SimBiology Model: TMDDmodel

Repeated Assignments:

1. [UnboundAbConc (mcg/ml)] = [UnboundAbAmt (mcg/kg)]/V1
2. [PeriConc (mcg/ml)] = [PeriAbAmt (mcg/kg)]/V2
3. [UnboundAb (nM)] = [UnboundAbConc (mcg/ml)] * 1e3/MWab
4. [TotalAbConc (mcg/ml)] = ([UnboundAb (nM)]+[Complex (nM)])*MWab/1e3
5. [FreeTarget (ng/ml)] = [FreeTarget (nM)]*MWtarget
6. [TotalTarget (ng/ml)] = [FreeTarget (ng/ml)]+[Complex (nM)]*MWtarget
7. TargetFracBound = min(1,max(0,(1-[FreeTarget (nM)]/target_init)))

ODEs:

1. d([UnboundAbAmt (mcg/kg)])/dt = 1/[TMDD model]*(-(CLd*([UnboundAbConc (mcg/ml)]-[PeriConc (mcg/ml)])) - (CL*[UnboundAbConc (mcg/ml)]) + ((fbio*kabs*[SCdepot (mcg/kg)])*[TMDD model]) - ((kon*[UnboundAb (nM)]*[FreeTarget (nM)]-kon*KD*[Complex (nM)])*MWab/1e3*V1))
2. d([PeriAbAmt (mcg/kg)])/dt = 1/[TMDD model]*((CLd*([UnboundAbConc (mcg/ml)]-[PeriConc (mcg/ml)])))
3. d([SCdepot (mcg/kg)])/dt = 1/[TMDD model]*(-((fbio*kabs*[SCdepot (mcg/kg)])*[TMDD model]) - (((1-fbio)*kabs*[SCdepot (mcg/kg)])*[TMDD model]))
4. d([FreeTarget (nM)])/dt = 1/[TMDD model]*(-(((kon*[UnboundAb (nM)]*[FreeTarget (nM)]-kon*KD*[Complex (nM)]))*[TMDD model]) + ((log(2)/target_thalf)*target_init) - ((log(2)/target_thalf)*[FreeTarget (nM)]))
5. d([Complex (nM)])/dt = 1/[TMDD model]*((((kon*[UnboundAb (nM)]*[FreeTarget (nM)]-kon*KD*[Complex (nM)]))*[TMDD model]) - ((complCLfactor*(CL/V1*[Complex (nM)]))*[TMDD model]))

Name	Type	Scope	Initial Value	Units
TMDD model	compartment	TMDDmodel	1.0	
Complex (nM)	species	TMDD model	0.0	
FreeTarget (ng/ml)	species	TMDD model	0.0	
FreeTarget (nM)	species	TMDD model	0.0	
PeriAbAmt (mcg/kg)	species	TMDD model	0.0	
PeriConc (mcg/ml)	species	TMDD model	0.0	
SCdepot (mcg/kg)	species	TMDD model	0.0	
TargetFracBound	species	TMDD model	0.0	
TotalAbConc (mcg/ml)	species	TMDD model	0.0	
TotalTarget (ng/ml)	species	TMDD model	0.0	
UnboundAb (nM)	species	TMDD model	0.0	
UnboundAbAmt (mcg/kg)	species	TMDD model	0.0	
UnboundAbConc (mcg/ml)	species	TMDD model	0.0	
CL	parameter	TMDDmodel	5.0	milliliter/day/kilogram
CLd	parameter	TMDDmodel	10.0	milliliter/day/kilogram
complCLfactor	parameter	TMDDmodel	1.0	fold
fbio	parameter	TMDDmodel	0.7	fraction
kabs	parameter	TMDDmodel	0.2	1/day
KD	parameter	TMDDmodel	0.1	nM
kon	parameter	TMDDmodel	400.0	1/nM/day
MWab	parameter	TMDDmodel	150.0	microgram/nanomolarity
MWtarget	parameter	TMDDmodel	38.0	microgram/nanomolarity
target_init	parameter	TMDDmodel	0.0	nM
target_thalf	parameter	TMDDmodel	1.0	day
V1	parameter	TMDDmodel	40.0	milliliter/kilogram
V2	parameter	TMDDmodel	40.0	milliliter/kilogram