

```

begin model
#####
#
begin parameters
# molecules
LCK_T 19.703
CD3z_T 20000

#####
#####
KmA1 96.548
KmA2 331.68
KmB1 270
KmB2 153.82
KmC1 484.9
KmC2 405.43

Xi 0.1153

KiA1 KmA1*Xi
KiA2 KmA2*Xi
KiB1 KmB1*Xi
KiB2 KmB2*Xi
KiC1 KmC1*Xi
KiC2 KmC2*Xi

Kcat 360

end parameters

#####
#

begin molecule types

LCK(b, Y394~U~P, Y505~U~P)
A1 (Y~U~P~X)
A2 (Y~U~P~X)
B1 (Y~U~P~X)
B2 (Y~U~P~X)
C1 (Y~U~P~X)
C2 (Y~U~P~X)

end molecule types

#####
#

begin seed species

LCK(b, Y394~P, Y505~U) LCK_T
A1 (Y~U) CD3z_T
A2 (Y~U) CD3z_T
B1 (Y~U) CD3z_T
B2 (Y~U) CD3z_T
C1 (Y~U) CD3z_T
C2 (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!?)
```

```
end observables
```

```
#####
#
```

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

```
A1(Y~U) + LCK(b,Y394~P,Y505~U) -> A1(Y~P) + LCK(b,Y394~P,Y505~U)
(Kcat/KmA1)/(1 + U_A1/KmA1 + U_A2/KmA2 + U_B1/KmB1 + U_B2/KmB2 + U_C1/KmC1
+ U_C2/KmC2 + Total_A1/KiA1 + Total_A2/KiA2 + Total_B1/KiB1 + Total_B2/KiB2
+ Total_C1/KiC1 + Total_C2/KiC2)
A2(Y~U) + LCK(b,Y394~P,Y505~U) -> A2(Y~P) + LCK(b,Y394~P,Y505~U)
(Kcat/KmA2)/(1 + U_A1/KmA1 + U_A2/KmA2 + U_B1/KmB1 + U_B2/KmB2 + U_C1/KmC1
+ U_C2/KmC2 + Total_A1/KiA1 + Total_A2/KiA2 + Total_B1/KiB1 + Total_B2/KiB2
+ Total_C1/KiC1 + Total_C2/KiC2)
```

```
B1(Y~U) + LCK(b,Y394~P,Y505~U) -> B1(Y~P) + LCK(b,Y394~P,Y505~U)
(Kcat/KmB1)/(1 + U_A1/KmA1 + U_A2/KmA2 + U_B1/KmB1 + U_B2/KmB2 + U_C1/KmC1
+ U_C2/KmC2 + Total_A1/KiA1 + Total_A2/KiA2 + Total_B1/KiB1 + Total_B2/KiB2
+ Total_C1/KiC1 + Total_C2/KiC2)
B2(Y~U) + LCK(b,Y394~P,Y505~U) -> B2(Y~P) + LCK(b,Y394~P,Y505~U)
(Kcat/KmB2)/(1 + U_A1/KmA1 + U_A2/KmA2 + U_B1/KmB1 + U_B2/KmB2 + U_C1/KmC1
+ U_C2/KmC2 + Total_A1/KiA1 + Total_A2/KiA2 + Total_B1/KiB1 + Total_B2/KiB2
+ Total_C1/KiC1 + Total_C2/KiC2)
```

```
C1(Y~U) + LCK(b,Y394~P,Y505~U) -> C1(Y~P) + LCK(b,Y394~P,Y505~U)
(Kcat/KmC1)/(1 + U_A1/KmA1 + U_A2/KmA2 + U_B1/KmB1 + U_B2/KmB2 + U_C1/KmC1
+ U_C2/KmC2 + Total_A1/KiA1 + Total_A2/KiA2 + Total_B1/KiB1 + Total_B2/KiB2
+ Total_C1/KiC1 + Total_C2/KiC2)
C2(Y~U) + LCK(b,Y394~P,Y505~U) -> C2(Y~P) + LCK(b,Y394~P,Y505~U)
(Kcat/KmC2)/(1 + U_A1/KmA1 + U_A2/KmA2 + U_B1/KmB1 + U_B2/KmB2 + U_C1/KmC1
+ U_C2/KmC2 + Total_A1/KiA1 + Total_A2/KiA2 + Total_B1/KiB1 + Total_B2/KiB2
+ Total_C1/KiC1 + Total_C2/KiC2)
```

```
end reaction rules
```

```
end model
```

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