

#	Reaction	Value	Unit	Description	Source of parameter value		
<b>TLR module</b>							
<b>TLR3</b>							
1	=> TLR3	1.0E-04	$\mu\text{M}^{-1}\text{min}^{-1}$	Protein Synth.	Fit		
2	TLR3 =>	5.8E-03	$\text{min}^{-1}$	Protein Deg.	Fit		
3	PIC + TLR3 => TLR3PIC	6.0E-01	$\mu\text{M}^{-1}\text{min}^{-1}$	Association	Fit		
4	TLR3PIC => PIC + TLR3	1.1E-01	$\text{min}^{-1}$	Dissociation	Fit		
5	TRIF => TRIF* ; TLR3PIC	0.39	$\mu\text{M}^{-1}\text{min}^{-1}$	Triff activation by receptor complex in the early endosome	Fit		
<b>TLR4</b>							
6	LPS => LPSpm	1.7E-01	$\text{min}^{-1}$	LPS bind to the plasma membrane	Fit		
7	LPSpm => LPSen	1.8E-01	$\text{min}^{-1}$	LPS translocate from plasma membrane to early endosome	Fit		
8	LPSen => LPS	2.6E-01	$\text{min}^{-1}$	Export LPS	Fit		
9	LPSen =>	1.3E+01	$\text{min}^{-1}$	Depletion of LPS from the early endosome	Fit		
10	LPSpm + TLR4pm => TLP4LPSpm	0.19	$\mu\text{M}^{-1}\text{min}^{-1}$	Association of LPS and TLR4 in the plasma membrane	Fixed, Table 1. Shin et al. 2007, 0.12~ 0.36		
11	TLP4LPSpm => LPSpm + TLR4pm	2.7	$\text{min}^{-1}$	Disassociation of TLR4LPS in the plasma membrane	Fixed, Table 1. Shin et al. 2007, 0.6~3.6		
12	LPSen + TLR4en => TLR4LPSen	0.19	$\mu\text{M}^{-1}\text{min}^{-1}$	Association of LPS and TLR4 in the early endosome	#5		
13	TLR4LPSen => LPSen + TLR4en	2.7	$\text{min}^{-1}$	Disassociation of TLR4LPS in the early endosome	#6		
14	=> TLR4pm	2.6E-02	$\mu\text{M}\text{min}^{-1}$	TLR4 generation at the plasma membrane	Fit		
15	TLR4pm =>	9.0E-01	$\text{min}^{-1}$	TLR4 depletion from the plasma membrane	Fit		
16	TLR4en =>	2.9E+00	$\text{min}^{-1}$	TLR4 depletion from the early endosome	Fit		
17	TLR4pm => TLR4en	1.3E-01	$\text{min}^{-1}$	TLR4 translocate from plasma membrane to early endosome	Fit		
18	TLR4en => TLR4pm	3.6E+00	$\text{min}^{-1}$	TLR4 translocate from early endosome to plasma membrane	Fit		
19	TLR4LPSpm => TLR4LPSen	2.4E-01	$\text{min}^{-1}$	Receptor complex translocate from plasma membrane to early endosome	Fit		
20	TLR4LPSen => TLR4LPSpm	0.04	$\text{min}^{-1}$	Receptor complex translocate from early endosome to plasma membrane	Fit		
21	TLR4LPSpm =>	14.41	$\text{min}^{-1}$	Receptor complex degradation in the plasma membrane	Fit		
22	TLR4LPSen =>	0.4	$\text{min}^{-1}$	Receptor complex degradation in the early endosome	Fit		
23		3	$\mu\text{M}^{-1}\text{min}^{-1}$		Fit		
24	MYD88 => MYD88* ; TLR4LPSpm	3	Hill coefficient	MyD88 activation (by receptor complex) in the plasma membrane	Derived from MyDDosome model		
25		5.8E-02	EC50: $\mu\text{M}$		Fit		
26	MYD88* => MYD88	0.3	$\text{min}^{-1}$	MyD88 Deactivation	Fit		
27	TRIF => TRIF* ; TLR4LPSen	0.39	$\mu\text{M}^{-1}\text{min}^{-1}$	Triff activation by receptor complex in the early endosome	Fit		
28	TRIF* => TRIF	1.2E-02	$\text{min}^{-1}$	Triff Deactivation	Fit		
<b>TLR9</b>							
29	=> TLR9	1.0E-04	$\mu\text{M}^{-1}\text{min}^{-1}$	Protein Synth.	Fit		
30	TLR9 =>	5.8E-03	$\text{min}^{-1}$	Protein Deg.	Fit		
31	CpG + TLR9 => TLR9CpG	6.0E-01	$\mu\text{M}^{-1}\text{min}^{-1}$	Association	Fit		
32	TLR9CpG => CpG + TLR9	2.7E+00	$\text{min}^{-1}$	Dissociation	Fit		
33		33	$\mu\text{M}^{-1}\text{min}^{-1}$		Fit		
34	MYD88 => MYD88* ; TLR4LPSpm	3	Hill coefficient	MyD88 activation (by receptor complex)	Derived from MyDDosome model		
35		5.8E-02	EC50: $\mu\text{M}$		Fit		
<b>TNFR module</b>							
36	=> tnfrm	2.0E-07	$\text{min}^{-1}$	Protein Synth.	(Werner et al. 2008)		
37	tnfrm =>	5.8E-03	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
38	3 tnfrm => TNFR	1.0E-05	$\mu\text{M}^{-1}\text{min}^{-1}$	Association	(Werner et al. 2008)		
39	TNFR => 3 tnfrm	1.0E-01	$\text{min}^{-1}$	Dissociation	(Werner et al. 2008)		
40	TNFR => (internalization)	1.7E-03	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
41	TNFR + TTR => C1_off	100.00	$\mu\text{M}^{-1}\text{min}^{-1}$	Association	(Werner et al. 2008)		
42	C1_off => TNFR + TTR	0.75	$\text{min}^{-1}$	Dissociation	(Werner et al. 2008)		
43	C1_off => C1	3.0E+01	$\text{min}^{-1}$	Activation	(Werner et al. 2008)		
44	C1 => C1_off	2.0E+00	$\text{min}^{-1}$	Deactivation	(Werner et al. 2008)		
45	C1 => C1_off (A20 mediated)	1000.00	$\mu\text{M}^{-1}\text{min}^{-1}$	Deactivation	(Werner et al. 2008)		
46	C1 => TNFR + TTR	7.5E-01	$\text{min}^{-1}$	Dissociation	(Werner et al. 2008)		
47	C1_off => (internalization)	1.7E-03	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
48	C1 => (internalization)	1.7E-03	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
49	tnf =>	1.5E-02	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
50	tnf + 3tnfrm => TNFRtnf	1.1E+03	$\text{min}^{-1}$	Association	(Werner et al. 2008)		
51	tnf + TNFR => TNRtnf	1.1E+03	$\text{min}^{-1}$	Association	(Werner et al. 2008)		
52	TNFRtnf => TNFR + tnf	2.1E-02	$\text{min}^{-1}$	Dissociation	(Werner et al. 2008)		
53	TNFRtnf => (internalization)	1.7E-03	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
54	TNFRtnf + TTR => C1tnf_off	1.0E+02	$\mu\text{M}^{-1}\text{min}^{-1}$	Association	(Werner et al. 2008)		
55	C1tnf_off => TNFRtnf + TTR	7.5E-01	$\text{min}^{-1}$	Dissociation	(Werner et al. 2008)		
56	C1tnf_off => C1tnf	3.0E+01	$\text{min}^{-1}$	Activation	(Werner et al. 2008)		
57	C1tnf => C1tnf_off	2.0E+00	$\text{min}^{-1}$	Deactivation	(Werner et al. 2008)		

58	C1tnf=>C1tnf off (A20 mediated)	1.0E+03	$\mu\text{M}^{-1} \text{min}^{-1}$	Deactivation	(Werner et al. 2008)		
59	C1tnf=> TNFRtnf + TTR	7.5E-01	$\text{min}^{-1}$	Dissociation	(Werner et al. 2008)		
60	C1tnf off=> (internalization)	1.7E-03	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
61	C1tnf=> (internalization)	1.7E-03	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
62	C1tnf off=> C1 off + tnf	2.1E-02	$\text{min}^{-1}$	Dissociation	(Werner et al. 2008)		
63	C1 off + tnf=> C1tnf off	1.1E+03	$\mu\text{M}^{-1} \text{min}^{-1}$	Association	(Werner et al. 2008)		
64	C1tnf=> C1 + tnf	2.1E-02	$\text{min}^{-1}$	Dissociation	(Werner et al. 2008)		
65	C1 + tnf=> C1tnf	1.1E+03	$\mu\text{M}^{-1} \text{min}^{-1}$	Association	(Werner et al. 2008)		
<b>IKK-NFkB module</b>							<i>wt</i>
66	TRAF6 => TRAF6* ; MyD88*	4.9E+00	$\mu\text{M}^{-1} \text{min}^{-1}$	TRAF6 activation by MyD88*	Fit	79	7.5E+00
67	TRAF6 => TRAF6* ; TRIF*	1.3E+00	$\mu\text{M}^{-1} \text{min}^{-1}$	TRAF6 activation by TRIF*	Fit	80	3.4E+00
68	TRAF6* => TRAF6	0.22	$\text{min}^{-1}$	TRAF6 Deactivation	Fit		
69	IKKK off=> IKKK (C1 mediated)						
70	IKKK off=> IKKK (C1tnf mediated)						
71	IKKK => IKKK* ; TRAF6*	3.4E-01	$\mu\text{M}^{-1} \text{min}^{-1}$	IKKK activation by TRAF6*	Fit		IKK total multiplier
72	IKKK => IKKK*	5.0E-07	$\text{min}^{-1}$	Basal activation	(Werner et al. 2008)	81	0.06791
73	IKKK* => IKKK	0.25	$\text{min}^{-1}$	Deactivation	(Werner et al. 2008)		
74	IKK => IKK* ; IKKK*	520.00	$\mu\text{M}^{-1} \text{min}^{-1}$	Activation	(Werner et al. 2008)		LPS scale
75	IKK => IKK*	5.0E-05	$\text{min}^{-1}$	Basal activation	(Werner et al. 2008)	82	633.55
76	IKK* => IKK	2.0E-02	$\text{min}^{-1}$	Deactivation	(Werner et al. 2008)		
77	IKK* => IKKi	0.15	$\text{min}^{-1}$	Deactivation	(Werner et al. 2008)		
78	IKKi => IKK	0.02	$\text{min}^{-1}$	Deactivation	(Werner et al. 2008)		
<b>IkB mRNA and Protein Synthesis Reactions</b>							
79	=> IkBat (constitutive)	7.0E-05	$\text{min}^{-1}$	RNA Synth.	(Werner et al. 2008)		
80	=> IkBbt (constitutive)	1.0E-05	$\text{min}^{-1}$	RNA Synth.	(Werner et al. 2008)		
81	=> IkBet (constitutive)	1.0E-06	$\text{min}^{-1}$	RNA Synth.	(Werner et al. 2008)		
82		8	$\text{min}^{-1}$		(Werner et al. 2008)		
83		3.0	Hill Coefficient		(Werner et al. 2008)		
84	=> IkBat (induced by NFkBn)	0	Delay: min	RNA Synth.	(Werner et al. 2008)		
85		0.02	$\text{min}^{-1}$		(Werner et al. 2008)		
86		3	Hill Coefficient		(Werner et al. 2008)		
87	=> IkBbt (induced by NFkBn)	37	Delay: min	RNA Synth.	(Werner et al. 2008)		
88		0.3	$\text{min}^{-1}$		(Werner et al. 2008)		
89		3	Hill Coefficient		(Werner et al. 2008)		
90	=> IkBet (induced by NFkBn)	37	Delay: min	RNA Synth.	(Werner et al. 2008)		
91	IkBat =>	0.035	$\text{min}^{-1}$	RNA Deg.	(Werner et al. 2008)		
92	IkBbt =>	8.0E-03	$\text{min}^{-1}$	RNA Deg.	(Werner et al. 2008)		
93	IkBet =>	4.0E-03	$\text{min}^{-1}$	RNA Deg.	(Werner et al. 2008)		
94	=> IkBa	0.25	$\mu\text{M} \text{min}^{-1}$	Protein Synth.	(Werner et al. 2008)		
95	=> IkBb	0.25	$\mu\text{M} \text{min}^{-1}$	Protein Synth.	(Werner et al. 2008)		
96	=> IkBe	0.25	$\mu\text{M} \text{min}^{-1}$	Protein Synth.	(Werner et al. 2008)		
<b>IkB and NFkB Cellular Localization Reactions</b>							
97	IkBa => IkBan	0.09	$\text{min}^{-1}$	Import	(Werner et al. 2008)		
98	IkBb => IkBbn	0.009	$\text{min}^{-1}$	Import	(Werner et al. 2008)		
99	IkBe => IkBen	0.045	$\text{min}^{-1}$	Import	(Werner et al. 2008)		
100	NFkB => NFkBn	5.4	$\text{min}^{-1}$	Import	(Werner et al. 2008)		
101	IkBan => IkBa	0.012	$\text{min}^{-1}$	Export	(Werner et al. 2008)		
102	IkBbn => IkBb	0.012	$\text{min}^{-1}$	Export	(Werner et al. 2008)		
103	IkBen => IkBe	0.012	$\text{min}^{-1}$	Export	(Werner et al. 2008)		
104	NFkBn => NFkB	0.0048	$\text{min}^{-1}$	Export	(Werner et al. 2008)		
105	IkBaNFkB => IkBaNFkBn	0.276	$\text{min}^{-1}$	Import	(Werner et al. 2008)		
106	IkBbNFkB => IkBbNFkBn	0.0276	$\text{min}^{-1}$	Import	(Werner et al. 2008)		
107	IkBeNFkB => IkBeNFkBn	0.138	$\text{min}^{-1}$	Import	(Werner et al. 2008)		
108	IkBaNFkBn => IkBaNFkB	0.828	$\text{min}^{-1}$	Export	(Werner et al. 2008)		
109	IkBbNFkBn => IkBbNFkB	0.414	$\text{min}^{-1}$	Export	(Werner et al. 2008)		
110	IkBeNFkBn => IkBeNFkB	0.414	$\text{min}^{-1}$	Export	(Werner et al. 2008)		
<b>IkB Protein Degradation Reactions</b>							
111	IkBa =>	0.12	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
112	IkBb =>	0.18	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
113	IkBe =>	0.18	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
114	IkBan =>	0.12	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
115	IkBbn =>	0.18	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
116	IkBen =>	0.18	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
117	IkBaNFkB => NFkB	6.0E-05	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
118	IkBbNFkB => NFkB	6.0E-05	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
119	IkBeNFkB => NFkB	6.0E-05	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
120	IkBaNFkBn => NFkBn	6.0E-05	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
121	IkBbNFkBn => NFkBn	6.0E-05	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
122	IkBeNFkBn => NFkBn	6.0E-05	$\text{min}^{-1}$	Protein Deg.	(Werner et al. 2008)		
<b>IkB:NFkB Association and Dissociation Reactions</b>							
123	IkBa + NFkB => IkBaNFkB	30	$\mu\text{M}^{-1} \text{min}^{-1}$	Association	(Werner et al. 2008)		
124	IkBb + NFkB => IkBbNFkB	30	$\mu\text{M}^{-1} \text{min}^{-1}$	Association	(Werner et al. 2008)		
125	IkBe + NFkB => IkBeNFkB	30	$\mu\text{M}^{-1} \text{min}^{-1}$	Association	(Werner et al. 2008)		
126	IkBa + NFkBn => IkBaNFkBn	30	$\mu\text{M}^{-1} \text{min}^{-1}$	Association	(Werner et al. 2008)		
127	IkBb + NFkBn => IkBbNFkBn	30	$\mu\text{M}^{-1} \text{min}^{-1}$	Association	(Werner et al. 2008)		
128	IkBe + NFkBn => IkBeNFkBn	30	$\mu\text{M}^{-1} \text{min}^{-1}$	Association	(Werner et al. 2008)		

129	IkBaNfKb => IkBa + NfKb	6.0E-05	min <sup>-1</sup>	Dissociation	(Werner et al. 2008)		
130	IkBbNfKb => IkBb + NfKb	6.0E-05	min <sup>-1</sup>	Dissociation	(Werner et al. 2008)		
131	IkBeNfKb => IkBe + NfKb	6.0E-05	min <sup>-1</sup>	Dissociation	(Werner et al. 2008)		
132	IkBaNfKbN => IkBa + NfKbN	6.0E-05	min <sup>-1</sup>	Dissociation	(Werner et al. 2008)		
133	IkBbNfKbN => IkBb + NfKbN	6.0E-05	min <sup>-1</sup>	Dissociation	(Werner et al. 2008)		
134	IkBeNfKbN => IkBe + NfKbN	6.0E-05	min <sup>-1</sup>	Dissociation	(Werner et al. 2008)		
<b>IKK-mediated IkB Degradation Reactions</b>							
135	IkBa =>	0.36	min <sup>-1</sup>	Protein Deg.	(Werner et al. 2008)		
136	IkBb =>	0.12	min <sup>-1</sup>	Protein Deg.	(Werner et al. 2008)		
137	IkBe =>	0.18	min <sup>-1</sup>	Protein Deg.	(Werner et al. 2008)		
138	IkBaNfKb => NfKb	0.36	min <sup>-1</sup>	Protein Deg.	(Werner et al. 2008)		
139	IkBbNfKb => NfKb	0.12	min <sup>-1</sup>	Protein Deg.	(Werner et al. 2008)		
140	IkBeNfKb => NfKb	0.18	min <sup>-1</sup>	Protein Deg.	(Werner et al. 2008)		
<b>A20 mRNA and Protein Synthesis and Degradation Reactions</b>							
141	=> A20t (constitutive)	2.00E-06	min <sup>-1</sup>	RNA Synth.	(Werner et al. 2008)		
142		0.40	μM <sup>-2</sup> min <sup>-1</sup>		(Werner et al. 2008)		
143		3.00	Hill Coefficient		(Werner et al. 2008)		
144		0	Delay: min		(Werner et al. 2008)		
145	=> A20t (induced by NfKbN)	120	Shutdown: min	RNA Synth.	(Werner et al. 2008)		
146	A20t =>	0.04	min <sup>-1</sup>	RNA Deg.	(Werner et al. 2008)		
147		0.25	min <sup>-1</sup>		(Werner et al. 2008)		
148	=> A20	30	Delay: min	Protein Deg.	(Werner et al. 2008)		
149	A20 =>	0.0029	min <sup>-1</sup>	Protein Deg.	(Werner et al. 2008)		
<b>TNF production module</b>							
	=> TNFnaCent (Constitute)	1.00E-05		RNA Synth.	Fit		
	=> TNFnaCent (induced by NfKbN)	1		RNA Synth.	Fixed		
		2			Fixed		
		0.65			Fit		
	TNFnaCent => TNFmRNA	0.4		mRNA process	Fit		
	TNFmRNA =>	0.02	/- (30min): min <sup>-1</sup>	mRNA Deg.	Measure		
			min <sup>-1</sup> / -				
		0.07	(30min): min <sup>-1</sup>				
	=> proTNF	0.05		Protein Synth.	Fit		
	proTNF =>	0.07		Protein Deg.	Fit		
	proTNF => TNF	0.07		Secretion	Fit		