

```

begin model
#####
#
begin parameters
# molecules
LCK_T 16.491
CD3z_T 20000

#####
#####
KmA1 1.60E+05
KmA2 5.55E+06
KmB1 4.05E+06
KmB2 3.88E+05
KmC1 2.55E+08
KmC2 6.86E+06

Kcat 381.73
L 3

end parameters

#####
#
begin molecule types

LCK(b,Y394~U~P,Y505~U~P)
count(num~0~1~2~3~4~5~6,A1,A2,B1,B2,C1,C2)
A1(I,Y~U~P~X)
A2(I,Y~U~P~X)
B1(I,Y~U~P~X)
B2(I,Y~U~P~X)
C1(I,Y~U~P~X)
C2(I,Y~U~P~X)

end molecule types

#####
#
begin seed species

LCK(b,Y394~P,Y505~U) LCK_T

count(num~0,A1!1,A2!2,B1!3,B2!4,C1!5,C2!6).A1(I!1,Y~U).A2(I!2,Y~U).B1(I!3,Y~U).B2(I!4,Y~U).C1(I!5,Y~U).C2(I!6,Y~U)
) CD3z_T

end seed species

#####
#
begin observables
Molecules Total_A1 A1(Y~P!?)
Molecules Total_A2 A2(Y~P!?)
Molecules Total_B1 B1(Y~P!?)
Molecules Total_B2 B2(Y~P!?)
Molecules Total_C1 C1(Y~P!?)
Molecules Total_C2 C2(Y~P!?)

Molecules U_A1 A1(Y~U!?)
Molecules U_A2 A2(Y~U!?)
Molecules U_B1 B1(Y~U!?)
Molecules U_B2 B2(Y~U!?)
Molecules U_C1 C1(Y~U!?)
Molecules U_C2 C2(Y~U!?)

Molecules F_A1 A1(Y~X!?)
Molecules F_A2 A2(Y~X!?)
Molecules F_B1 B1(Y~X!?)
Molecules F_B2 B2(Y~X!?)
Molecules F_C1 C1(Y~X!?)
Molecules F_C2 C2(Y~X!?)

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end observables

#

begin reaction rules # CD3z (A1~?, A2~?, B1~?, B2~?, C1~?, C2~?)

count (num~0, A1!1) .A1 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~1, A1!1) .A1 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmA1) + U_A1)
count (num~1, A1!1) .A1 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~2, A1!1) .A1 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmA1/L) +
U_A1)
count (num~2, A1!1) .A1 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~3, A1!1) .A1 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmA1/L/L) +
U_A1)
count (num~3, A1!1) .A1 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~4, A1!1) .A1 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmA1/L/L/L) +
U_A1)
count (num~4, A1!1) .A1 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~5, A1!1) .A1 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmA1/L/L/L/L)
+ U_A1)
count (num~5, A1!1) .A1 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~6, A1!1) .A1 (I!1, Y~P) + LCK (b, Y394~P, Y505~U)
(Kcat) / ((KmA1/L/L/L/L/L) + U_A1)

count (num~0, A2!1) .A2 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~1, A2!1) .A2 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmA2) + U_A2)
count (num~1, A2!1) .A2 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~2, A2!1) .A2 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmA2/L) +
U_A2)
count (num~2, A2!1) .A2 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~3, A2!1) .A2 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmA2/L/L) +
U_A2)
count (num~3, A2!1) .A2 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~4, A2!1) .A2 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmA2/L/L/L) +
U_A2)
count (num~4, A2!1) .A2 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~5, A2!1) .A2 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmA2/L/L/L/L)
+ U_A2)
count (num~5, A2!1) .A2 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~6, A2!1) .A2 (I!1, Y~P) + LCK (b, Y394~P, Y505~U)
(Kcat) / ((KmA2/L/L/L/L/L) + U_A2)

count (num~0, B1!1) .B1 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~1, B1!1) .B1 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmB1) + U_B1)
count (num~1, B1!1) .B1 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~2, B1!1) .B1 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmB1/L) +
U_B1)
count (num~2, B1!1) .B1 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~3, B1!1) .B1 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmB1/L/L) +
U_B1)
count (num~3, B1!1) .B1 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~4, B1!1) .B1 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmB1/L/L/L) +
U_B1)
count (num~4, B1!1) .B1 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~5, B1!1) .B1 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmB1/L/L/L/L)
+ U_B1)
count (num~5, B1!1) .B1 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~6, B1!1) .B1 (I!1, Y~P) + LCK (b, Y394~P, Y505~U)
(Kcat) / ((KmB1/L/L/L/L/L) + U_B1)

count (num~0, B2!1) .B2 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~1, B2!1) .B2 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmB2) + U_B2)
count (num~1, B2!1) .B2 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~2, B2!1) .B2 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmB2/L) +
U_B2)
count (num~2, B2!1) .B2 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~3, B2!1) .B2 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmB2/L/L) +
U_B2)
count (num~3, B2!1) .B2 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~4, B2!1) .B2 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmB2/L/L/L) +
U_B2)
count (num~4, B2!1) .B2 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->
count (num~5, B2!1) .B2 (I!1, Y~P) + LCK (b, Y394~P, Y505~U) (Kcat) / ((KmB2/L/L/L/L)
+ U_B2)
count (num~5, B2!1) .B2 (I!1, Y~U) + LCK (b, Y394~P, Y505~U) ->

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count(num~6,B2!1).B2(I!1,Y~P) + LCK(b,Y394~P,Y505~U)
(Kcat)/((KmB2/L/L/L/L/L) + U_B2)

count(num~0,C1!1).C1(I!1,Y~U) + LCK(b,Y394~P,Y505~U) ->
count(num~1,C1!1).C1(I!1,Y~P) + LCK(b,Y394~P,Y505~U) (Kcat)/((KmC1) + U_C1)
count(num~1,C1!1).C1(I!1,Y~U) + LCK(b,Y394~P,Y505~U) ->
count(num~2,C1!1).C1(I!1,Y~P) + LCK(b,Y394~P,Y505~U) (Kcat)/((KmC1/L) +
U_C1)
count(num~2,C1!1).C1(I!1,Y~U) + LCK(b,Y394~P,Y505~U) ->
count(num~3,C1!1).C1(I!1,Y~P) + LCK(b,Y394~P,Y505~U) (Kcat)/((KmC1/L/L) +
U_C1)
count(num~3,C1!1).C1(I!1,Y~U) + LCK(b,Y394~P,Y505~U) ->
count(num~4,C1!1).C1(I!1,Y~P) + LCK(b,Y394~P,Y505~U) (Kcat)/((KmC1/L/L/L) +
U_C1)
count(num~4,C1!1).C1(I!1,Y~U) + LCK(b,Y394~P,Y505~U) ->
count(num~5,C1!1).C1(I!1,Y~P) + LCK(b,Y394~P,Y505~U) (Kcat)/((KmC1/L/L/L/L)
+ U_C1)
count(num~5,C1!1).C1(I!1,Y~U) + LCK(b,Y394~P,Y505~U) ->
count(num~6,C1!1).C1(I!1,Y~P) + LCK(b,Y394~P,Y505~U)
(Kcat)/((KmC1/L/L/L/L/L) + U_C1)

count(num~0,C2!1).C2(I!1,Y~U) + LCK(b,Y394~P,Y505~U) ->
count(num~1,C2!1).C2(I!1,Y~P) + LCK(b,Y394~P,Y505~U) (Kcat)/((KmC2) + U_C2)
count(num~1,C2!1).C2(I!1,Y~U) + LCK(b,Y394~P,Y505~U) ->
count(num~2,C2!1).C2(I!1,Y~P) + LCK(b,Y394~P,Y505~U) (Kcat)/((KmC2/L) +
U_C2)
count(num~2,C2!1).C2(I!1,Y~U) + LCK(b,Y394~P,Y505~U) ->
count(num~3,C2!1).C2(I!1,Y~P) + LCK(b,Y394~P,Y505~U) (Kcat)/((KmC2/L/L) +
U_C2)
count(num~3,C2!1).C2(I!1,Y~U) + LCK(b,Y394~P,Y505~U) ->
count(num~4,C2!1).C2(I!1,Y~P) + LCK(b,Y394~P,Y505~U) (Kcat)/((KmC2/L/L/L) +
U_C2)
count(num~4,C2!1).C2(I!1,Y~U) + LCK(b,Y394~P,Y505~U) ->
count(num~5,C2!1).C2(I!1,Y~P) + LCK(b,Y394~P,Y505~U) (Kcat)/((KmC2/L/L/L/L)
+ U_C2)
count(num~5,C2!1).C2(I!1,Y~U) + LCK(b,Y394~P,Y505~U) ->
count(num~6,C2!1).C2(I!1,Y~P) + LCK(b,Y394~P,Y505~U)
(Kcat)/((KmC2/L/L/L/L/L) + U_C2)

end reaction rules

end model

generate_network({overwrite=>1});
writeMfile({});

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