

```

begin model
#####
#
begin parameters
# molecules
LCK_T    1000
CD3z_T   1
Phos_T   1000

#####
#####
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

PmA1  10.56
PmA2  36.3
PmB1  32.4
PmB2  18.36
PmC1  67.2
PmC2  56.7

PXi  0.1

PiA1  PmA1*PXi
PiA2  PmA2*PXi
PiB1  PmB1*PXi
PiB2  PmB2*PXi
PiC1  PmC1*PXi
PiC2  PmC2*PXi

Pcat  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)

Phos()

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
```

```
Phos() Phos_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!?)
```

```
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)
```

```

A1(Y~P) + Phos() -> A1(Y~U) + Phos() (Pcat/PmA1)/(1 + Total_A1/PmA1 +
Total_A2/PmA2 + Total_B1/PmB1 + Total_B2/PmB2 + Total_C1/PmC1 +
Total_C2/PmC2 + U_A1/PiA1 + U_A2/PiA2 + U_B1/PiB1 + U_B2/PiB2 + U_C1/PiC1 +
U_C2/PiC2)
A2(Y~P) + Phos() -> A2(Y~U) + Phos() (Pcat/PmA2)/(1 + Total_A1/PmA1 +
Total_A2/PmA2 + Total_B1/PmB1 + Total_B2/PmB2 + Total_C1/PmC1 +
Total_C2/PmC2 + U_A1/PiA1 + U_A2/PiA2 + U_B1/PiB1 + U_B2/PiB2 + U_C1/PiC1 +
U_C2/PiC2)
B1(Y~P) + Phos() -> B1(Y~U) + Phos() (Pcat/PmB1)/(1 + Total_A1/PmA1 +
Total_A2/PmA2 + Total_B1/PmB1 + Total_B2/PmB2 + Total_C1/PmC1 +
Total_C2/PmC2 + U_A1/PiA1 + U_A2/PiA2 + U_B1/PiB1 + U_B2/PiB2 + U_C1/PiC1 +
U_C2/PiC2)
B2(Y~P) + Phos() -> B2(Y~U) + Phos() (Pcat/PmB2)/(1 + Total_A1/PmA1 +
Total_A2/PmA2 + Total_B1/PmB1 + Total_B2/PmB2 + Total_C1/PmC1 +
Total_C2/PmC2 + U_A1/PiA1 + U_A2/PiA2 + U_B1/PiB1 + U_B2/PiB2 + U_C1/PiC1 +
U_C2/PiC2)
C1(Y~P) + Phos() -> C1(Y~U) + Phos() (Pcat/PmC1)/(1 + Total_A1/PmA1 +
Total_A2/PmA2 + Total_B1/PmB1 + Total_B2/PmB2 + Total_C1/PmC1 +
Total_C2/PmC2 + U_A1/PiA1 + U_A2/PiA2 + U_B1/PiB1 + U_B2/PiB2 + U_C1/PiC1 +
U_C2/PiC2)
C2(Y~P) + Phos() -> C2(Y~U) + Phos() (Pcat/PmC2)/(1 + Total_A1/PmA1 +
Total_A2/PmA2 + Total_B1/PmB1 + Total_B2/PmB2 + Total_C1/PmC1 +
Total_C2/PmC2 + U_A1/PiA1 + U_A2/PiA2 + U_B1/PiB1 + U_B2/PiB2 + U_C1/PiC1 +
U_C2/PiC2)

```

```
end reaction rules
```

```
end model
```

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