag{8}$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.001		☑
k2	k2		0.001		☑

6.3 Reaction reaction_3

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

Name MYD883) TAK/TAB Binds to TRAF6

Reaction equation

$$\text{species\_11} + \text{species\_12} \xrightleftharpoons{\text{species\_11, species\_12, species\_13}} \text{species\_13} \tag{9}$$

Reactants

Table 13: Properties of each reactant.

Id	Name	SBO
species_11	TRAF6:IRAK1[P]	
species_12	TAK1:TAB1:TAB2	

Modifiers

Table 14: Properties of each modifier.

Id	Name	SBO
species_11	TRAF6:IRAK1[P]	
species_12	TAK1:TAB1:TAB2	
species_13	TAK1:TAB1:TAB2:TRAF6	

Product

Table 15: Properties of each product.

Id	Name	SBO
species_13	TAK1:TAB1:TAB2:TRAF6	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}(\text{compartment\_1}) \cdot (\text{k1} \cdot [\text{species\_11}] \cdot [\text{species\_12}] - \text{k2} \cdot [\text{species\_13}]) \tag{10}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.003		☑
k2	k2		0.010		☑

6.4 Reaction reaction_4

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

Name MYD884) IKK Phosphorylation by TAK1

Reaction equation

$$\text{species\_14} \xrightarrow{\text{species\_13, species\_13, species\_14}} \text{species\_15} \tag{11}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
species_14	IKK	

Modifiers

Table 18: Properties of each modifier.

Id	Name	SBO
species_13	TAK1:TAB1:TAB2:TRAF6	
species_13	TAK1:TAB1:TAB2:TRAF6	
species_14	IKK	

Product

Table 19: Properties of each product.

Id	Name	SBO
species_15	IKK[P]	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{vol}\left(\text{compartment\_1}\right) \cdot \text{function\_2}\left(\text{k}, [\text{species\_13}], [\text{species\_14}], \text{Km}\right) \tag{12}$$

$$\text{function\_2}\left(\text{k}, \text{Enzyme}, \text{Substrate}, \text{Km}\right) = \frac{\text{k} \cdot \text{Enzyme} \cdot \text{Substrate}}{\text{Km} + \text{Substrate}} \tag{13}$$

$$\text{function\_2}\left(\text{k}, \text{Enzyme}, \text{Substrate}, \text{Km}\right) = \frac{\text{k} \cdot \text{Enzyme} \cdot \text{Substrate}}{\text{Km} + \text{Substrate}} \tag{14}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k	k		0.1		☑
Km	Km		0.1		☑

6.5 Reaction reaction_5

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

Name MYD885) IKK[P] Dephosphorylation

Reaction equation

$$\text{species\_15} \xrightarrow{\text{species\_15}} \text{species\_14} \tag{15}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
species_15	IKK[P]	

Modifier

Table 22: Properties of each modifier.

Id	Name	SBO
species_15	IKK[P]	

Product

Table 23: Properties of each product.

Id	Name	SBO
species_14	IKK	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_15}] \tag{16}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.1		☑

6.6 Reaction reaction_6

This is a reversible reaction of eight reactants forming one product influenced by nine modifiers.

Name TRIF01) Receptor Complex Formation

Reaction equation

$$\mathrm{species\_4} + \mathrm{species\_3} + \mathrm{species\_1} + \mathrm{species\_8} + \mathrm{species\_18} + \mathrm{species\_17} + \mathrm{species\_16} + \mathrm{species\_53} \xrightleftharpoons{\mathrm{species\_4,\ specie}} \tag{17}$$

Reactants

Table 25: Properties of each reactant.

Id	Name	SBO
species_4	LPS	
species_3	LBP	
species_1	CD14	
species_8	TLR4	
species_18	TRIF	
species_17	TRAM	
species_16	RIP1	
species_53	TBK1/IKKe	

Modifiers

Table 26: Properties of each modifier.

Id	Name	SBO
species_4	LPS	
species_3	LBP	
species_1	CD14	
species_8	TLR4	
species_18	TRIF	
species_17	TRAM	
species_16	RIP1	
species_53	TBK1/IKKe	
species_52	LPS:LBP:CD14:TLR4:RIP1:TRAM:TRIF:TBK/IKKe	

Product

Table 27: Properties of each product.

Id	Name	SBO
species_52	LPS:LBP:CD14:TLR4:RIP1:TRAM:TRIF:TBK/IKKe	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot (\mathrm{k1} \cdot [\mathrm{species\_4}] \cdot [\mathrm{species\_3}] \cdot [\mathrm{species\_1}] \cdot [\mathrm{species\_8}] \cdot [\mathrm{species\_18}] \cdot [\mathrm{species\_17}] \cdot [\mathrm{species\_16}] \cdot [\mathrm{species\_53}] - \mathrm{k2} \cdot [\mathrm{species\_52}]) \quad (18)$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		10^{-4}		☑
k2	k2		10^{-4}		☑

6.7 Reaction reaction_7

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

Name TRIF02) IRF3 Phosphorylation

Reaction equation

$$\text{species\_19} \xrightarrow{\text{species\_52, species\_52, species\_19}} \text{species\_20} \tag{19}$$

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
species_19	IRF3	

Modifiers

Table 30: Properties of each modifier.

Id	Name	SBO
species_52	LPS:LBP:CD14:TLR4:RIP1:TRAM:TRIF:TBK/IKKe	
species_52	LPS:LBP:CD14:TLR4:RIP1:TRAM:TRIF:TBK/IKKe	
species_19	IRF3	

Product

Table 31: Properties of each product.

Id	Name	SBO
species_20	IRF3[P]	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{vol}\left(\text{compartment\_1}\right) \cdot \text{function\_2}\left(\text{k}, [\text{species\_52}], [\text{species\_19}], \text{Km}\right) \tag{20}$$

$$\text{function\_2}\left(\text{k}, \text{Enzyme}, \text{Substrate}, \text{Km}\right) = \frac{\text{k} \cdot \text{Enzyme} \cdot \text{Substrate}}{\text{Km} + \text{Substrate}} \tag{21}$$

$$\text{function\_2}\left(\text{k}, \text{Enzyme}, \text{Substrate}, \text{Km}\right) = \frac{\text{k} \cdot \text{Enzyme} \cdot \text{Substrate}}{\text{Km} + \text{Substrate}} \tag{22}$$

Table 32: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k	k		0.1		☑
Km	Km		0.1		☑

6.8 Reaction reaction_8

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

Name TRIF03) IRF3 Dephosphorylation

Reaction equation

$$\text{species\_20} \xrightarrow{\text{species\_20}} \text{species\_19} \tag{23}$$

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
species_20	IRF3[P]	

Modifier

Table 34: Properties of each modifier.

Id	Name	SBO
species_20	IRF3[P]	

Product

Table 35: Properties of each product.

Id	Name	SBO
species_19	IRF3	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_20}] \tag{24}$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.1		☑

6.9 Reaction reaction_9

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

Name TRIF04) IRF3 Nuclear Import/Export

Reaction equation

$$\mathrm{species\_20} \xrightleftharpoons{\mathrm{species\_20},\ \mathrm{species\_21}} \mathrm{species\_21} \tag{25}$$

Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
species_20	IRF3[P]	

Modifiers

Table 38: Properties of each modifier.

Id	Name	SBO
species_20	IRF3[P]	
species_21	IRF3[P](nuc)	

Product

Table 39: Properties of each product.

Id	Name	SBO
species_21	IRF3[P](nuc)	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot (\mathrm{k1} \cdot [\mathrm{species\_20}] - \mathrm{k2} \cdot [\mathrm{species\_21}]) \tag{26}$$

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.1		☑
k2	k2		0.1		☑

6.10 Reaction reaction_10

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

Name TRIF05) Inducible TNFa Synthesis

Reaction equation

$$2\,\mathrm{species\_21} \xrightarrow{\mathrm{species\_21}} \mathrm{species\_24} + 2\,\mathrm{species\_21} \tag{27}$$

Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
species_21	IRF3[P](nuc)	

Modifier

Table 42: Properties of each modifier.

Id	Name	SBO
species_21	IRF3[P](nuc)	

Products

Table 43: Properties of each product.

Id	Name	SBO
species_24	TNFa	
species_21	IRF3[P](nuc)	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_21}]^2 \tag{28}$$

Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.02		☑

6.11 Reaction reaction_11

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

Name TRIF06) Constitutive TNFa Synthesis

Reaction equation

$$\mathrm{species\_22} \xrightarrow{\mathrm{species\_22}} \mathrm{species\_24} \tag{29}$$

Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
species_22	source	

Modifier

Table 46: Properties of each modifier.

Id	Name	SBO
species_22	source	

Product

Table 47: Properties of each product.

Id	Name	SBO
species_24	TNFa	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_22}] \tag{30}$$

Table 48: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.001		☑

6.12 Reaction reaction_12

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

Name TRIF09) TNFa Degradation

Reaction equation

$$\mathrm{species\_24} \xrightarrow{\mathrm{species\_24}} \mathrm{species\_23} \tag{31}$$

Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
species_24	TNFa	

Modifier

Table 50: Properties of each modifier.

Id	Name	SBO
species_24	TNFa	

Id	Name	SBO

Product

Table 51: Properties of each product.

Id	Name	SBO
species_23	sink	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_24}] \tag{32}$$

Table 52: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.1		☑

6.13 Reaction reaction_13

This is a reversible reaction of five reactants forming one product influenced by six modifiers.

Name TRIF10) TNFa Receptor Complex Formation

Reaction equation

$$\mathrm{species\_24} + \mathrm{species\_25} + \mathrm{species\_27} + \mathrm{species\_26} + \mathrm{species\_16} \xrightleftharpoons{\mathrm{species\_24,\ species\_25,\ species\_27,\ species\_26,\ spec}} \tag{33}$$

Reactants

Table 53: Properties of each reactant.

Id	Name	SBO
species_24	TNFa	
species_25	TNFR1	
species_27	TRAF2	
species_26	TRADD	

Id	Name	SBO
species_16	RIP1	

Modifiers

Table 54: Properties of each modifier.

Id	Name	SBO
species_24	TNFa	
species_25	TNFR1	
species_27	TRAF2	
species_26	TRADD	
species_16	RIP1	
species_28	TNFa:TNFR1:TRAF2:TRADD:RIP1	

Product

Table 55: Properties of each product.

Id	Name	SBO
species_28	TNFa:TNFR1:TRAF2:TRADD:RIP1	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot (\mathrm{k1} \cdot [\mathrm{species\_24}] \cdot [\mathrm{species\_25}] \cdot [\mathrm{species\_27}] \cdot [\mathrm{species\_26}] \cdot [\mathrm{species\_16}] - \mathrm{k2} \cdot [\mathrm{species\_28}]) \quad (34)$$

Table 56: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.1		☑
k2	k2		0.1		☑

6.14 Reaction reaction_14

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

Name TRIF11) IKK Phosphorylation by RIP1

Reaction equation

$$\text{species\_14} \xrightarrow{\text{species\_28, species\_28, species\_14}} \text{species\_15} \tag{35}$$

Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
species_14	IKK	

Modifiers

Table 58: Properties of each modifier.

Id	Name	SBO
species_28	TNFa:TNFR1:TRAF2:TRADD:RIP1	
species_28	TNFa:TNFR1:TRAF2:TRADD:RIP1	
species_14	IKK	

Product

Table 59: Properties of each product.

Id	Name	SBO
species_15	IKK[P]	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \text{vol}\left(\text{compartment\_1}\right) \cdot \text{function\_2}\left(\text{k}, [\text{species\_28}], [\text{species\_14}], \text{Km}\right) \tag{36}$$

$$\text{function\_2}\left(\text{k}, \text{Enzyme}, \text{Substrate}, \text{Km}\right) = \frac{\text{k} \cdot \text{Enzyme} \cdot \text{Substrate}}{\text{Km} + \text{Substrate}} \tag{37}$$

$$\text{function\_2}\left(\text{k}, \text{Enzyme}, \text{Substrate}, \text{Km}\right) = \frac{\text{k} \cdot \text{Enzyme} \cdot \text{Substrate}}{\text{Km} + \text{Substrate}} \tag{38}$$

Table 60: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k	k		0.1		☑
Km	Km		0.1		☑

6.15 Reaction reaction_15

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

Name NFkB01) IkBa:NFkB Binding

Reaction equation

$$\text{species\_29} + \text{species\_31} \xrightleftharpoons{\text{species\_29, species\_31, species\_30}} \text{species\_30} \tag{39}$$

Reactants

Table 61: Properties of each reactant.

Id	Name	SBO
species_29	IkBa	
species_31	NFkB	

Modifiers

Table 62: Properties of each modifier.

Id	Name	SBO
species_29	IkBa	
species_31	NFkB	
species_30	IkBa:NFkB	

Product

Table 63: Properties of each product.

Id	Name	SBO
species_30	IkBa:NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot (\mathrm{k1} \cdot [\mathrm{species\_29}] \cdot [\mathrm{species\_31}] - \mathrm{k2} \cdot [\mathrm{species\_30}]) \quad (40)$$

Table 64: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.500		☑
k2	k2		$5 \cdot 10^{-4}$		☑

6.16 Reaction `reaction_16`

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

Name NFkB02) IKK:IkBa:NFkB Binding (1)

Reaction equation

$$\mathrm{species\_15} + \mathrm{species\_30} \xrightleftharpoons{\mathrm{species\_15,\ species\_30,\ species\_32}} \mathrm{species\_32} \quad (41)$$

Reactants

Table 65: Properties of each reactant.

Id	Name	SBO
species_15	IKK[P]	
species_30	IkBa:NFkB	

Modifiers

Table 66: Properties of each modifier.

Id	Name	SBO
species_15	IKK[P]	
species_30	IkBa:NFkB	
species_32	IKK[P]:IkBa:NFkB	

Product

Table 67: Properties of each product.

Id	Name	SBO
species_32	IKK[P]:IkBa:NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot (\mathrm{k1} \cdot [\mathrm{species\_15}] \cdot [\mathrm{species\_30}] - \mathrm{k2} \cdot [\mathrm{species\_32}]) \quad (42)$$

Table 68: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.185		☑
k2	k2		0.013		☑

6.17 Reaction reaction_17

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

Name NFkB03) IkBb:NFkB Binding

Reaction equation

$$\mathrm{species\_33} + \mathrm{species\_31} \xrightleftharpoons{\mathrm{species\_33,\ species\_31,\ species\_34}} \mathrm{species\_34} \quad (43)$$

Reactants

Table 69: Properties of each reactant.

Id	Name	SBO
species_33	IkBb	
species_31	NFkB	

Modifiers

Table 70: Properties of each modifier.

Id	Name	SBO
species_33	IkBb	

Id	Name	SBO
species_31	NFkB	
species_34	IkBb:NFkB	

Product

Table 71: Properties of each product.

Id	Name	SBO
species_34	IkBb:NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot (\mathrm{k1} \cdot [\mathrm{species\_33}] \cdot [\mathrm{species\_31}] - \mathrm{k2} \cdot [\mathrm{species\_34}]) \quad (44)$$

Table 72: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.500		☑
k2	k2		$5 \cdot 10^{-4}$		☑

6.18 Reaction reaction_18

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

Name NFkB04) IKK:IkBb:NFkB Binding (1)

Reaction equation

$$\mathrm{species\_15} + \mathrm{species\_34} \underset{}{\overset{\mathrm{species\_15,\ species\_34,\ species\_35}}{\rightleftharpoons}} \mathrm{species\_35} \quad (45)$$

Reactants

Table 73: Properties of each reactant.

Id	Name	SBO
species_15	IKK[P]	
species_34	IkBb:NFkB	

Modifiers

Table 74: Properties of each modifier.

Id	Name	SBO
species_15	IKK[P]	
species_34	IkBb:NFkB	
species_35	IKK[P]:IkBb:NFkB	

Product

Table 75: Properties of each product.

Id	Name	SBO
species_35	IKK[P]:IkBb:NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot (\mathrm{k1} \cdot [\mathrm{species\_15}] \cdot [\mathrm{species\_34}] - \mathrm{k2} \cdot [\mathrm{species\_35}]) \quad (46)$$

Table 76: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.048		☑
k2	k2		0.002		☑

6.19 Reaction reaction_19

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

Name NFkB05) IkBe:NFkB Binding

Reaction equation

$$\mathrm{species\_36} + \mathrm{species\_31} \underset{}{\overset{\mathrm{species\_36,\ species\_31,\ species\_37}}{\rightleftharpoons}} \mathrm{species\_37} \quad (47)$$

Reactants

Table 77: Properties of each reactant.

Id	Name	SBO
species_36	IkBe	
species_31	NFkB	

Modifiers

Table 78: Properties of each modifier.

Id	Name	SBO
species_36	IkBe	
species_31	NFkB	
species_37	IkBe:NFkB	

Product

Table 79: Properties of each product.

Id	Name	SBO
species_37	IkBe:NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot (\mathrm{k1} \cdot [\mathrm{species\_36}] \cdot [\mathrm{species\_31}] - \mathrm{k2} \cdot [\mathrm{species\_37}]) \quad (48)$$

Table 80: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.500		☑
k2	k2		$5 \cdot 10^{-4}$		☑

6.20 Reaction reaction_20

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

Name NFkB06) IKK:IkBe:NFkB Binding (1)

Reaction equation

$$\text{species\_15} + \text{species\_37} \xrightleftharpoons{\text{species\_15, species\_37, species\_38}} \text{species\_38} \tag{49}$$

Reactants

Table 81: Properties of each reactant.

Id	Name	SBO
species_15	IKK[P]	
species_37	IkBe:NFkB	

Modifiers

Table 82: Properties of each modifier.

Id	Name	SBO
species_15	IKK[P]	
species_37	IkBe:NFkB	
species_38	IKK[P]:IkBe:NFkB	

Product

Table 83: Properties of each product.

Id	Name	SBO
species_38	IKK[P]:IkBe:NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \text{vol}\,(\text{compartment\_1}) \cdot (\text{k1} \cdot [\text{species\_15}] \cdot [\text{species\_37}] - \text{k2} \cdot [\text{species\_38}]) \tag{50}$$

Table 84: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.070		☑
k2	k2		0.002		☑

6.21 Reaction reaction_21

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

Name NFkB07) IKK:IkBa:NFkB Catalysis

Reaction equation

$$\text{species\_32} \xrightarrow{\text{species\_32}} \text{species\_15} + \text{species\_31} \tag{51}$$

Reactant

Table 85: Properties of each reactant.

Id	Name	SBO
species_32	IKK[P]:IkBa:NFkB	

Modifier

Table 86: Properties of each modifier.

Id	Name	SBO
species_32	IKK[P]:IkBa:NFkB	

Products

Table 87: Properties of each product.

Id	Name	SBO
species_15	IKK[P]	
species_31	NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \text{vol}(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_32}] \tag{52}$$

Table 88: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.020		☑

6.22 Reaction reaction_22

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

Name NFkB08) IKK:IkBb:NFkB Catalysis

Reaction equation

$$\text{species\_35} \xrightarrow{\text{species\_35}} \text{species\_15} + \text{species\_31} \tag{53}$$

Reactant

Table 89: Properties of each reactant.

Id	Name	SBO
species_35	IKK[P]:IkBb:NFkB	

Modifier

Table 90: Properties of each modifier.

Id	Name	SBO
species_35	IKK[P]:IkBb:NFkB	

Products

Table 91: Properties of each product.

Id	Name	SBO
species_15	IKK[P]	
species_31	NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_35}] \tag{54}$$

Table 92: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.008		☑

6.23 Reaction reaction_23

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

Name NFkB09) IKK:IkBe:NFkB Catalysis

Reaction equation

$$\mathrm{species\_38} \xrightarrow{\mathrm{species\_38}} \mathrm{species\_15} + \mathrm{species\_31} \tag{55}$$

Reactant

Table 93: Properties of each reactant.

Id	Name	SBO
species_38	IKK[P]:IkBe:NFkB	

Modifier

Table 94: Properties of each modifier.

Id	Name	SBO
species_38	IKK[P]:IkBe:NFkB	

Products

Table 95: Properties of each product.

Id	Name	SBO
species_15	IKK[P]	
species_31	NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_38}] \tag{56}$$

Table 96: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.011		☑

6.24 Reaction reaction_24

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

Name NFkB10) IkBa:NFkB Constitutive Degradation

Reaction equation

$$\mathrm{species\_30} \xrightarrow{\mathrm{species\_30}} \mathrm{species\_31} \tag{57}$$

Reactant

Table 97: Properties of each reactant.

Id	Name	SBO
species_30	IkBa:NFkB	

Modifier

Table 98: Properties of each modifier.

Id	Name	SBO
species_30	IkBa:NFkB	

Product

Table 99: Properties of each product.

Id	Name	SBO
species_31	NFkB	

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_30}] \tag{58}$$

Table 100: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$2.25 \cdot 10^{-5}$		☑

6.25 Reaction reaction_25

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

Name NFkB11) IkBb:NFkB Constitutive Degradation

Reaction equation

$$\mathrm{species\_34} \xrightarrow{\mathrm{species\_34}} \mathrm{species\_31} \tag{59}$$

Reactant

Table 101: Properties of each reactant.

Id	Name	SBO
species_34	IkBb:NFkB	

Modifier

Table 102: Properties of each modifier.

Id	Name	SBO
species_34	IkBb:NFkB	

Product

Table 103: Properties of each product.

Id	Name	SBO
species_31	NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_34}] \tag{60}$$

Table 104: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$2.25 \cdot 10^{-5}$		☑

6.26 Reaction reaction_26

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

Name NFkB12) IkBe:NFkB Constitutive Degradation

Reaction equation

$$\mathrm{species\_37} \xrightarrow{\mathrm{species\_37}} \mathrm{species\_31} \tag{61}$$

Reactant

Table 105: Properties of each reactant.

Id	Name	SBO
species_37	IkBe:NFkB	

Modifier

Table 106: Properties of each modifier.

Id	Name	SBO
species_37	IkBe:NFkB	

Product

Table 107: Properties of each product.

Id	Name	SBO
species_31	NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_37}] \tag{62}$$

Table 108: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$2.25 \cdot 10^{-5}$		☑

6.27 Reaction reaction_27

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

Name NFkB13) NFkB Nuclear Import/Export

Reaction equation

$$\mathrm{species\_31} \xrightleftharpoons{\mathrm{species\_31,\ species\_39}} \mathrm{species\_39} \tag{63}$$

Reactant

Table 109: Properties of each reactant.

Id	Name	SBO
species_31	NFkB	

Modifiers

Table 110: Properties of each modifier.

Id	Name	SBO
species_31	NFkB	
species_39	NFkB(nuc)	

Product

Table 111: Properties of each product.

Id	Name	SBO
species_39	NFkB(nuc)	

Kinetic Law

Derived unit contains undeclared units

$$v_{27} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot (\mathrm{k1} \cdot [\mathrm{species\_31}] - \mathrm{k2} \cdot [\mathrm{species\_39}]) \tag{64}$$

Table 112: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.090		☑
k2	k2		$8 \cdot 10^{-5}$		☑

6.28 Reaction reaction_28

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

Name NFkB14) Nuclear IkBa:NFkB Binding

Reaction equation

$$\mathrm{species\_40} + \mathrm{species\_39} \xrightleftharpoons{\mathrm{species\_40,\ species\_39,\ species\_41}} \mathrm{species\_41} \tag{65}$$

Reactants

Table 113: Properties of each reactant.

Id	Name	SBO
species_40	IkBa(nuc)	

Id	Name	SBO
species_39	NFkB(nuc)	

Modifiers

Table 114: Properties of each modifier.

Id	Name	SBO
species_40	IkBa(nuc)	
species_39	NFkB(nuc)	
species_41	IkBa:NFkB(nuc)	

Product

Table 115: Properties of each product.

Id	Name	SBO
species_41	IkBa:NFkB(nuc)	

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot (\mathrm{k1} \cdot [\mathrm{species\_40}] \cdot [\mathrm{species\_39}] - \mathrm{k2} \cdot [\mathrm{species\_41}]) \quad (66)$$

Table 116: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.500		☑
k2	k2		$5 \cdot 10^{-4}$		☑

6.29 Reaction reaction_29

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

Name NFkB15) Nuclear IkBb:NFkB Binding

Reaction equation

$$\mathrm{species\_42} + \mathrm{species\_39} \underset{\leftarrow}{\overset{\mathrm{species\_42,\ species\_39,\ species\_43}}{\rightarrow}} \mathrm{species\_43} \quad (67)$$

Reactants

Table 117: Properties of each reactant.

Id	Name	SBO
species_42	IkBb(nuc)	
species_39	NFkB(nuc)	

Modifiers

Table 118: Properties of each modifier.

Id	Name	SBO
species_42	IkBb(nuc)	
species_39	NFkB(nuc)	
species_43	IkBb:NFkB(nuc)	

Product

Table 119: Properties of each product.

Id	Name	SBO
species_43	IkBb:NFkB(nuc)	

Kinetic Law

Derived unit contains undeclared units

$$v_{29} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot (\mathrm{k1} \cdot [\mathrm{species\_42}] \cdot [\mathrm{species\_39}] - \mathrm{k2} \cdot [\mathrm{species\_43}]) \quad (68)$$

Table 120: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.500		☑
k2	k2		$5 \cdot 10^{-4}$		☑

6.30 Reaction reaction_30

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

Name NFkB16) Nuclear IkBe:NFkB Binding

Reaction equation

$$\text{species\_44} + \text{species\_39} \underset{}{\overset{\text{species\_44, species\_39, species\_45}}{\rightleftharpoons}} \text{species\_45} \tag{69}$$

Reactants

Table 121: Properties of each reactant.

Id	Name	SBO
species_44	IkBe(nuc)	
species_39	NFkB(nuc)	

Modifiers

Table 122: Properties of each modifier.

Id	Name	SBO
species_44	IkBe(nuc)	
species_39	NFkB(nuc)	
species_45	IkBe:NFkB(nuc)	

Product

Table 123: Properties of each product.

Id	Name	SBO
species_45	IkBe:NFkB(nuc)	

Kinetic Law

Derived unit contains undeclared units

$$v_{30} = \text{vol}\,(\text{compartment\_1}) \cdot (\text{k1} \cdot [\text{species\_44}] \cdot [\text{species\_39}] - \text{k2} \cdot [\text{species\_45}]) \tag{70}$$

Table 124: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.500		☑
k2	k2		$5 \cdot 10^{-4}$		☑

6.31 Reaction reaction_31

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

Name NFkB17) Constitutive IkBa mRNA Synthesis

Reaction equation

$$\text{species\_22} \xrightarrow{\text{species\_22}} \text{species\_46} \tag{71}$$

Reactant

Table 125: Properties of each reactant.

Id	Name	SBO
species_22	source	

Modifier

Table 126: Properties of each modifier.

Id	Name	SBO
species_22	source	

Product

Table 127: Properties of each product.

Id	Name	SBO
species_46	IkBa_mRNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{31} = \text{vol}(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_22}] \tag{72}$$

Table 128: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$1.54 \cdot 10^{-6}$		☑

6.32 Reaction reaction_32

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

Name NFkB18) Inducible IkBa mRNA Synthesis

Reaction equation

$$2\,\text{species\_39} \xrightarrow{\text{species\_39}} \text{species\_46} + 2\,\text{species\_39} \tag{73}$$

Reactant

Table 129: Properties of each reactant.

Id	Name	SBO
species_39	NFkB(nuc)	

Modifier

Table 130: Properties of each modifier.

Id	Name	SBO
species_39	NFkB(nuc)	

Products

Table 131: Properties of each product.

Id	Name	SBO
species_46	IkBa_mRNA	
species_39	NFkB(nuc)	

Kinetic Law

Derived unit contains undeclared units

$$v_{32} = \text{vol}\,(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_39}]^2 \tag{74}$$

Table 132: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.017		☑

6.33 Reaction reaction_33

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

Name NFkB19) IkBa mRNA degradation

Reaction equation

$$\text{species\_46} \xrightarrow{\text{species\_46}} \text{species\_23} \tag{75}$$

Reactant

Table 133: Properties of each reactant.

Id	Name	SBO
species_46	IkBa_mRNA	

Modifier

Table 134: Properties of each modifier.

Id	Name	SBO
species_46	IkBa_mRNA	

Product

Table 135: Properties of each product.

Id	Name	SBO
species_23	sink	

Kinetic Law

Derived unit contains undeclared units

$$v_{33} = \text{vol}(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_46}] \tag{76}$$

Table 136: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$2.8 \cdot 10^{-4}$		☑

6.34 Reaction reaction_34

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

Name NFkB20) Constitutive IkBb mRNA Synthesis

Reaction equation

$$\text{species\_22} \xrightarrow{\text{species\_22}} \text{species\_47} \tag{77}$$

Reactant

Table 137: Properties of each reactant.

Id	Name	SBO
species_22	source	

Modifier

Table 138: Properties of each modifier.

Id	Name	SBO
species_22	source	

Product

Table 139: Properties of each product.

Id	Name	SBO
species_47	IkBb_mRNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{34} = \text{vol}(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_22}] \tag{78}$$

Table 140: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$1.78 \cdot 10^{-7}$		☑

6.35 Reaction reaction_35

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

Name NFkB21) IkBb mRNA degradation

Reaction equation

$$\text{species\_47} \xrightarrow{\text{species\_47}} \text{species\_23} \tag{79}$$

Reactant

Table 141: Properties of each reactant.

Id	Name	SBO
species_47	IkBb_mRNA	

Modifier

Table 142: Properties of each modifier.

Id	Name	SBO
species_47	IkBb_mRNA	

Product

Table 143: Properties of each product.

Id	Name	SBO
species_23	sink	

Kinetic Law

Derived unit contains undeclared units

$$v_{35} = \text{vol}(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_47}] \tag{80}$$

Table 144: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$2.8 \cdot 10^{-4}$		☑

6.36 Reaction reaction_36

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

Name NFkB22) Constitutive IkBe mRNA Synthesis

Reaction equation

$$\text{species\_22} \xrightarrow{\text{species\_22}} \text{species\_48} \tag{81}$$

Reactant

Table 145: Properties of each reactant.

Id	Name	SBO
species_22	source	

Modifier

Table 146: Properties of each modifier.

Id	Name	SBO
species_22	source	

Product

Table 147: Properties of each product.

Id	Name	SBO
species_48	IkBe_mRNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{36} = \text{vol}(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_22}] \tag{82}$$

Table 148: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$1.27 \cdot 10^{-7}$		☑

6.37 Reaction reaction_37

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

Name NFkB23) IkBe mRNA degradation

Reaction equation

$$\text{species\_48} \xrightarrow{\text{species\_48}} \text{species\_23} \tag{83}$$

Reactant

Table 149: Properties of each reactant.

Id	Name	SBO
species_48	IkBe_mRNA	

Modifier

Table 150: Properties of each modifier.

Id	Name	SBO
species_48	IkBe_mRNA	

Product

Table 151: Properties of each product.

Id	Name	SBO
species_23	sink	

Kinetic Law

Derived unit contains undeclared units

$$v_{37} = \text{vol}(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_48}] \tag{84}$$

Table 152: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$2.8 \cdot 10^{-4}$		☑

6.38 Reaction reaction_38

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

Name NFkB24) IKK:IkBa Binding

Reaction equation

$$\text{species\_15} + \text{species\_29} \xrightleftharpoons{\text{species\_15, species\_29, species\_49}} \text{species\_49} \tag{85}$$

Reactants

Table 153: Properties of each reactant.

Id	Name	SBO
species_15	IKK[P]	
species_29	IkBa	

Modifiers

Table 154: Properties of each modifier.

Id	Name	SBO
species_15	IKK[P]	
species_29	IkBa	
species_49	IKK[P]:IkBa	

Product

Table 155: Properties of each product.

Id	Name	SBO
species_49	IKK[P]:IkBa	

Kinetic Law

Derived unit contains undeclared units

$$v_{38} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot (\mathrm{k1} \cdot [\mathrm{species\_15}] \cdot [\mathrm{species\_29}] - \mathrm{k2} \cdot [\mathrm{species\_49}]) \quad (86)$$

Table 156: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.023		☑
k2	k2		0.001		☑

6.39 Reaction reaction_39

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

Name NFkB25) IkBa Translation

Reaction equation

$$\mathrm{species\_46} \xrightarrow{\mathrm{species\_46}} \mathrm{species\_29} + \mathrm{species\_46} \quad (87)$$

Reactant

Table 157: Properties of each reactant.

Id	Name	SBO
species_46	IkBa_mRNA	

Modifier

Table 158: Properties of each modifier.

Id	Name	SBO
species_46	IkBa_mRNA	

Products

Table 159: Properties of each product.

Id	Name	SBO
species_29	IkBa	
species_46	IkBa_mRNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{39} = \mathrm{vol}(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_46}] \tag{88}$$

Table 160: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.004		☑

6.40 Reaction reaction_40

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

Name NFkB26) IkBa Degradation

Reaction equation

$$\mathrm{species\_29} \xrightarrow{\mathrm{species\_29}} \mathrm{species\_23} \tag{89}$$

Reactant

Table 161: Properties of each reactant.

Id	Name	SBO
species_29	IkBa	

Modifier

Table 162: Properties of each modifier.

Id	Name	SBO
species_29	IkBa	

Product

Table 163: Properties of each product.

Id	Name	SBO
species_23	sink	

Kinetic Law

Derived unit contains undeclared units

$$v_{40} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{k1} \cdot [\mathrm{species\_29}] \tag{90}$$

Table 164: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$1.13 \cdot 10^{-4}$		☑

6.41 Reaction reaction_41

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

Name NFkB27) IkBa Nuclear Import/Export

Reaction equation

$$\mathrm{species\_29} \xrightleftharpoons{\mathrm{species\_29,\ species\_40}} \mathrm{species\_40} \tag{91}$$

Reactant

Table 165: Properties of each reactant.

Id	Name	SBO
species_29	IkBa	

Modifiers

Table 166: Properties of each modifier.

Id	Name	SBO
species_29	IkBa	
species_40	IkBa(nuc)	

Product

Table 167: Properties of each product.

Id	Name	SBO
species_40	IkBa(nuc)	

Kinetic Law

Derived unit contains undeclared units

$$v_{41} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot (\mathrm{k1} \cdot [\mathrm{species\_29}] - \mathrm{k2} \cdot [\mathrm{species\_40}]) \tag{92}$$

Table 168: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$3 \cdot 10^{-4}$		☑
k2	k2		$2 \cdot 10^{-4}$		☑

6.42 Reaction reaction_42

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

Name NFkB28) IKK:IkBb Binding

Reaction equation

$$\mathrm{species\_15} + \mathrm{species\_33} \xrightleftharpoons{\mathrm{species\_15,\ species\_33,\ species\_50}} \mathrm{species\_50} \tag{93}$$

Reactants

Table 169: Properties of each reactant.

Id	Name	SBO
species_15	IKK[P]	

Id	Name	SBO
species_33	IkBb	

Modifiers

Table 170: Properties of each modifier.

Id	Name	SBO
species_15	IKK[P]	
species_33	IkBb	
species_50	IKK[P]:IkBb	

Product

Table 171: Properties of each product.

Id	Name	SBO
species_50	IKK[P]:IkBb	

Kinetic Law

Derived unit contains undeclared units

$$v_{42} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot (\mathrm{k1} \cdot [\mathrm{species\_15}] \cdot [\mathrm{species\_33}] - \mathrm{k2} \cdot [\mathrm{species\_50}]) \quad (94)$$

Table 172: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.006		☑
k2	k2		0.002		☑

6.43 Reaction reaction_43

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

Name NFkB29) IkBb Translation

Reaction equation

$$\mathrm{species\_47} \xrightarrow{\mathrm{species\_47}} \mathrm{species\_33} + \mathrm{species\_47} \quad (95)$$

Reactant

Table 173: Properties of each reactant.

Id	Name	SBO
species_47	IkBb_mRNA	

Modifier

Table 174: Properties of each modifier.

Id	Name	SBO
species_47	IkBb_mRNA	

Products

Table 175: Properties of each product.

Id	Name	SBO
species_33	IkBb	
species_47	IkBb_mRNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{43} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{k1} \cdot [\mathrm{species\_47}] \tag{96}$$

Table 176: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.004		☑

6.44 Reaction reaction_44

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

Name NFkB30) IkBb Degradation

Reaction equation

$$\text{species\_33} \xrightarrow{\text{species\_33}} \text{species\_23} \tag{97}$$

Reactant

Table 177: Properties of each reactant.

Id	Name	SBO
species_33	IkBb	

Modifier

Table 178: Properties of each modifier.

Id	Name	SBO
species_33	IkBb	

Product

Table 179: Properties of each product.

Id	Name	SBO
species_23	sink	

Kinetic Law

Derived unit contains undeclared units

$$v_{44} = \text{vol}(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_33}] \tag{98}$$

Table 180: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$1.13 \cdot 10^{-4}$		☑

6.45 Reaction reaction_45

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

Name NFkB31) IkBb Nuclear Import/Export

Reaction equation

$$\text{species\_33} \underset{}{\overset{\text{species\_33, species\_42}}{\rightleftharpoons}} \text{species\_42} \tag{99}$$

Reactant

Table 181: Properties of each reactant.

Id	Name	SBO
species_33	IkBb	

Modifiers

Table 182: Properties of each modifier.

Id	Name	SBO
species_33	IkBb	
species_42	IkBb(nuc)	

Product

Table 183: Properties of each product.

Id	Name	SBO
species_42	IkBb(nuc)	

Kinetic Law

Derived unit contains undeclared units

$$v_{45} = \text{vol}\,(\text{compartment\_1}) \cdot (\text{k1} \cdot [\text{species\_33}] - \text{k2} \cdot [\text{species\_42}]) \tag{100}$$

Table 184: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$1.5 \cdot 10^{-4}$		☑
k2	k2		10^{-4}		☑

6.46 Reaction reaction_46

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

Name NFkB32) IKK:IkBe Binding

Reaction equation

$$\text{species\_15} + \text{species\_36} \xrightleftharpoons{\text{species\_15, species\_36, species\_51}} \text{species\_51} \tag{101}$$

Reactants

Table 185: Properties of each reactant.

Id	Name	SBO
species_15	IKK[P]	
species_36	IkBe	

Modifiers

Table 186: Properties of each modifier.

Id	Name	SBO
species_15	IKK[P]	
species_36	IkBe	
species_51	IKK[P]:IkBe	

Product

Table 187: Properties of each product.

Id	Name	SBO
species_51	IKK[P]:IkBe	

Kinetic Law

Derived unit contains undeclared units

$$v_{46} = \text{vol}\,(\text{compartment\_1}) \cdot (\text{k1} \cdot [\text{species\_15}] \cdot [\text{species\_36}] - \text{k2} \cdot [\text{species\_51}]) \tag{102}$$

Table 188: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.009		☑
k2	k2		0.002		☑

6.47 Reaction reaction_47

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

Name NFkB33) IkBe Translation

Reaction equation

$$\text{species\_48} \xrightarrow{\text{species\_48}} \text{species\_36} + \text{species\_48} \tag{103}$$

Reactant

Table 189: Properties of each reactant.

Id	Name	SBO
species_48	IkBe_mRNA	

Modifier

Table 190: Properties of each modifier.

Id	Name	SBO
species_48	IkBe_mRNA	

Products

Table 191: Properties of each product.

Id	Name	SBO
species_36	IkBe	
species_48	IkBe_mRNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{47} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_48}] \tag{104}$$

Table 192: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.004		☑

6.48 Reaction reaction_48

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

Name NFkB34) IkBe Degradation

Reaction equation

$$\mathrm{species\_36} \xrightarrow{\mathrm{species\_36}} \mathrm{species\_23} \tag{105}$$

Reactant

Table 193: Properties of each reactant.

Id	Name	SBO
species_36	IkBe	

Modifier

Table 194: Properties of each modifier.

Id	Name	SBO
species_36	IkBe	

Product

Table 195: Properties of each product.

Id	Name	SBO
species_23	sink	

Kinetic Law

Derived unit contains undeclared units

$$v_{48} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{k1} \cdot [\mathrm{species\_36}] \tag{106}$$

Table 196: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$1.13 \cdot 10^{-4}$		☑

6.49 Reaction reaction_49

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

Name NFkB35) IkBe Nuclear Import/Export

Reaction equation

$$\mathrm{species\_36} \xrightleftharpoons{\mathrm{species\_36,\ species\_44}} \mathrm{species\_44} \tag{107}$$

Reactant

Table 197: Properties of each reactant.

Id	Name	SBO
species_36	IkBe	

Modifiers

Table 198: Properties of each modifier.

Id	Name	SBO
species_36	IkBe	
species_44	IkBe(nuc)	

Product

Table 199: Properties of each product.

Id	Name	SBO
species_44	IkBe(nuc)	

Kinetic Law

Derived unit contains undeclared units

$$v_{49} = \mathrm{vol}(\mathrm{compartment\_1}) \cdot (\mathrm{k1} \cdot [\mathrm{species\_36}] - \mathrm{k2} \cdot [\mathrm{species\_44}]) \tag{108}$$

Table 200: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		$1.5 \cdot 10^{-4}$		☑
k2	k2		10^{-4}		☑

6.50 Reaction reaction_50

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

Name NFkB36) IKK:IkBa:NFkB Binding (2)

Reaction equation

$$\mathrm{species\_49} + \mathrm{species\_31} \xrightleftharpoons{\mathrm{species\_49},\ \mathrm{species\_31},\ \mathrm{species\_32}} \mathrm{species\_32} \tag{109}$$

Reactants

Table 201: Properties of each reactant.

Id	Name	SBO
species_49	IKK[P]:IkBa	
species_31	NFkB	

Modifiers

Table 202: Properties of each modifier.

Id	Name	SBO
species_49	IKK[P]:IkBa	

Id	Name	SBO
species_31	NFkB	
species_32	IKK[P]:IkBa:NFkB	

Product

Table 203: Properties of each product.

Id	Name	SBO
species_32	IKK[P]:IkBa:NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{50} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot (\mathrm{k1} \cdot [\mathrm{species\_49}] \cdot [\mathrm{species\_31}] - \mathrm{k2} \cdot [\mathrm{species\_32}]) \quad (110)$$

Table 204: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.500		☑
k2	k2		$5 \cdot 10^{-4}$		☑

6.51 Reaction reaction_51

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

Name NFkB37) IkBa:NFkB Nuclear Export

Reaction equation

$$\mathrm{species\_41} \xrightarrow{\mathrm{species\_41}} \mathrm{species\_30} \quad (111)$$

Reactant

Table 205: Properties of each reactant.

Id	Name	SBO
species_41	IkBa:NFkB(nuc)	

Modifier

Table 206: Properties of each modifier.

Id	Name	SBO
species_41	IkBa:NFkB(nuc)	

Product

Table 207: Properties of each product.

Id	Name	SBO
species_30	IkBa:NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{51} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{k1} \cdot \left[\mathrm{species\_41}\right] \tag{112}$$

Table 208: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.014		☑

6.52 Reaction reaction_52

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

Name NFkB38) IKK:IkBb:NFkB Binding (2)

Reaction equation

$$\mathrm{species\_50} + \mathrm{species\_31} \underset{}{\overset{\mathrm{species\_50,\ species\_31,\ species\_35}}{\rightleftharpoons}} \mathrm{species\_35} \tag{113}$$

Reactants

Table 209: Properties of each reactant.

Id	Name	SBO
species_50	IKK[P]:IkBb	
species_31	NFkB	

Modifiers

Table 210: Properties of each modifier.

Id	Name	SBO
species_50	IKK[P]:IkBb	
species_31	NFkB	
species_35	IKK[P]:IkBb:NFkB	

Product

Table 211: Properties of each product.

Id	Name	SBO
species_35	IKK[P]:IkBb:NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{52} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot (\mathrm{k1} \cdot [\mathrm{species\_50}] \cdot [\mathrm{species\_31}] - \mathrm{k2} \cdot [\mathrm{species\_35}]) \quad (114)$$

Table 212: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.500		☑
k2	k2		$5 \cdot 10^{-4}$		☑

6.53 Reaction reaction_53

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

Name NFkB39) IkBb:NFkB Nuclear Export

Reaction equation

$$\text{species\_43} \xrightarrow{\text{species\_43}} \text{species\_34} \tag{115}$$

Reactant

Table 213: Properties of each reactant.

Id	Name	SBO
species_43	IkBb:NFkB(nuc)	

Modifier

Table 214: Properties of each modifier.

Id	Name	SBO
species_43	IkBb:NFkB(nuc)	

Product

Table 215: Properties of each product.

Id	Name	SBO
species_34	IkBb:NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{53} = \text{vol}\left(\text{compartment\_1}\right) \cdot \text{k1} \cdot [\text{species\_43}] \tag{116}$$

Table 216: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.005		☑

6.54 Reaction reaction_54

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

Name NFkB40) IKK:IkBe:NFkB Binding (2)

Reaction equation

$$\text{species\_51} + \text{species\_31} \underset{\text{species\_51, species\_31, species\_38}}{\rightleftharpoons} \text{species\_38} \tag{117}$$

Reactants

Table 217: Properties of each reactant.

Id	Name	SBO
species_51	IKK[P]:IkBe	
species_31	NFkB	

Modifiers

Table 218: Properties of each modifier.

Id	Name	SBO
species_51	IKK[P]:IkBe	
species_31	NFkB	
species_38	IKK[P]:IkBe:NFkB	

Product

Table 219: Properties of each product.

Id	Name	SBO
species_38	IKK[P]:IkBe:NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{54} = \text{vol}(\text{compartment\_1}) \cdot (\text{k1} \cdot [\text{species\_51}] \cdot [\text{species\_31}] - \text{k2} \cdot [\text{species\_38}]) \tag{118}$$

Table 220: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.500		☑
k2	k2		$5 \cdot 10^{-4}$		☑

6.55 Reaction reaction_55

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

Name NFkB41) IkBe:NFkB Nuclear Export

Reaction equation

$$\text{species\_45} \xrightarrow{\text{species\_45}} \text{species\_37} \tag{119}$$

Reactant

Table 221: Properties of each reactant.

Id	Name	SBO
species_45	IkBe:NFkB(nuc)	

Modifier

Table 222: Properties of each modifier.

Id	Name	SBO
species_45	IkBe:NFkB(nuc)	

Product

Table 223: Properties of each product.

Id	Name	SBO
species_37	IkBe:NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{55} = \text{vol}(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_45}] \tag{120}$$

Table 224: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.005		☑

6.56 Reaction reaction_56

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

Name NFkB42) IKK:IkBa Catalysis

Reaction equation

$$\text{species\_49} \xrightarrow{\text{species\_49}} \text{species\_15} \tag{121}$$

Reactant

Table 225: Properties of each reactant.

Id	Name	SBO
species_49	IKK[P]:IkBa	

Modifier

Table 226: Properties of each modifier.

Id	Name	SBO
species_49	IKK[P]:IkBa	

Product

Table 227: Properties of each product.

Id	Name	SBO
species_15	IKK[P]	

Kinetic Law

Derived unit contains undeclared units

$$v_{56} = \text{vol}(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_49}] \tag{122}$$

Table 228: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.004		☑

6.57 Reaction reaction_57

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

Name NFkB43) IKK:IkBb Catalysis

Reaction equation

$$\text{species\_50} \xrightarrow{\text{species\_50}} \text{species\_15} \tag{123}$$

Reactant

Table 229: Properties of each reactant.

Id	Name	SBO
species_50	IKK[P]:IkBb	

Modifier

Table 230: Properties of each modifier.

Id	Name	SBO
species_50	IKK[P]:IkBb	

Product

Table 231: Properties of each product.

Id	Name	SBO
species_15	IKK[P]	

Kinetic Law

Derived unit contains undeclared units

$$v_{57} = \text{vol}(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_50}] \tag{124}$$

Table 232: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.002		☑

6.58 Reaction reaction_58

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

Name NFkB44) IKK:IkBe Catalysis

Reaction equation

$$\text{species\_51} \xrightarrow{\text{species\_51}} \text{species\_15} \tag{125}$$

Reactant

Table 233: Properties of each reactant.

Id	Name	SBO
species_51	IKK[P]:IkBe	

Modifier

Table 234: Properties of each modifier.

Id	Name	SBO
species_51	IKK[P]:IkBe	

Product

Table 235: Properties of each product.

Id	Name	SBO
species_15	IKK[P]	

Kinetic Law

Derived unit contains undeclared units

$$v_{58} = \text{vol}(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_51}] \tag{126}$$

Table 236: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.002		☑

6.59 Reaction reaction_59

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

Name TRIF06a)Inducible TNFa Synthesis by NFkB

Reaction equation

$$2\,\text{species\_39} \xrightarrow{\text{species\_39}} \text{species\_24} + 2\,\text{species\_39} \tag{127}$$

Reactant

Table 237: Properties of each reactant.

Id	Name	SBO
species_39	NFkB(nuc)	

Modifier

Table 238: Properties of each modifier.

Id	Name	SBO
species_39	NFkB(nuc)	

Products

Table 239: Properties of each product.

Id	Name	SBO
species_24	TNFa	
species_39	NFkB(nuc)	

Kinetic Law

Derived unit contains undeclared units

$$v_{59} = \text{vol}\,(\text{compartment\_1}) \cdot \text{k1} \cdot [\text{species\_39}]^2 \tag{128}$$

Table 240: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.001		☑

7 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.

7.1 Species species_1

Name CD14

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

This species takes part in four reactions (as a reactant in reaction_1, reaction_6 and as a modifier in reaction_1, reaction_6), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_1} = 0 \tag{129}$$

7.2 Species species_2

Name IRAK4

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

This species takes part in two reactions (as a reactant in reaction_1 and as a modifier in reaction_1), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_2} = 0 \tag{130}$$

7.3 Species species_3

Name LBP

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

This species takes part in four reactions (as a reactant in reaction_1, reaction_6 and as a modifier in reaction_1, reaction_6), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_3} = 0 \tag{131}$$

7.4 Species species_4

Name LPS

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

This species takes part in four reactions (as a reactant in reaction_1, reaction_6 and as a modifier in reaction_1, reaction_6), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_4} = 0 \tag{132}$$

7.5 Species species_5

Name LPS:LBP:CD14:TLR4:TIRAP:MyD88:IRAK4

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

This species takes part in four reactions (as a product in reaction_1 and as a modifier in reaction_1, reaction_2, reaction_2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_5} = v_1 \tag{133}$$

7.6 Species species_6

Name MyD88

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

This species takes part in two reactions (as a reactant in reaction_1 and as a modifier in reaction_1), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_6} = 0 \tag{134}$$

7.7 Species species_7

Name TIRAP

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

This species takes part in two reactions (as a reactant in reaction_1 and as a modifier in reaction_1), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_7} = 0 \tag{135}$$

7.8 Species species_8

Name TLR4

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

This species takes part in four reactions (as a reactant in reaction_1, reaction_6 and as a modifier in reaction_1, reaction_6), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_8} = 0 \tag{136}$$

7.9 Species species_9

Name IRAK1

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

This species takes part in two reactions (as a reactant in reaction_2 and as a modifier in reaction_2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_9} = -v_2 \tag{137}$$

7.10 Species species_10

Name TRAF6

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

This species takes part in two reactions (as a reactant in reaction_2 and as a modifier in reaction_2), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_10} = 0 \tag{138}$$

7.11 Species species_11

Name TRAF6:IRAK1[P]

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

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

$$\frac{\text{d}}{\text{d}t}\text{species\_11} = v_2 - v_3 \tag{139}$$

7.12 Species species_12

Name TAK1:TAB1:TAB2

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

This species takes part in two reactions (as a reactant in reaction_3 and as a modifier in reaction_3), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\text{d}}{\text{d}t}\text{species\_12} = 0 \tag{140}$$

7.13 Species species_13

Name TAK1:TAB1:TAB2:TRAF6

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

This species takes part in four reactions (as a product in reaction_3 and as a modifier in reaction_3, reaction_4, reaction_4).

$$\frac{\text{d}}{\text{d}t}\text{species\_13} = v_3 \tag{141}$$

7.14 Species species_14

Name IKK

Initial concentration $0.1\ \mu\text{mol} \cdot \text{ml}^{-1}$

This species takes part in five reactions (as a reactant in reaction_4, reaction_14 and as a product in reaction_5 and as a modifier in reaction_4, reaction_14).

$$\frac{\text{d}}{\text{d}t}\text{species\_14} = v_5 - v_4 - v_{14} \tag{142}$$

7.15 Species species_15

Name IKK[P]

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

This species takes part in 22 reactions (as a reactant in reaction_5, reaction_16, reaction_18, reaction_20, reaction_38, reaction_42, reaction_46 and as a product in reaction_4, reaction_14, reaction_21, reaction_22, reaction_23, reaction_56, reaction_57, reaction_58 and as a modifier in reaction_5, reaction_16, reaction_18, reaction_20, reaction_38, reaction_42, reaction_46).

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_15} = {} & v_4 + v_{14} + v_{21} + v_{22} + v_{23} + v_{56} + v_{57} + v_{58} \\ & - v_5 - v_{16} - v_{18} - v_{20} - v_{38} - v_{42} - v_{46}\end{aligned} \tag{143}$$

7.16 Species species_16

Name RIP1

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

This species takes part in four reactions (as a reactant in reaction_6, reaction_13 and as a modifier in reaction_6, reaction_13), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_16} = 0 \tag{144}$$

7.17 Species species_17

Name TRAM

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

This species takes part in two reactions (as a reactant in reaction_6 and as a modifier in reaction_6), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_17} = 0 \tag{145}$$

7.18 Species species_18

Name TRIF

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

This species takes part in two reactions (as a reactant in reaction_6 and as a modifier in reaction_6), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_18} = 0 \tag{146}$$

7.19 Species species_19

Name IRF3

Initial concentration $1\ \mu\mathrm{mol}\cdot\mathrm{ml}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_19} = v_8 - v_7 \tag{147}$$

7.20 Species species_20

Name IRF3[P]

Initial concentration $0\ \mu\mathrm{mol}\cdot\mathrm{ml}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_20} = v_7 - v_8 - v_9 \tag{148}$$

7.21 Species species_21

Name IRF3[P](nuc)

Initial concentration $0\ \mu\mathrm{mol}\cdot\mathrm{ml}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_21} = v_9 + 2\,v_{10} - 2\,v_{10} \tag{149}$$

7.22 Species species_22

Name source

SBO:0000291 empty set

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

This species takes part in eight reactions (as a reactant in reaction_11, reaction_31, reaction_34, reaction_36 and as a modifier in reaction_11, reaction_31, reaction_34, reaction_36), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_22} = 0 \tag{150}$$

7.23 Species species_23

Name sink

SBO:0000291 empty set

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

This species takes part in seven reactions (as a product in reaction_12, reaction_33, reaction_35, reaction_37, reaction_40, reaction_44, reaction_48), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_23} = 0 \tag{151}$$

7.24 Species species_24

Name TNFa

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

This species takes part in seven reactions (as a reactant in reaction_12, reaction_13 and as a product in reaction_10, reaction_11, reaction_59 and as a modifier in reaction_12, reaction_13).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_24} = v_{10} + v_{11} + v_{59} - v_{12} - v_{13} \tag{152}$$

7.25 Species species_25

Name TNFR1

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

This species takes part in two reactions (as a reactant in reaction_13 and as a modifier in reaction_13), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\text{d}}{\text{d}t}\text{species\_25} = 0 \tag{153}$$

7.26 Species species_26

Name TRADD

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

This species takes part in two reactions (as a reactant in reaction_13 and as a modifier in reaction_13), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\text{d}}{\text{d}t}\text{species\_26} = 0 \tag{154}$$

7.27 Species species_27

Name TRAF2

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

This species takes part in two reactions (as a reactant in reaction_13 and as a modifier in reaction_13), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\text{d}}{\text{d}t}\text{species\_27} = 0 \tag{155}$$

7.28 Species species_28

Name TNFa:TNFR1:TRAF2:TRADD:RIP1

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

This species takes part in four reactions (as a product in reaction_13 and as a modifier in reaction_13, reaction_14, reaction_14).

$$\frac{\text{d}}{\text{d}t}\text{species\_28} = v_{13} \tag{156}$$

7.29 Species species_29

Name IkBa

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

This species takes part in nine reactions (as a reactant in reaction_15, reaction_38, reaction_40, reaction_41 and as a product in reaction_39 and as a modifier in reaction_15, reaction_38, reaction_40, reaction_41).

$$\frac{\text{d}}{\text{d}t}\text{species\_29} = v_{39} - v_{15} - v_{38} - v_{40} - v_{41} \tag{157}$$

7.30 Species species_30

Name IkBa:NFkB

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

This species takes part in seven reactions (as a reactant in reaction_16, reaction_24 and as a product in reaction_15, reaction_51 and as a modifier in reaction_15, reaction_16, reaction_24).

$$\frac{\text{d}}{\text{d}t}\text{species\_30} = v_{15} + v_{51} - v_{16} - v_{24} \tag{158}$$

7.31 Species species_31

Name NFkB

Initial concentration $0.1\ \mu\text{mol} \cdot \text{ml}^{-1}$

This species takes part in 20 reactions (as a reactant in reaction_15, reaction_17, reaction_19, reaction_27, reaction_50, reaction_52, reaction_54 and as a product in reaction_21, reaction_22, reaction_23, reaction_24, reaction_25, reaction_26 and as a modifier in reaction_15, reaction_17, reaction_19, reaction_27, reaction_50, reaction_52, reaction_54).

$$\begin{aligned}\frac{\text{d}}{\text{d}t}\text{species\_31} = {} & v_{21} + v_{22} + v_{23} + v_{24} + v_{25} + v_{26} - v_{15} \\ & - v_{17} - v_{19} - v_{27} - v_{50} - v_{52} - v_{54}\end{aligned} \tag{159}$$

7.32 Species species_32

Name IKK[P]:IkBa:NFkB

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

This species takes part in six reactions (as a reactant in reaction_21 and as a product in reaction_16, reaction_50 and as a modifier in reaction_16, reaction_21, reaction_50).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_32} = v_{16} + v_{50} - v_{21} \tag{160}$$

7.33 Species species_33

Name IkBb

Initial concentration $0\ \mu\mathrm{mol}\cdot\mathrm{ml}^{-1}$

This species takes part in nine reactions (as a reactant in reaction_17, reaction_42, reaction_44, reaction_45 and as a product in reaction_43 and as a modifier in reaction_17, reaction_42, reaction_44, reaction_45).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_33} = v_{43} - v_{17} - v_{42} - v_{44} - v_{45} \tag{161}$$

7.34 Species species_34

Name IkBb:NFkB

Initial concentration $0\ \mu\mathrm{mol}\cdot\mathrm{ml}^{-1}$

This species takes part in seven reactions (as a reactant in reaction_18, reaction_25 and as a product in reaction_17, reaction_53 and as a modifier in reaction_17, reaction_18, reaction_25).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_34} = v_{17} + v_{53} - v_{18} - v_{25} \tag{162}$$

7.35 Species species_35

Name IKK[P]:IkBb:NFkB

Initial concentration $0\ \mu\mathrm{mol}\cdot\mathrm{ml}^{-1}$

This species takes part in six reactions (as a reactant in reaction_22 and as a product in reaction_18, reaction_52 and as a modifier in reaction_18, reaction_22, reaction_52).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_35} = v_{18} + v_{52} - v_{22} \tag{163}$$

7.36 Species species_36

Name IkBe

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

This species takes part in nine reactions (as a reactant in reaction_19, reaction_46, reaction_48, reaction_49 and as a product in reaction_47 and as a modifier in reaction_19, reaction_46, reaction_48, reaction_49).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_36} = v_{47} - v_{19} - v_{46} - v_{48} - v_{49} \tag{164}$$

7.37 Species species_37

Name IkBe:NFkB

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

This species takes part in seven reactions (as a reactant in reaction_20, reaction_26 and as a product in reaction_19, reaction_55 and as a modifier in reaction_19, reaction_20, reaction_26).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_37} = v_{19} + v_{55} - v_{20} - v_{26} \tag{165}$$

7.38 Species species_38

Name IKK[P]:IkBe:NFkB

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

This species takes part in six reactions (as a reactant in reaction_23 and as a product in reaction_20, reaction_54 and as a modifier in reaction_20, reaction_23, reaction_54).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_38} = v_{20} + v_{54} - v_{23} \tag{166}$$

7.39 Species species_39

Name NFkB(nuc)

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

This species takes part in 14 reactions (as a reactant in reaction_28, reaction_29, reaction_30, reaction_32, reaction_59 and as a product in reaction_27, reaction_32, reaction_59 and as a modifier in reaction_27, reaction_28, reaction_29, reaction_30, reaction_32, reaction_59).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_39} = v_{27} + 2\,v_{32} + 2\,v_{59} - v_{28} - v_{29} - v_{30} - 2\,v_{32} - 2\,v_{59} \tag{167}$$

7.40 Species species_40

Name IkBa(nuc)

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

This species takes part in four reactions (as a reactant in reaction_28 and as a product in reaction_41 and as a modifier in reaction_28, reaction_41).

$$\frac{\text{d}}{\text{d}t}\text{species\_40} = v_{41} - v_{28} \tag{168}$$

7.41 Species species_41

Name IkBa:NFkB(nuc)

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

This species takes part in four reactions (as a reactant in reaction_51 and as a product in reaction_28 and as a modifier in reaction_28, reaction_51).

$$\frac{\text{d}}{\text{d}t}\text{species\_41} = v_{28} - v_{51} \tag{169}$$

7.42 Species species_42

Name IkBb(nuc)

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

This species takes part in four reactions (as a reactant in reaction_29 and as a product in reaction_45 and as a modifier in reaction_29, reaction_45).

$$\frac{\text{d}}{\text{d}t}\text{species\_42} = v_{45} - v_{29} \tag{170}$$

7.43 Species species_43

Name IkBb:NFkB(nuc)

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

This species takes part in four reactions (as a reactant in reaction_53 and as a product in reaction_29 and as a modifier in reaction_29, reaction_53).

$$\frac{\text{d}}{\text{d}t}\text{species\_43} = v_{29} - v_{53} \tag{171}$$

7.44 Species species_44

Name IkBe(nuc)

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

This species takes part in four reactions (as a reactant in reaction_30 and as a product in reaction_49 and as a modifier in reaction_30, reaction_49).

$$\frac{\text{d}}{\text{d}t}\text{species\_44} = v_{49} - v_{30} \tag{172}$$

7.45 Species species_45

Name IkBe:NFkB(nuc)

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

This species takes part in four reactions (as a reactant in reaction_55 and as a product in reaction_30 and as a modifier in reaction_30, reaction_55).

$$\frac{\text{d}}{\text{d}t}\text{species\_45} = v_{30} - v_{55} \tag{173}$$

7.46 Species species_46

Name IkBa_mRNA

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

This species takes part in seven reactions (as a reactant in reaction_33, reaction_39 and as a product in reaction_31, reaction_32, reaction_39 and as a modifier in reaction_33, reaction_39).

$$\frac{\text{d}}{\text{d}t}\text{species\_46} = v_{31} + v_{32} + v_{39} - v_{33} - v_{39} \tag{174}$$

7.47 Species species_47

Name IkBb_mRNA

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

This species takes part in six reactions (as a reactant in reaction_35, reaction_43 and as a product in reaction_34, reaction_43 and as a modifier in reaction_35, reaction_43).

$$\frac{\text{d}}{\text{d}t}\text{species\_47} = v_{34} + v_{43} - v_{35} - v_{43} \tag{175}$$

7.48 Species species_48

Name IkBe_mRNA

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

This species takes part in six reactions (as a reactant in reaction_37, reaction_47 and as a product in reaction_36, reaction_47 and as a modifier in reaction_37, reaction_47).

$$\frac{\text{d}}{\text{d}t}\text{species\_48} = v_{36} + v_{47} - v_{37} - v_{47} \tag{176}$$

7.49 Species species_49

Name IKK[P]:IkBa

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

This species takes part in six reactions (as a reactant in reaction_50, reaction_56 and as a product in reaction_38 and as a modifier in reaction_38, reaction_50, reaction_56).

$$\frac{\text{d}}{\text{d}t}\text{species\_49} = v_{38} - v_{50} - v_{56} \tag{177}$$

7.50 Species species_50

Name IKK[P]:IkBb

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

This species takes part in six reactions (as a reactant in reaction_52, reaction_57 and as a product in reaction_42 and as a modifier in reaction_42, reaction_52, reaction_57).

$$\frac{\text{d}}{\text{d}t}\text{species\_50} = v_{42} - v_{52} - v_{57} \tag{178}$$

7.51 Species species_51

Name IKK[P]:IkBe

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

This species takes part in six reactions (as a reactant in reaction_54, reaction_58 and as a product in reaction_46 and as a modifier in reaction_46, reaction_54, reaction_58).

$$\frac{\text{d}}{\text{d}t}\text{species\_51} = v_{46} - v_{54} - v_{58} \tag{179}$$

7.52 Species species_52

Name LPS:LBP:CD14:TLR4:RIP1:TRAM:TRIF:TBK/IKKe

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

This species takes part in four reactions (as a product in reaction_6 and as a modifier in reaction_6, reaction_7, reaction_7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_52} = v_6 \tag{180}$$

7.53 Species species_53

Name TBK1/IKKe

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

This species takes part in two reactions (as a reactant in reaction_6 and as a modifier in reaction_6), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_53} = 0 \tag{181}$$

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

SBO:0000291 empty set: Entity defined by the absence of any actual object. An empty set is often used to represent the source of a creation process or the result of a degradation process.

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