	Reaction name	Reaction equation	Rate equation	kf¹	Kinetic parameters  0.0001 ml^6/(μmol^6*s)
1	MYD881) Receptor Complex Formation	LPS+LBP+CD14+TLR4+MyD88+IRAK4+TIRAP=LPS:LBP:CD14:TLR4:TIRAP:MyD88:IRAK4	$v^1 = {}^{kf^L} [LPS] [LBP] [CD14] [TLR4] [MYD88] [IRAK4] [TIRAP] - {}^{kf^L} [LPS:LBP:CD14:TLR4:TIRAP:MyD88:IRAK4]$	kr1	0.0001 1/s
2	MYD882) IRAK1 and TRAF6 Phosphorylation	IRAK1 + TRAF6 = TRAF6:IRAK1[P]; LPS:LBP:CD14:TLR4:TIRAP:MyD88:IRAK4	$v^2 = ^{kf^{\circ}\cdot \text{[LPS:LBP:CD14:TLR4:TIRAP:MyD88:IRAK4]}\cdot \text{[TRAF6]}\cdot \text{[IRAK1]} - \\ \text{$k$^{\circ}\cdot \text{[TRAF6:IRAK1[P]]}$}$	kf² kr²	0.001 ml^2/(µmol^2*s) 0.001 1/s
3	MYD883) TAK/TAB Binds to TRAF6	TRAF6:IRAK1[P] + TAK1:TAB1:TAB2 = TAK1:TAB1:TAB2:TRAF6	$v^3 = {}^{kf^3.} [TRAF6:IRAK1[P]] \cdot [TAK1:TAB1:TAB2] - {}_{kr^3.} [TAK1:TAB1:TAB2:TRAF6]$	kf³ kr³	0.003 ml/(μmol*s) 0.01 1/s
4	MYD884) IKK Phosphorylation by TAK1	IKK->IKK[P]; TAK1:TAB1:TAB2:TRAF6	$v^4 = \frac{k^4 \cdot [TAK1:TAB1:TAB2:TRAF6] \cdot [IKK]}{km^4 + [IKK]}$	k <sup>4</sup> km <sup>4</sup>	0.1 1/s 0.1 μmol/ml
5	MYD885) IKK[P] Dephosphorylation	IKK[P] -> IKK	$v^5 = kf^5 \cdot [IKK[P]]$	kf <sup>5</sup>	0.1 1/s
6	TRIF01) Receptor Complex Formation	LPS+LBP+CD14+TLR4+TRIF+TRAM+RIP1+TBK1/IKKe=LPS:LBP:CD14:TLR4:RIP1:TRAM:TRIF:TBK1/IKKe	$v^6 = {}^{kf^4.} \texttt{[LPS]-[LBP]-[CD14]-[TR4]-[TRIF]-[TRAM]-[RIP1]-[TBK1/IKKe] - } \\ {}^{kf^4.} \texttt{-[LPS:LBP:CD14:TLR4:TRAM:TRIF:TBK1/IKKe]}$	kf <sup>6</sup>	0.0001 ml^7/(µmol^7*s)
7	TRIF02) IRF3 Phosphorylation	IRF3 -> IRF3[P]; LPS:LBP:CD14:TLR4:RIP1:TRAM:TRIF:TBK/IKKe	<sub>7</sub> _ k <sup>7</sup> · [LPS:LBP:CD14:TLR4:RIP1:TRAM:TRIF:TBK/IKKe]·[IRF3]	kr <sup>6</sup>	0.0001 1/s 0.1 1/s
8	TRIF03) IRF3 Dephosphorylation	IRF3[P] -> IRF3	$v = -\frac{km^7 + [IRF3]}{v^8 = kf^8 \cdot [IRF3[P]]}$	km <sup>7</sup>	0.1 μmol/ml 0.1 1/s
9	TRIF04) IRF3 Nuclear Import/Export	IRF3[P] = IRF3[P](nuc)	$v = kf^9 \cdot [\text{IRF3[P]}] \cdot kr^9 \cdot [\text{IRF3[P](nuc)}]$	kf°	0.1 1/s
	TRIF05) Inducible TNFa Synthesis	2 * IRF3[P](nuc) -> TNFa + 2 * IRF3[P](nuc)		kr <sup>9</sup>	0.1 1/s 0.02 ml/(μmol*s)
	TRIF06) Constitutive TNFa Synthesis	source -> TNFa	v <sup>10</sup> = kf <sup>10</sup> · 2 · [IRF3[P](nuc)]	kf 11	0.001 1/s
	TRIF07)Inducible TNFa Synthesis by NFkB	2 * NFkB(nuc) -> TNFa + 2 * NFkB(nuc)	$v^{11} = kf^{11} \cdot [\text{source}]$ $v^{12} = kf^{12} \cdot 2 \cdot [\text{NFkB(nuc)}]$	kf 12	0.001 1/3 0.001 ml/(μmol*s)
	TRIF08) TNFa Degradation	TNFa -> sink	$v^{-1} = k f^{-1} \cdot 2^{-1} [NFKB(fluc)]$ $v^{13} = k f^{13} \cdot [TNFa]$	kf 13	0.1 1/s
	TRIF09) TNFa Receptor Complex Formation	TNFa + TNFR1 + TRAF2 + TRADD + RIP1 = TNFa:TNFR1:TRAF2:TRADD:RIP1	$v^{14} = k_f^{14}.[TNFa].[TNFA1].[TRAF2].[TRADD].[RIP1]-$ $k_f^{14}.[TNFa:TNFR1:TRAF:2:TRADD:RIP1]$	kf <sup>24</sup>	0.1 ml^4/(µmol^4*s)
			$v^{15} = \frac{k^{15} \cdot [\text{TNFa:TNFR1:TRAF:2:TRADD:RIP1}]}{v^{15} = \frac{k^{15} \cdot [\text{TNFa:TNFR1:TRAF2:TRADD:RIP1}] \cdot [\text{IKK}]}{v^{15} \cdot [\text{TNFa:TNFR1:TRAF2:TRADD:RIP1}] \cdot [\text{TNFA:TNFR1:TRAF2:TRADD:RIP1]}}$	kr <sup>14</sup>	0.1 1/s 0.1 1/s
15	TRIF10) IKK Phosphorylation by RIP1	IKK -> IKK[P]; TNFa:TNFR1:TRAF2:TRADD:RIP1	$v^{zz} = \frac{1}{km^{zz} + [IKK]}$	km <sup>15</sup>	0.1 µmol/ml 0.5 ml/(µmol*s)
16	NFkB01) IkBa:NFkB Binding	IkBa + NFkB = IkBa:NFkB	$v^{16} = kf^{16} \cdot [\text{IkBa}] \cdot [\text{NFkB}] - kr^{16} \cdot [\text{IkBa}:\text{NFkB}]$	kr <sup>16</sup>	0.0005 1/s
17	NFkB02) IKK:IkBa:NFkB Binding (1)	IKK[P] + IkBa:NFkB = IKK[P]:IkBa:NFkB	$v^{17} = kf^{17} \cdot \left[ \text{IKK[P]]} \cdot \left[ \text{IkBa:NFkB} \right] \cdot kr^{16} \cdot \left[ \text{IKK[P]:IkBa:NFkB} \right]$	kf <sup>17</sup>	0.185 ml/(μmol*s) 0.0125 1/s
18	NFkB03) IkBb:NFkB Binding	IkBb + NFkB = IkBb:NFkB	$v^{\text{18}} = kf^{\text{18}} \cdot [\text{IkBb}] \cdot [\text{NFkB}] \cdot kr^{\text{18}} \cdot [\text{IkBb:NFkB}]$	kf <sup>18</sup> kr <sup>18</sup>	0.5 ml/(μmol*s) 0.0005 1/s
19	NFkB04) IKK:IkBb:NFkB Binding (1)	IKK[P] + IkBb:NFkB = IKK[P]:IkBb:NFkB	$v^{19} = kf^{19} \cdot [\mathrm{IKK[P]]} \cdot [\mathrm{IkBb:NFkB}] \cdot kr^{19} \cdot [\mathrm{IKK[P]:IkBb:NFkB}]$	kf <sup>19</sup> kr <sup>19</sup>	0.048 ml/(μmol*s) 0.00175 1/s
20	NFkB05) IkBe:NFkB Binding	IkBe + NFkB = IkBe:NFkB	$v^{20} = kf^{20} \cdot [\text{IkBe}] \cdot [\text{NFkB}] \cdot kr^{20} \cdot [\text{IkBe:NFkB}]$	kf <sup>20</sup> kr <sup>20</sup>	0.5 ml/(μmol*s) 0.0005 1/s
21	NFkB06) IKK:IkBe:NFkB Binding (1)	IKK[P] + IkBe:NFkB = IKK[P]:IkBe:NFkB	$v^{21} = kf^{21} \cdot [\text{IKK[P]}] \cdot [\text{IKBe:NFkB}] \cdot kr^{21} \cdot [\text{IKK[P]}] \cdot [\text{IkBe:NFkB}]$	kf <sup>21</sup>	0.07 ml/(µmol*s)
	NFkB07) IKK:IkBa:NFkB Catalysis	IKK[P]:ikBa:NFkB -> IKK[P] + NFkB	$v^{-1} = kf^{-1} \cdot [IKK[P]] \cdot [IKBE:NFKB] - kf^{-1} \cdot [IKK[P]:IKBE:NFKB]$ $v^{22} = kf^{22} \cdot [IKK[P]:IkBa:NFkB]$	kr <sup>21</sup>	0.00175 1/s 0.0204 1/s
	NFkB08) IKK:IkBb:NFkB Catalysis	IKK[P]:IkBb:NFkB -> IKK[P] + NFkB	$v^{23} = kf^{23} \cdot [IKK[P]:IkBb:NFkB]$	kf <sup>23</sup>	0.0075 1/s
	NFkB09) IKK:IkBe:NFkB Catalysis	IKK[P]:IkBe:NFkB -> IKK[P] + NFkB	$v^{24} = kf^{24} \cdot [IKK[P]:IkBe:NFkB]$	kf <sup>24</sup>	0.011 1/s
25			$v^{25} = kf^{25} \cdot [IkBa:NFkB]$	kf <sup>25</sup>	2.25E-05 1/s
26	NFkB11) IkBb:NFkB Constitutive Degradation	IkBb:NFkB -> NFkB	$v^{26} = kf^{26} \cdot [\text{IkBb:NFkB}]$	kf <sup>26</sup>	2.25E-05 1/s
27	NFkB12) IkBe:NFkB Constitutive Degradation	IkBe:NFkB -> NFkB	$v^{27} = kf^{27} \cdot [\text{IkBe:NFkB}]$	kf <sup>27</sup>	2.25E-05 1/s
28	NFkB13) NFkB Nuclear Import/Export	NFkB = NFkB(nuc)	$v^{28} = kf^{28} \cdot [NFkB] - kr^{28} \cdot [NFkB(nuc)]$	kf <sup>28</sup>	0.09 1/s
29	NFkB14) Nuclear IkBa:NFkB Binding	IkBa(nuc) + NFkB(nuc) = IkBa:NFkB(nuc)		kr <sup>28</sup> kf <sup>29</sup>	8.00E-05 1/s 0.5 ml/(μmol*s)
30	NFkB15) Nuclear IkBb:NFkB Binding	IkBb(nuc) + NFkB(nuc) = IkBb:NFkB(nuc)	$v^{29} = kf^{29} \cdot \text{[IkBa(nuc)]} \cdot \text{[NFkB(nuc)]} - kr^{29} \cdot \text{[IkBa:NFkB(nuc)]}$	kr <sup>29</sup> kf <sup>30</sup>	0.0005 1/s 0.5 ml/(μmol*s)
			$v^{30} = kf^{30} \cdot [lkBb(nuc)] \cdot [NFkB(nuc)] \cdot kr^{30} \cdot [lkBb:NFkB(nuc)]$	kr <sup>30</sup> kf <sup>31</sup>	0.0005 1/s 0.5 ml/(μmol*s)
	NFkB16) Nuclear IkBe:NFkB Binding	IkBe(nuc) + NFkB(nuc) = IkBe:NFkB(nuc)	$v^{31} = kf^{31} \cdot [lkBe(nuc)] \cdot [NFkB(nuc)] - kr^{31} \cdot [lkBe:NFkB(nuc)]$	kr <sup>31</sup>	0.0005 1/s
	NFkB17) Constitutive IkBa mRNA Synthesis	source -> lkBa_mRNA	$v^{32} = kf^{32} \cdot [\text{source}]$	kf <sup>32</sup>	1.54E-06 1/s
	NFkB18) Inducible IkBa mRNA Synthesis	2 * NFkB(nuc) -> IkBa_mRNA + 2 * NFkB(nuc)	$v^{33} = kf^{33} \cdot 2 \cdot [\text{NFkB(nuc)}]$	kf <sup>33</sup>	0.0165 ml/(μmol*s)
	NFkB19) IkBa mRNA degradation  NFkB20) Constitutive IkBb mRNA Synthesis	IkBa_mRNA->sink	v <sup>34</sup> = kf <sup>34</sup> · [IkBa_mRNA]	kf <sup>34</sup>	0.00028 1/s 1.78E-07 1/s
		source -> IKBb_mRNA  IkBb_mRNA -> sink	$v^{35} = kf^{35} \cdot [\text{source}]$	kf <sup>35</sup>	0.00028 1/s
	NFkB21) IkBb mRNA degradation  NFkB22) Constitutive IkBe mRNA Synthesis	source -> lkBe_mRNA	v <sup>36</sup> = kf <sup>36</sup> · [IkBb_mRNA]	kf <sup>37</sup>	1.27E-07 1/s
38	NFkB23) IkBe mRNA degradation	IkBe_mRNA -> sink	$v^{37} = kf^{37} \cdot [\text{source}]$ $v^{38} = kf^{38} \cdot [\text{IkBe mRNA}]$	kf <sup>38</sup>	0.00028 1/s
		IKK[P] + IkBa = IKK[P]:IkBa	$v^{39} = kf^{39} \cdot [IKK[P]] \cdot [IKBa] \cdot kr^{39} \cdot [IKK[P] \cdot lkBa]$	kf 39	0.0225 ml/(μmol*s)
	NFkB24) IKK:IkBa Binding			kr <sup>39</sup>	0.00125 1/s 0.00408 1/s
	NFkB25) IkBa Translation	IkBa_mRNA -> IkBa + IkBa_mRNA	v <sup>40</sup> = kf <sup>40</sup> · [IkBa_mRNA]	kf <sup>40</sup>	
	NFkB26) IkBa Degradation	IkBa -> sink	v <sup>41</sup> = kf <sup>41</sup> · [IkBa]	kf <sup>41</sup>	0.000113 1/s 0.0003 1/s
	NFkB27) IkBa Nuclear Import/Export	IkBa = IkBa(nuc)	$v^{42} = kf^{42} \cdot [IKBa] \cdot kr^{42} \cdot [IkBa(nuc)]$	kr <sup>42</sup>	0.0002 1/s 0.006 ml/(µmol*s)
	NFkB28) IKK:IkBb Binding	IKK[P] + IkBb = IKK[P]:IkBb	$v^{43} = kf^{43} \cdot [\text{IKK[P]]} \cdot [\text{IKBb}] - kr^{43} \cdot [\text{IKK[P]} \cdot \text{lkBb}]$	kr <sup>43</sup>	0.00175 1/s
	NFkB29) IkBb Translation	IkBb_mRNA -> IkBb + IkBb_mRNA	$v^{44} = kf^{44} \cdot [IkBb\_mRNA]$	kf <sup>44</sup>	0.00408 1/s
	NFkB30) IkBb Degradation	IkBb-> sink	$v^{45} = kf^{45} \cdot [lkBb]$	kf <sup>45</sup>	0.000113 1/s 0.00015 1/s
46	NFkB31) IkBb Nuclear Import/Export	IkBb = IkBb(nuc)	$v^{46} = kf^{46} \cdot [\text{IKBb}] \cdot kr^{46} \cdot [\text{lkBb(nuc)}]$	kf <sup>46</sup> kr <sup>46</sup>	0.0001 1/s
47	NFkB32) IKK:IkBe Binding	IKK[P] + IkBe = IKK[P]:IkBe	$v^{47} = kf^{47} \cdot [\text{IKK[P]]} \cdot [\text{IKBe}] \cdot kr^{47} \cdot [\text{IKK[P]} : \text{IkBe}]$	kf <sup>47</sup> kr <sup>47</sup>	0.009 ml/(μmol*s) 0.00175 1/s
48	NFkB33) IkBe Translation	IkBe_mRNA -> IkBe + IkBe_mRNA	$v^{\rm 48} = kf^{\rm 48} \cdot {\rm [lkBe\_mRNA]}$	kf <sup>48</sup>	0.00408 1/s
49	NFkB34) IkBe Degradation	IkBe -> sink	$v^{49} = kf^{49} \cdot [lkBe]$	kf 49	0.000113 1/s
50	NFkB35) IkBe Nuclear Import/Export	IkBe = IkBe(nuc)	$v^{\rm SO} = kf^{\rm SO} \cdot [\rm IKBe] \cdot kr^{\rm SO} \cdot [\rm IkBe(nuc)]$	kf <sup>50</sup> kr <sup>50</sup>	0.00015 1/s 0.0001 1/s
51	NFkB36) IKK:IkBa:NFkB Binding (2)	IKK[P]:lkBa + NFkB = IKK[P]:lkBa:NFkB	$v^{\rm 51} = kf^{\rm 51} \cdot [{\rm IKK[P]:lkBa]} \cdot [{\rm NFkB}]  \cdot  kr^{\rm 51} \cdot [{\rm IKK[P]:lkBa:NFkB}]$	kf <sup>51</sup> kr <sup>51</sup>	0.5 ml/(μmol*s) 0.0005 1/s
52	NFkB37) IkBa:NFkB Nuclear Export	IkBa:NFkB(nuc) -> IkBa:NFkB	$v^{52} = kf^{52} \cdot [\text{IkBa:NFkB(nuc)}]$	kf 52	0.0138 1/s
53	NFkB38) IKK:IkBb:NFkB Binding (2)	IKK[P]:IkBb + NFkB = IKK[P]:IkBb:NFkB	$v^{\rm 53} = kf^{\rm 53} \cdot [\rm IKK[P]:lkBb] \cdot [\rm NFkB]  \cdot  kr^{\rm 53} \cdot [\rm IKK[P]:lkBb:NFkB]$	kf <sup>53</sup> kr <sup>53</sup>	0.5 ml/(μmol*s) 0.0005 1/s
54	NFkB39) IkBb:NFkB Nuclear Export	IkBb:NFkB(nuc) -> IkBb:NFkB	$v^{54} = kf^{54} \cdot [\text{IkBb:NFkB(nuc)}]$	kf 54	0.0052 1/s
55	NFkB40) IKK:IkBe:NFkB Binding (2)	IKK[P]:IkBe + NFkB = IKK[P]:IkBe:NFkB	$v^{\rm 55} = kf^{\rm 55} \cdot [\rm IKK[P]:lkBe] \cdot [\rm NFkB] - kr^{\rm 55} \cdot [\rm IKK[P]:lkBe:NFkB]$	kf <sup>55</sup> kr <sup>55</sup>	0.5 ml/(μmol*s) 0.0005 1/s
56	NFkB41) IkBe:NFkB Nuclear Export	IkBe:NFkB(nuc) -> IkBe:NFkB	$v^{56} = kf^{56} \cdot [\text{IkBe:NFkB(nuc)}]$	kf 56	0.0052 1/s
57	NFkB42) IKK:IkBa Catalysis	IKK[P]:IkBa->IKK[P]	$v^{57} = kf^{57} \cdot [\text{IKK[P]:IkBa}]$	kf 57	0.00407 1/s
58	NFkB43) IKK:IkBb Catalysis	IKK[P]:IkBb->IKK[P]	$v^{\rm S8} = kf^{\rm S8} \cdot [\rm IKK[P]:lkBb]$	kf <sup>58</sup>	0.0015 1/s
59	NFkB44) IKK:IkBe Catalysis	IKK[P]:lkBe -> IKK[P]	$v^{59} = kf^{59} \cdot [IKK[P]:IkBe]$	kf 59	0.0022 1/s