

SimBiology Model: two compartment PK

Repeated Assignments:

- 1. [CentralConc(mcg/mL)] = [CentralAmt(mcg/kg)]/V1
- 2. [PeriConc(mcg/mL)] = [PeriAmt(mcg/kg)]/V2
- 3. log10Conc = log10([CentralConc(mcg/mL)]+1e-6)

ODEs:

- 1.  $d([CentralAmt(mcg/kg)]) / dt = 1/PK * (- (CLd * ([CentralConc(mcg/mL)] - [PeriConc(mcg/mL)])) - (CL * [CentralConc(mcg/mL)]) - (Vm * [CentralConc(mcg/mL)] / (Km + [CentralConc(mcg/mL)])) + ((kabs * fbio * [SCdepot(mcg/kg)]) * PK))$
- 2.  $d([PeriAmt(mcg/kg)]) / dt = 1/PK * ((CLd * ([CentralConc(mcg/mL)] - [PeriConc(mcg/mL)]))$
- 3.  $d([SCdepot(mcg/kg)]) / dt = 1/PK * (- ((kabs * fbio * [SCdepot(mcg/kg)]) * PK) - ((kabs * (1 - fbio) * [SCdepot(mcg/kg)]) * PK))$
- 4.  $d(AUC) / dt = 1/PK * (([CentralConc(mcg/mL)])$
- 5.  $d(Cmax) / dt = 1/PK * ((50 * ([CentralConc(mcg/mL)] - Cmax) * ([CentralConc(mcg/mL)] > Cmax))$

Name	Type	Scope	Initial Value	Units
PK	compartment	two compartment PK	1.0	
AUC	species	PK	0.0	
CentralAmt(mcg/kg)	species	PK	0.0	
CentralConc(mcg/mL)	species	PK	0.0	
Cmax	species	PK	0.0	
log10Conc	species	PK	-6.0	
PeriAmt(mcg/kg)	species	PK	0.0	
PeriConc(mcg/mL)	species	PK	0.0	
SCdepot(mcg/kg)	species	PK	0.0	
CL	parameter	two compartment PK	5.0	milliliter/day/kilogram
CLd	parameter	two compartment PK	10.0	milliliter/day/kilogram
fbio	parameter	two compartment PK	0.7	fraction
kabs	parameter	two compartment PK	10.0	1/day
Km	parameter	two compartment PK	5.0	microgram/milliliter
V1	parameter	two compartment PK	40.0	milliliter/kilogram
V2	parameter	two compartment PK	40.0	milliliter/kilogram
Vm	parameter	two compartment PK	0.0	microgram/day/kilogram