

Version=3.21301
EndTime=1.800000e 팔
Points=200
OutputTimeZero=1
RealTime=0
SleepTime=0
TimeUnit=s
ConcentrationUnit=M
VolumeUnit=L
TimeElasticities=0
Dynamics=1
SteadyState=0
Report=1
DynTitles=1
SSTitles=0
DynQuotes=1
SSQuotes=0
DynColWidth=12
SSColWidth=12
DynSeparator=32
SSSeparator=32
SSMCAUnscaled=0
SSStrategy=0
SSBackIntegration=1
RepStructuralAnalysis=1
RepStabilityAnalysis=1
RepMCA=1
NewtonLimit=50
SSResolution=1.000000e-009
RelativeTolerance=1.000000e-006
AbsoluteTolerance=1.000000e-012
AdamsMaxOrder=12
BDFMaxOrder=5
DerivationFactor=1.000000e-003
ReportFile=upynapy7_goed_300secminimaal_1HNMR_flux.txt
DynamicsFile=upynapy2.dyn
SSFile=simresults.ss
Title=UNkin
TotalMetabolites=5
TotalSteps=4
TotalMoieties=2
TotalCompartments=1
TotalUDKinetics=0
Metabolite=U
Concentration=1e-008
Compartment=0
Type=1
Metabolite=Uk
Concentration=5e-006
Compartment=0
Type=1
Metabolite=N
Concentration=0.005
Compartment=0
Type=1
Metabolite=NU
Concentration=0

Compartment=0
Type=2
Metabolite=U2
Concentration=0.0024992
Compartment=0
Type=2
Metabolite= N NU
Concentration=0.04999999999999999
Compartment=0
Type=7
Metabolite= 0.5*U 0.5*Uk - 0.5*N U2
Concentration=2.505000000003338e-006
Compartment=0
Type=7
Step=R4
Equation=Uk N = NU
KineticType=Mass action (reversible)
Flux=0
Reversible=1
Substrates=2
Products=1
Modifiers=0
Constants=2
Subs0=1
Subs1=2
Prod0=3
Param0=11800000000
Param1=100
Step=R1
Equation=U2 = U U
KineticType=Mass action (reversible)
Flux=0
Reversible=1
Substrates=1
Products=2
Modifiers=0
Constants=2
Subs0=4
Prod0=0
Prod1=0
Param0=1
Param1=10000000000
Step=R2
Equation=U U = Uk U
KineticType=Mass action (reversible)
Flux=0
Reversible=1
Substrates=2
Products=2
Modifiers=0
Constants=2
Subs0=0
Subs1=0
Prod0=1
Prod1=0
Param0=8109037.395347904
Param1=2013996.821631786

Step=R3
Equation=U N = Uk N
KineticType=Mass action (reversible)
Flux=0
Reversible=1
Substrates=2
Products=2
Modifiers=0
Constants=2
Subs0=0
Subs1=2
Prod0=1
Prod1=2
Param0=16704.42622315591
Param1=0.2575774779254673
Compartment=compartment
Volume=1.000000e 팔
Comments

EndComments
PlotType=2
PlotDyn=0
Plot3d=0
PlotGrid=1
PlotKey=1
PlotTitles=1
PlotMultiplot=0
PlotContour=0
PlotHidden3d=0
PlotLogX=0
PlotLogY=0
PlotLogZ=0
PlotXEntry=0
PlotYTotal=1
PlotZTotal=1
PlotY0=3
PlotZ0=-1
User-defined functions
Items=5
Name=Kdimconc
Description= $k/(m)^2$
Nodes=10
Node=37,64
Node=73,107
Title=[U2]
Type=2
I=U2
Node=79,47
Node=79,40
Node=73,109
Title=[U]
Type=2
I=U
Node=79,43
Node=73,110
Title=[Uk]
Type=2

I=Uk
 Node=79,41
 Node=79,94
 Node=78,64
 Value=2.000000e $\frac{a}{b}$
 Name=Kassconc
 Description= $a/(b*(c))$
 Nodes=12
 Node=37,64
 Node=73,97
 Title=[NU]
 Type=2
 I=NU
 Node=79,47
 Node=79,40
 Node=73,98
 Title=[N]
 Type=2
 I=N
 Node=79,42
 Node=79,40
 Node=73,99
 Title=[Uk]
 Type=2
 I=Uk
 Node=79,43
 Node=73,100
 Title=[U]
 Type=2
 I=U
 Node=79,41
 Node=79,41
 Name=conversion
 Description= a/b
 Nodes=4
 Node=37,64
 Node=73,97
 Title=[NU]
 Type=2
 I=NU
 Node=79,47
 Node=73,98
 Title=[N] i
 Type=1
 I=N
 Name=Ktaut
 Description= $(a*d)/(c*b)$
 Nodes=12
 Node=37,64
 Node=79,40
 Node=73,97
 Title=R2(k1)
 Type=6
 I=R2
 J=k1
 Node=79,42
 Node=73,100

Title=R3 (k2)
Type=6
I=R3
J=k2
Node=79,41
Node=79,47
Node=79,40
Node=73,99
Title=R2 (k2)
Type=6
I=R2
J=k2
Node=79,42
Node=73,98
Title=R3 (k1)
Type=6
I=R3
J=k1
Node=79,41
Name=Tautflux
Description=a/b
Nodes=4
Node=37,64
Node=73,97
Title=J (R2)
Type=4
I=R2
Node=79,47
Node=73,98
Title=J (R3)
Type=4
I=R3
Interactive time course
Items=3
Title= [N] t
Type=3
I=N
Title= [NU] t
Type=3
I=NU
Title= [U2] t
Type=3
I=U2
Time-course output
Items=14
Title=time
Type=14
Title= [N] t
Type=3
I=N
Title= [NU] t
Type=3
I=NU
Title=conversion
Type=24
Title= [U] t
Type=3

I=U
Title=[Uk] t
Type=3
I=Uk
Title=Ktaut
Type=24
Title=Kassconc
Type=24
Title=Kdimconc
Type=24
Title=J (R4)
Type=5
I=R4
Title=J (R1)
Type=5
I=R1
Title=J (R2)
Type=5
I=R2
Title=J (R3)
Type=5
I=R3
Title=Tautflux
Type=24
Steady-state output
Items=0
Scan
Enabled=1
Dimension=2
Title=[N] i
Type=1
I=N
Min=0.000253000000000000
Max=0.050000000000000000
Density=5
Log=1
Independent=1
Grid=0
Title=[U2] i
Type=1
I=U2
Min=0.000249920000000000
Max=0.025000000000000000
Density=3
Log=1
Independent=0
Grid=0
Parameter Links
Items=0
Optimisation
Enabled=0
SetModel=0
Sign=1.0
OptimiseDyn=1
Constrained=0
Method=Evolutionary programming
P0=500

P1=10
P2=0.85
P3=1
P4=1
Title=Kdim
Type=24
Parameters=1
MinType=1
MaxType=1
MinIneq=0
MaxIneq=0
MinD=1000000000
MaxD=1000000000
IsParameter=0
Title=Kdim
Type=24
Min=1.0000000000000000
Max=2.0000000000000000
Density=2
Log=0
Independent=1
Grid=-1
Title=
Type=0
Title=
Type=0
Fitting
Enabled=0
SetModel=1
FitDyn=1
Constrained=0
FitDataFile=5mM.dat
FitSeparator=9
FitLines=15
Method=Evolutionary programming
P0=500
P1=10
P2=0.85
P3=1
P4=1
Parameters=8
MinType=1
MaxType=1
MinIneq=1
MaxIneq=1
MinD=10000000
MaxD=500000000
IsParameter=0
Title=Kassconc
Type=24
Min=1.0000000000000000
Max=2.0000000000000000
Density=2
Log=0
Independent=1
Grid=-1
Title=

Type=0
Title=
Type=0
MinType=1
MaxType=1
MinIneq=1
MaxIneq=1
MinD=100000000
MaxD=800000000
IsParameter=0
Title=Kdimconc
Type=24
Min=1.0000000000000000
Max=2.0000000000000000
Density=2
Log=0
Independent=1
Grid=-1
Title=
Type=0
Title=
Type=0
MinType=1
MaxType=1
MinIneq=1
MaxIneq=0
MinD=0.0001
MaxD=10000000000
IsParameter=1
Title=R2 (k1)
Type=6
I=R2
J=k1
Min=1.0000000000000000
Max=2.0000000000000000
Density=2
Log=0
Independent=1
Grid=-1
Title=
Type=0
Title=
Type=0
MinType=1
MaxType=1
MinIneq=1
MaxIneq=0
MinD=0.0001
MaxD=10000000000
IsParameter=1
Title=R2 (k2)
Type=6
I=R2
J=k2
Min=1.0000000000000000
Max=2.0000000000000000
Density=2

Log=0
Independent=1
Grid=-1
Title=
Type=0
Title=
Type=0
MinType=1
MaxType=1
MinIneq=0
MaxIneq=0
MinD=0.0001
MaxD=10000000000
IsParameter=1
Title=R3 (k2)
Type=6
I=R3
J=k2
Min=1.0000000000000000
Max=2.0000000000000000
Density=2
Log=0
Independent=1
Grid=-1
Title=
Type=0
Title=
Type=0
MinType=1
MaxType=1
MinIneq=1
MaxIneq=0
MinD=1e-005
MaxD=10000000000
IsParameter=1
Title=R3 (k1)
Type=6
I=R3
J=k1
Min=1.0000000000000000
Max=2.0000000000000000
Density=2
Log=0
Independent=1
Grid=-1
Title=
Type=0
Title=
Type=0
MinType=1
MaxType=1
MinIneq=0
MaxIneq=0
MinD=5000000000
MaxD=11800000000
IsParameter=1
Title=R4 (k1)

Type=6
I=R4
J=k1
Min=1.0000000000000000
Max=2.0000000000000000
Density=2
Log=0
Independent=1
Grid=-1
Title=
Type=0
Title=
Type=0
MinType=1
MaxType=1
MinIneq=0
MaxIneq=0
MinD=100
MaxD=1000000
IsParameter=1
Title=R4 (k2)
Type=6
I=R4
J=k2
Min=1.0000000000000000
Max=2.0000000000000000
Density=2
Log=0
Independent=1
Grid=-1
Title=
Type=0
Title=
Type=0
AdjConcentrations=0
FitXItems=1
Title=time
Type=14
FitYItems=1
Title= [NU] t
Type=3
I=NU