Example code of the QE approximation with non-constant total receptors in MONOLIX

DESCRIPTION:

BsAb QE approximation

[LONGITUDINAL]

input = {kel,KD1,KD2,a,ksynA,kdegA,ksynB,kdegB,kintA,kintB,kintAB,k12,k21,ka,V,F}

PK:

tdur = 0.0001

; tdur = 14

depot(adm = 1,target = In,p = 1/tdur) ; IV

depot(adm = 1,target = In,p = -1/tdur, Tlag = tdur)

depot(adm = 2,target = AB, p = F) ; SC

EQUATION:

odeType=stiff

t\_0=0

C\_0 = 0

RA\_0 = ksynA/kdegA

RB\_0 = ksynB/kdegB

AP\_0 = 0

AB\_0 = 0

In\_0 = 0

gam = a\*KD1\*KD2

det = ( C\*KD2\*RA^2 + C^2\*KD2\*RA + C\*KD1\*RB^2 + C^2\*KD1\*RB + C^2\*RA\*RB + a\*KD1^2\*KD2^2 + C\*KD1\*KD2\*RA + C\*KD1\*KD2\*RB

+ KD1\*KD2\*RA\*RB + a\*C\*KD1\*KD2^2 + a\*C\*KD1^2\*KD2 + a\*C^2\*KD1\*KD2 + a\*KD1\*KD2^2\*RA + a\*KD1^2\*KD2\*RB + a\*C\*KD1\*KD2\*RA + a\*C\*KD1\*KD2\*RB )/ (a\*KD1^2\*KD2^2);

m11 = (C^2\*KD2\*RA + C^2\*KD1\*RB + a\*KD1^2\*KD2^2 + C\*KD1\*KD2\*RA + C\*KD1\*KD2\*RB + a\*C\*KD1\*KD2^2 + a\*C\*KD1^2\*KD2 + a\*C^2\*KD1\*KD2 ) / (a\*KD1^2\*KD2^2);

m12 = - (C^2\*RA + C\*KD1\*RB + a\*C^2\*KD1 + a\*C\*KD1\*KD2)/(a\*KD1^2\*KD2);

m13 = - (C^2\*RB + C\*KD2\*RA + a\*C^2\*KD2 + a\*C\*KD1\*KD2)/(a\*KD1\*KD2^2);

m21 = - (C\*RA^2 + KD1\*RA\*RB + a\*C\*KD1\*RA + a\*KD1\*KD2\*RA)/(a\*KD1^2\*KD2);

m22 = (C\*RA^2 + C\*KD1\*RA + KD1\*RA\*RB + a\*C\*KD1^2 + a\*KD1^2\*KD2 + a\*KD1^2\*RB + a\*C\*KD1\*RA + a\*KD1\*KD2\*RA)/(a\*KD1^2\*KD2);

m23 = - (C\*RA-a\*C\*RA)/(a\*KD1\*KD2);

m31 = -(C\*RB^2 + KD2\*RA\*RB + a\*C\*KD2\*RB + a\*KD1\*KD2\*RB)/(a\*KD1\*KD2^2);

m32 = -(C\*RB - a\*C\*RB)/(a\*KD1\*KD2);

m33 = (C\*RB^2 + C\*KD2\*RB + KD2\*RA\*RB + a\*C\*KD2^2 + a\*KD1\*KD2^2 + a\*KD2^2\*RA + a\*C\*KD2\*RB + a\*KD1\*KD2\*RB)/(a\*KD1\*KD2^2);

g1 = In/V - kel\*C - kintA\*(RA\*C)/KD1 - kintB\*(RB\*C)/KD2 - kintAB\*(RA\*RB\*C)/gam - k12\*C + k21\*AP/V + ka\*AB/V

g2 = ksynA - kdegA\*RA - kintA\*(RA\*C)/KD1 - kintAB\*(RA\*RB\*C)/gam

g3 = ksynB - kdegB\*RB - kintB\*(RB\*C)/KD2 - kintAB\*(RA\*RB\*C)/gam

ddt\_C = (m11/det)\*g1 + (m12/det)\*g2 + (m13/det)\*g3

ddt\_RA = (m21/det)\*g1 + (m22/det)\*g2 + (m23/det)\*g3

ddt\_RB = (m31/det)\*g1 + (m32/det)\*g2 + (m33/det)\*g3

ddt\_AP = k12\*C\*V - k21\*AP

ddt\_AB = - ka\*AB

ddt\_In = 0

OUTPUT:

output = {C}

Example of the dataset with dosing – IV bolus:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| #ID | TIME | DV | AMT | ADM | EVID | MDV |
| 1 | 0 | . | 335 | 1 | 1 | 1 |
| 1 | 0.001 | 10.7 | . | 1 | 0 | 0 |

Example of the dataset with dosing – IV infusion:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| #ID | TIME | DV | AMT | ADM | EVID | MDV |
| 1 | 0 | . | 670 | 1 | 1 | 1 |
| 1 | 0 | 0 | . | 1 | 0 | 0 |
| 1 | 0.5 | 3.79E-07 | . | 1 | 0 | 0 |

Example of the dataset with dosing – SC:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| #ID | TIME | DV | AMT | ADM | EVID | MDV |
| 1 | 0 | . | 4020 | 2 | 1 | 1 |
| 1 | 0 | 0 | . | 1 | 0 | 0 |
| 1 | 0.5 | 0.12206 | . | 1 | 0 | 0 |