Scripts

Herein, the model and solver script used to predict the outcome of the generic model and the in silico experiments is described.

Model Script

The first script is termed the "Model script" which describes the model framework. This script included the assignment of fixed parameter values (section 1) and each metabolite as a number (for example y(1), y(2), etc) (section 2). Every uncertain parameter was assigned as a global value (section 3). The parameters and metabolites were then connected via rate laws (section 4), and the rate laws were then connected via ODEs for each metabolite (section 5).

```matlab
% Model script


function dydt = Model(t, y)
%% Units of the model

% time = min
% quantity = mmol
% volume = L


%% Section 1: Parameters (Fixed)


global LAT KfR1 c c2 AADT AAHL ABCdG TEMP R ATP ADP c3 c4 COX2DT COX2HL


KfR1= 0.1;
LAT=0;
AAHL=420; %AA Half life
AADT=420; %AA Doubling Time
ABCdG=-50000; %Gibbs free energy of ABC transporter
TEMP=310; %Kelvin
R=8.314;
ATP=0.00274;
```

```matlab
ADP=0.00134;

COX2DT =180;

COX2HL=1;


%% Section 2: Metabolite number


% BAA = y(1)

% AA = y(2)

% PGH2 = y(3)

% PGF2A = y(4)

% TXA2 = y(5)

% PGI2 = y(6)

% TXB2 = y(7)

% 6-Keto-PGF1A = y(8)

% PGJ2 = y(9)

% PGD2 = y(10)

% 15-DEOXY-PGJ2 = y(11)

% PGE2 = y(12)

% 5-HPETE = y(13)

% 5-HETE =y(14)

% LTA4 = y(15)

% 5-OXO-ETE = y(16)

% LTB4 = y(17)

% LTC4 = y(18)

% 15-HPETE = y(19)

% 15-HETE = y(20)

% 12-HPETE = y(21)

% 12-HETE = y(22)

% exPGF2A = y(23)

% exTXB2 = y(24)

% ex6-KETO-PGF1A = y(25)

% exPGE2 = y(26)

% ex15-DEOXY-PGJ2 = y(27)

% ex5-OXO-ETE = y(28)

% ex15-HETE =y(29)

% exLTB4 = y(30)

% exLTC4 = y(31)

% exHETE12 = y(32)

% exTXA2 = y(33)
```

```matlab
% exPGI2 = y(34)
% exPGH2 = y(35)
% exPGD2 = y(36)
% exPGJ2 = y(37)
% ex12-HPETE = y(38)
% ex15-HPETE = y(39)
% ex5-HPETE = y(40)
% ex5-HETE = y(41)
% exLTA4 = y(42)
% exAA = y(43)
% 15-KETO-PGE2 = y(44)
% ex15-KETO-PGE2 = y(45)
% 13,14-DIHYDRO-15-KETO-PGE2 = y(46)
% ex13,14-DIHYDRO-15-KETO-PGE2 = y(47)
% COX2 = y(48)
% Mischellanous species = y(49)


%% Section 3: Assignment of parameters as global values


%INTRACELLULAR REACTION Parameters
global KmsR1 KmpR1 PLA2Kcat KeqR1 %R1 Parameters
global KmsR2 KmpR2 COX2Kcat KeqR2 %R2 Parameters
global KmsR3 KmpR3 PGFSKcat KeqR3 %R3 Parameters
global KmsR4 KmpR4 TXASKcat KeqR4 %R4 Parameters
global KmsR5 KmpR5 PGISKcat KeqR5 %R5 Parameters
global KfR6 KrR6 %R6 Parameters
global KfR7 KrR7 %R7 Parameters
global KfR8 KrR8 %R8 Parameters
global KfR9 KrR9 %R9 Parameters
global KmsR10 KmpR10 PGESKcat KeqR10 %R10 Parameters
global KmsR11 KmpR11 LOX5Kcat KeqR11 %R11 Parameters
global KmsR12 KmpR12 PHGPxKcatR12 KeqR12 %R12 Parameters
global KmsR13 KmpR13 LOX5FLAPKcat KeqR13 %R13 Parameters
global KmsR14 KmpR14 HEDH5Kcat KeqR14 %R14 Parameters
global KmsR15 KmpR15 LTA4HKcat KeqR15 %R15 Parameters
global KmsR16 KmpR16 LTC4SKcat KeqR16 %R16 Parameters
global KmsR17 KmpR17 LOX15Kcat KeqR17 %R17 Parameters
global KmsR19 KmpR19 LOX12Kcat KeqR19 %R19 Parameters
global KmsR21 KmpR21 PGDSKcat KeqR21 %R21 Parameters
```

```matlab
global KmsR65 KmpR65 COX1Kcat KeqR65 %R65 Parameters

global KmsR66 KmpR66 PGDH15Kcat KeqR66 %R66 Parameters

global KmsR69 KmpR69 PTGR2Kcat KeqR69 %R69 Parameters

global KmsR100 KmpR100 LATKcat KeqR100 %R100 Parameters


% Other reaction parameters

global ABCKcat     ABCKmR22    ABCKmR23    ABCKmR24    ABCKmR25    ABCKmR26
ABCKmR27    ABCKmR28    ABCKmR29    ABCKmR30    ABCKmR31    ABCKmR32
ABCKmR33    ABCKmR34    ABCKmR35    ABCKmR36    ABCKmR37    ABCKmR38
ABCKmR39    ABCKmR40    ABCKmR41    ABCKmR42    ABCKmR67    ABCKmR70
PGTKcat     PGTKmR101   PGTKmR102   PGTKmR103   PGTKmR104   PGTKmR105
PGTKmR106   PGTKmR107   PGTKmR108   PGTKmR109   PGTKmR110   PGTKmR111
KfR44 KfR45 KfR46 KfR47 KfR48 KfR49 KfR50 KfR51 KfR52 KfR53 KfR54 KfR55
KfR56 KfR57 KfR58 KfR59 KfR60 KfR61 KfR62 KfR63 KfR64 KfR68 KfR71   ABCVmax
ABCKeq  PGDH15 ABC COX1    HEDH5   LOX12   LOX15   LOX5    LTA4H   LTC4S
PGDS    PGES    PGFS    PGIS    PGT PHGPX   PLA2    PTGR2   TXAS



%% Section 4: Reaction rate laws


%R1(PLA2) - Turned off
%BAA y(1) <-> AA y(2)
% r1=(PLA2Kcat*PLA2*(y(1)-(y(2)/KeqR1)))/((KmsR1*(1+(y(2)/KmpR1)))+y(1));
r1=(KfR1*y(1));


%R2(COX2)y(48)
%AA y(2)  <-> PGH2 y(3)
r2=(COX2Kcat*y(48)*(y(2)-(y(3)/KeqR2)))/((KmsR2*(1+(y(3)/KmpR2)))+y(2));


%R3(PGFS)
% PGH2 y(3) <-> PGF2A y(4)
r3= (PGFSKcat*PGFS*(y(3) -(y(4)/KeqR3)))/((KmsR3*(1+(y(4)/KmpR3)))+y(3));


%R4(TXAS)
% PGH2 y(3)<-> TXA2 y(5)
r4= (TXASKcat*TXAS*(y(3) -(y(5)/KeqR4)))/((KmsR4*(1+(y(5)/KmpR4)))+y(3));


%R5(PGIS)
% PGH2 y(3)<-> PGI2 y(6)
r5= (PGISKcat*PGIS*(y(3) -(y(6)/KeqR5)))/((KmsR5*(1+(y(6)/KmpR5)))+y(3));
```

```
% R6
% TXA2 y(5) <-> TXB2 y(7)
r6=(KfR6*y(5))-(KrR6*y(7));


% R7
% PGI2 y(6)<-> 6-Keto-PGF1A y(8)
r7= (KfR7*y(6))-(KrR7*y(8));


% R8
% PGD2 y(10) <-> PGJ2 y(9)
r8= (KfR8*y(10))-(KrR8*y(9));


% R9
% PGJ2  y(9)<-> 15-DEOXY-PGJ2 y(11)
r9= (KfR9*y(9))-(KrR9*y(11));


%R10 (PGES)
% PGH2 y(3)<-> PGE2 y(12)
r10=                             (PGESKcat*PGES*(y(3)-
(y(12)/KeqR10)))/((KmsR10*(1+(y(12)/KmpR10)))+y(3));


% R11 (LOX5)
% AA y(2)<-> 5-HPETE y(13)
r11=                     (LOX5Kcat*LOX5*(y(2)               -
(y(13)/KeqR11)))/((KmsR11*(1+(y(13)/KmpR11)))+y(2));


% R12 (PHGPX)
% 5-HPETE y(13)<-> 5-HETE y(14)
r12=                    (PHGPxKcatR12*PHGPX*(y(13)           -
(y(14)/KeqR12)))/((KmsR12*(1+(y(14)/KmpR12)))+y(13));


% R13 (LOX5FLAP)
% 5-HPETE y(13) <-> LTA4 y(15)
r13=                                  (LOX5FLAPKcat*LOX5*(y(13)-
(y(15)/KeqR13)))/((KmsR13*(1+(y(15)/KmpR13)))+y(13));


% R14 (HEDH5)
% 5-HETE y(14) <-> 5-OXO-ETE y(16)
r14=                                  (HEDH5Kcat*HEDH5*(y(14)-
(y(16)/KeqR14)))/((KmsR14*(1+(y(16)/KmpR14)))+y(14));
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% R15 (LTA4H)
% LTA4 y(15) <-> LTB4 y(17)
r15=                        (LTA4HKcat*LTA4H*(y(15)                        -
(y(17)/KeqR15)))/((KmsR15*(1+(y(17)/KmpR15)))+y(15));


% R16 (LTC4S)
% LTA4 y(15)<-> LTC4 y(18)
r16=                        (LTC4SKcat*LTC4S*(y(15)                        -
(y(18)/KeqR16)))/((KmsR16*(1+(y(18)/KmpR16)))+y(15));


% R17 (LOX15)
% AA y(2)<-> 15-HPETE y(19)
r17=                        (LOX15Kcat*LOX15*(y(2)                         -
(y(19)/KeqR17)))/((KmsR17*(1+(y(19)/KmpR17)))+y(2));


% R18 (PHGPX)
% 15-HPETE y(19)<-> 15-HETE y(20)
r18=                        (PHGPxKcatR12*PHGPX*(y(19)                     -
(y(20)/KeqR12)))/((KmsR12*(1+(y(20)/KmpR12)))+y(19));


% R19 (LOX12)
% AA y(2)<-> 12-HPETE y(21)
r19=                        (LOX12Kcat*LOX12*(y(2)                         -
(y(21)/KeqR19)))/((KmsR19*(1+(y(21)/KmpR19)))+y(2));


% R20 (PHGPX)
% 12-HPETE y(21)<-> 12-HETE y(22)
r20=                        (PHGPxKcatR12*PHGPX*(y(21)                     -
(y(22)/KeqR12)))/((KmsR12*(1+(y(22)/KmpR12)))+y(21));


% R21 (PGDS)
% PGH2 y(3)<-> PGD2 y(10)
r21=                        (PGDSKcat*PGDS*(y(3)                           -
(y(10)/KeqR21)))/((KmsR21*(1+(y(10)/KmpR21)))+y(3));


% R22 (ABC)
% PGF2A y(4) <-> exPGF2A y(23)
r22=            ABC*ABCKcat*((y(4)/ABCKmR22)*(1-((y(23)/(y(4)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(4)/ABCKmR22)+(y(
23)/ABCKmR22)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/AB
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CKmR38)+(y(3)/ABCKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR31
)+(y(20)/ABCKmR28)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(5
)/ABCKmR32)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/ABCKmR27)+(y(9)/ABCK
mR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));


% R23 (ABC)

% TXB2  y(7)<-> exTXB2 y(24)

r23=            ABC*ABCKcat*((y(7)/ABCKmR23)*(1-((y(24)/(y(7)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(7)/ABCKmR23)+(y(
24)/ABCKmR23)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/AB
CKmR38)+(y(3)/ABCKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR31
)+(y(20)/ABCKmR28)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(5
)/ABCKmR32)+(y(4)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/ABCK
mR27)+(y(9)/ABCKmR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));


% R24 (ABC)

% 6-KETO-PGF1A y(8)<-> ex6-KETO-PGF1A y(25)

r24=            ABC*ABCKcat*((y(8)/ABCKmR24)*(1-((y(25)/(y(8)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(8)/ABCKmR24)+(y(
25)/ABCKmR24)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/AB
CKmR38)+(y(3)/ABCKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR31
)+(y(20)/ABCKmR28)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(5
)/ABCKmR32)+(y(4)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/ABCK
mR27)+(y(9)/ABCKmR36)+(y(44)/ABCKmR67)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));


% R25 (ABC)

% PGE2 y(12)<-> exPGE2 y(26)

r25=            ABC*ABCKcat*((y(12)/ABCKmR25)*(1-((y(26)/(y(12)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(12)/ABCKmR25)+(y
(26)/ABCKmR25)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/A
BCKmR38)+(y(3)/ABCKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR3
1)+(y(20)/ABCKmR28)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(5)/ABCKmR32)+(y(4
)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/ABCKmR27)+(y(9)/ABCK
mR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));
%                       r25=(ABCVmax*(y(12)                      -
(y(26)/ABCKeq)))/((ABCKmR25*(1+(y(26)/ABCKmR25)))+y(12));


% R26 (ABC)

% 15-DEOXY-PGJ2 y(11)<-> ex15-DEOXY-PGJ2 y(27)

r26=            ABC*ABCKcat*((y(11)/ABCKmR26)*(1-((y(27)/(y(11)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(11)/ABCKmR26)+(y
(27)/ABCKmR26)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/A
BCKmR38)+(y(3)/ABCKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR3
1)+(y(20)/ABCKmR28)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(
5)/ABCKmR32)+(y(4)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/ABC
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KmR27)+(y(9)/ABCKmR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(
y(46)/ABCKmR70)));


% R27 (ABC)

% 5-Oxo-ETE y(16)<-> ex5-OXO-ETE y(28)

r27=          ABC*ABCKcat*((y(16)/ABCKmR27)*(1-((y(28)/(y(16)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(16)/ABCKmR27)+(y
(28)/ABCKmR27)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/A
BCKmR38)+(y(3)/ABCKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR3
1)+(y(20)/ABCKmR28)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(
5)/ABCKmR32)+(y(4)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(9)/ABCK
mR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));


% R28 (ABC)

% 15-HETE y(20)<-> ex15-HETE y(29)

r28=          ABC*ABCKcat*((y(20)/ABCKmR28)*(1-((y(29)/(y(20)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(20)/ABCKmR28)+(y
(29)/ABCKmR28)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/A
BCKmR38)+(y(3)/ABCKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR3
1)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(5)/ABCKmR32)+(y(4
)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/ABCKmR27)+(y(9)/ABCK
mR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));


% R29 (ABC)

% LTB4 y(17)<-> exLTB4 y(30)

r29=          ABC*ABCKcat*((y(17)/ABCKmR29)*(1-((y(30)/(y(17)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(17)/ABCKmR29)+(y
(30)/ABCKmR29)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/A
BCKmR38)+(y(3)/ABCKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR3
1)+(y(20)/ABCKmR28)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(
5)/ABCKmR32)+(y(4)/ABCKmR22)+(y(18)/ABCKmR30)+(y(16)/ABCKmR27)+(y(9)/ABCK
mR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));


% R30 (ABC)

% LTC4 y(18)<-> exLTC4 y(31)

r30=          ABC*ABCKcat*((y(18)/ABCKmR30)*(1-((y(31)/(y(18)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(18)/ABCKmR30)+(y
(31)/ABCKmR30)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/A
BCKmR38)+(y(3)/ABCKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR3
1)+(y(20)/ABCKmR28)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(
5)/ABCKmR32)+(y(4)/ABCKmR22)+(y(17)/ABCKmR29)+(y(16)/ABCKmR27)+(y(9)/ABCK
mR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));


% R31 (ABC)

% 12-HETE y(22)<-> ex12-HETE y(32)
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```matlab
r31=                ABC*ABCKcat*((y(22)/ABCKmR31)*(1-((y(32)/(y(22)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(22)/ABCKmR31)+(y
(32)/ABCKmR31)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/A
BCKmR38)+(y(3)/ABCKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(20)/ABCKmR2
8)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(5)/ABCKmR32)+(y(4
)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/ABCKmR27)+(y(9)/ABCK
mR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));


% R32 (ABC)

% TXA2 y(5)<-> exTXA2 y(33)

r32=                ABC*ABCKcat*((y(5)/ABCKmR32)*(1-((y(33)/(y(5)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(5)/ABCKmR32)+(y(
33)/ABCKmR32)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/AB
CKmR38)+(y(3)/ABCKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR31
)+(y(20)/ABCKmR28)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(4
)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/ABCKmR27)+(y(9)/ABCK
mR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));


% R33 (ABC)

% PGI2 y(6)<-> exPGI2 y(34)

r33=                ABC*ABCKcat*((y(6)/ABCKmR33)*(1-((y(34)/(y(6)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(6)/ABCKmR33)+(y(
34)/ABCKmR33)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/AB
CKmR38)+(y(3)/ABCKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR31
)+(y(20)/ABCKmR28)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(5)/ABCKmR32)+(y(4
)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/ABCKmR27)+(y(9)/ABCK
mR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));


% R34 (ABC)

% PGH2 y(3)<-> exPGH2 y(35)

r34=                ABC*ABCKcat*((y(3)/ABCKmR34)*(1-((y(35)/(y(3)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(3)/ABCKmR34)+(y(
35)/ABCKmR34)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/AB
CKmR38)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR31)+(y(20)/ABCKmR2
8)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(5)/ABCKmR32)+(y(4
)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/ABCKmR27)+(y(9)/ABCK
mR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));


% R35 (ABC)

% PGD2 y(10)<-> exPGD2 y(36)

r35=                ABC*ABCKcat*((y(10)/ABCKmR35)*(1-((y(36)/(y(10)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(10)/ABCKmR35)+(y
(36)/ABCKmR35)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/A
BCKmR38)+(y(3)/ABCKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR3
1)+(y(20)/ABCKmR28)+(y(12)/ABCKmR25)+(y(6)/ABCKmR33)+(y(5)/ABCKmR32)+(y(4
)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/ABCKmR27)+(y(9)/ABCK
```

```
mR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));
```

```
% R36 (ABC)
```

```
% PGJ2 y(9)<-> exPGJ2 y(37)
```

```
r36=                   ABC*ABCKcat*((y(9)/ABCKmR36)*(1-((y(37)/(y(9)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(9)/ABCKmR36)+(y(
37)/ABCKmR36)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/AB
CKmR38)+(y(3)/ABCKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR31
)+(y(20)/ABCKmR28)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(5
)/ABCKmR32)+(y(4)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/ABCK
mR27)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));
```

```
% R37 (ABC)
```

```
% 12-HPETE y(21) <-> ex12-HPETE y(38)
```

```
r37=                   ABC*ABCKcat*((y(21)/ABCKmR37)*(1-((y(38)/(y(21)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(21)/ABCKmR37)+(y
(38)/ABCKmR37)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(19)/ABCKmR38)+(y(3)/AB
CKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR31)+(y(20)/ABCKmR2
8)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(5)/ABCKmR32)+(y(4
)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/ABCKmR27)+(y(9)/ABCK
mR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));
```

```
% R38 (ABC)
```

```
% 15-HPETE y(19) <-> ex15-HPETE  y(39)
```

```
r38=                   ABC*ABCKcat*((y(19)/ABCKmR38)*(1-((y(39)/(y(19)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(19)/ABCKmR38)+(y
(39)/ABCKmR38)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(3)/AB
CKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR31)+(y(20)/ABCKmR2
8)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(5)/ABCKmR32)+(y(4
)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/ABCKmR27)+(y(9)/ABCK
mR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));
```

```
% R39 (ABC)
```

```
% 5-HPETE y(13)<-> ex5-HPETE y(40)
```

```
r39=                   ABC*ABCKcat*((y(13)/ABCKmR39)*(1-((y(40)/(y(13)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(13)/ABCKmR39)+(y
(40)/ABCKmR39)+(y(2)/ABCKmR42)+(y(21)/ABCKmR37)+(y(19)/ABCKmR38)+(y(3)/AB
CKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR31)+(y(20)/ABCKmR2
8)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(5)/ABCKmR32)+(y(4
)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/ABCKmR27)+(y(9)/ABCK
mR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));
```

```
% R40 (ABC)
```

```
% 5-HETE y(14)<-> ex5-HETE y(41)
```

```
r40=              ABC*ABCKcat*((y(14)/ABCKmR40)*(1-((y(41)/(y(14)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(14)/ABCKmR40)+(y
(41)/ABCKmR40)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/A
BCKmR38)+(y(3)/ABCKmR34)+(y(15)/ABCKmR41)+(y(22)/ABCKmR31)+(y(20)/ABCKmR2
8)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(5)/ABCKmR32)+(y(4
)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/ABCKmR27)+(y(9)/ABCK
mR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));


% R41 (ABC)

% LTA4 y(15) <-> exLTA4 y(42)

r41=              ABC*ABCKcat*((y(15)/ABCKmR41)*(1-((y(42)/(y(15)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(15)/ABCKmR41)+(y
(42)/ABCKmR41)+(y(2)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/A
BCKmR38)+(y(3)/ABCKmR34)+(y(14)/ABCKmR40)+(y(22)/ABCKmR31)+(y(20)/ABCKmR2
8)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(5)/ABCKmR32)+(y(4
)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/ABCKmR27)+(y(9)/ABCK
mR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));


% R42 (ABC)

% AA y(2)<-> exAA y(43)

r42       =       ABC*ABCKcat*((y(2)/ABCKmR42)*(1-((y(43)/(y(2)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(2)/ABCKmR42)+(y(
43)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/ABCKmR38)+(y(3)/AB
CKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR31)+(y(20)/ABCKmR2
8)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y(5)/ABCKmR32)+(y(4
)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/ABCKmR27)+(y(9)/ABCK
mR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+(
y(46)/ABCKmR70)));


% NO R43


% R44

% exPGF2A y(23)-> Mischellanous species

r44 = KfR44*y(23);


% R45

% exTXB2 y(24)-> Mischellanous species

r45= KfR45*y(24);


% R46

% exTXA2 y(33)-> Mischellanous species

r46= KfR46*y(33);
```

```matlab
% R47
% ex6-KETO-PGF1A y(25)-> Mischellanous species
r47= KfR47*y(25);


% R48
% exPGI2 y(34)-> Mischellanous species
r48= KfR48*y(34);


% R49
% exPGE2 y(26)-> Mischellanous species
r49= KfR49*y(26);


% R50
% ex15-DEOXY-PGJ2 y(27)-> Mischellanous species
r50= KfR50*y(27);


% R51
% exPGJ2 y(37)-> Mischellanous species
r51= KfR51* y(37);


% R52
% exPGD2 y(36)-> Mischellanous species
r52= KfR52*y(36);


% R53
% exPGH2 y(35)-> Mischellanous species
r53= KfR53*y(35);


% R54
% ex-5-OXO-ETE y(28)-> Mischellanous species
r54= KfR54*y(28);


% R55
% ex5-HETE y(41)-> Mischellanous species
r55= KfR55*y(41);


% R56
% exLTB4 y(30)-> Mischellanous species
```

```matlab
r56= KfR56*y(30);


% R57
% exLTC4 y(31)-> Mischellanous species
r57= KfR57*y(31);


% R58
% exLTA4 y(42)-> Mischellanous species
r58= KfR58*y(42);


% R59
% ex5-HPETE y(40)-> Mischellanous species
r59 = KfR59*y(40);


% R60
% ex15-HETE y(29)-> Mischellanous species
r60= KfR60*y(29);


% R61
% ex15-HPETE y(39)-> Mischellanous species
r61= KfR61*y(39);


% R62
% ex12-HETE y(32)-> Mischellanous species
r62= KfR62*y(32);


% R63
% ex12-HPETE y(38)-> Mischellanous species
r63= KfR63*y(38);


% R64
% exAA y(43)-> Mischellanous species
r64= KfR64*y(43);


% R65
% AA y(2)<-> PGH2 y(3) (COX1)
r65=(COX1Kcat*COX1*(y(2)-
(y(3)/KeqR65)))/((KmsR65*(1+(y(3)/KmpR65)))+y(2));
```

```
% R66 (PGDH15)

% PGE2 y(12)<-> 15-KETO-PGE2 y(44)

r66=                          (PGDH15Kcat*PGDH15*(y(12)          -
(y(44)/KeqR66)))/((KmsR66*(1+(y(44)/KmpR66)))+y(12));




% R67 (ABC)

% 15-KETO-PGE2 y(44) <-> ex15-KETO-PGE2 y(45)

r67=            ABC*ABCKcat*((y(44)/ABCKmR67)*(1-((y(45)/(y(44)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(44)/ABCKmR67)+(y
(45)/ABCKmR67)+(y(21)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/
ABCKmR38)+(y(3)/ABCKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR
31)+(y(20)/ABCKmR28)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y
(5)/ABCKmR32)+(y(4)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/AB
CKmR27)+(y(9)/ABCKmR36)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+(y(11)/ABCKmR26)+
(y(46)/ABCKmR70)));




% R68

% ex15-KETO-PGE2 y(45)-> Mischellanous species

r68= KfR68*y(45);


% R69 (PTGR2)

% 15-KETO-PGE2 y(44) <-> 13,14-DIHYDRO-15-KETO-PGE2 y(46)

r69=                                    (PTGR2Kcat*PTGR2*(y(44)-
(y(46)/KeqR69)))/((KmsR69*(1+(y(46)/KmpR69)))+y(44));


% R70 (ABC)

% 13,14-DIHYDRO-15-KETO-PGE2  y(46) <-> ex13,14-DIHYDRO-15-KETO-PGE2 y(47)

r70=            ABC*ABCKcat*((y(46)/ABCKmR70)*(1-((y(47)/(y(46)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(46)/ABCKmR70)+(y
(47)/ABCKmR70)+(y(21)/ABCKmR42)+(y(13)/ABCKmR39)+(y(21)/ABCKmR37)+(y(19)/
ABCKmR38)+(y(3)/ABCKmR34)+(y(15)/ABCKmR41)+(y(14)/ABCKmR40)+(y(22)/ABCKmR
31)+(y(20)/ABCKmR28)+(y(12)/ABCKmR25)+(y(10)/ABCKmR35)+(y(6)/ABCKmR33)+(y
(5)/ABCKmR32)+(y(4)/ABCKmR22)+(y(18)/ABCKmR30)+(y(17)/ABCKmR29)+(y(16)/AB
CKmR27)+(y(9)/ABCKmR36)+(y(44)/ABCKmR67)+(y(8)/ABCKmR24)+(y(7)/ABCKmR23)+
(y(11)/ABCKmR26)));



% R71

% ex13,14-DIHYDRO-15-KETO-PGE2 y(47)-> Mischellanous species

r71= KfR71*y(47);
```

```matlab
% INTRACELLULAR DECAY REACTIONS


% R72
% PGF2A y(4-> Mischellanous species
r72 = KfR44*y(4);


% R73
% TXB2 y(7-> Mischellanous species
r73= KfR45*y(7);


% R74
% TXA2 y(5)-> Mischellanous species
r74= KfR46*y(5);


% R75
% 6-KETO-PGF1A y(8)-> Mischellanous species
r75= KfR47*y(8);


% R76
% PGI2 y(6)-> Mischellanous species
r76= KfR48*y(6);


% R77
% PGE2 y(12)-> Mischellanous species
r77= KfR49*y(12);


% R78
% 15-DEOXY-PGJ2 y(11)-> Mischellanous species
r78= KfR50*y(11);


% R79
% PGJ2 y(9)-> Mischellanous species
r79= KfR51* y(9);


% R80
% PGD2 y(10)-> Mischellanous species
r80= KfR52*y(10);
```

```matlab
% R81
% PGH2 y(3)-> Mischellanous species
r81= KfR53*y(3);


% R82
% 5-OXO-ETE y(16)-> Mischellanous species
r82= KfR54*y(16);


% R83
% 5-HETE y(14)-> Mischellanous species
r83= KfR55*y(14);


% R84
% LTB4 y(17)-> Mischellanous species
r84= KfR56*y(17);


% R85
% LTC4 y(18)-> Mischellanous species
r85= KfR57*y(18);


% R86
% LTA4 y(15)-> Mischellanous species
r86= KfR58*y(15);


% R87
% 5-HPETE y(13)-> Mischellanous species
r87 = KfR59*y(13);


% R88
% 15-HETE y(20)-> Mischellanous species
r88= KfR60*y(20);


% R89
% 15-HPETE y(19)-> Mischellanous species
r89= KfR61*y(19);


% R90
% 12-HETE  y(22)-> Mischellanous species
```

```matlab
r90= KfR62*y(22);


% R91
% 12-HPETE y(21)-> Mischellanous species
r91= KfR63*y(21);


% R92
% AA y(2)-> Mischellanous species
r92= KfR64*y(2);


% R93
% 13,14-DIHYDRO-15-KETO-PGE2 y(46)-> Mischellanous species
r93= KfR71*y(46);


% R94
% 15-KETO-PGE2 y(44)-> Mischellanous species
r94= KfR68*y(44);


% AA ACTIVATION
% -> AA
r95= (c/AADT)-((c2*log(2)*y(2))/AAHL);


% R96
% exTXA2 y(33) <-> exTXB2 y(24)
r96=(KfR6*y(33))-(KrR6*y(24));


% R97
% exPGI2 y(34)<-> ex6-Keto-PGF1A y(25)
r97= (KfR7*y(34))-(KrR7*y(25));


% R98
% exPGD2 y(36) <-> exPGJ2 y(37)
r98= (KfR8*y(36))-(KrR8*y(37));


% R99
% exPGJ2  y(37)<-> ex15-DEOXY-PGJ2 y(27)
r99= (KfR9*y(37))-(KrR9*y(27));
```

```
%R100 - Turned off
%AA y(2) <-> BAA y(1)
r100=(LATKcat*LAT*(y(2)-
(y(1)/KeqR100)))/((KmsR100*(1+(y(1)/KmpR100)))+y(2));



% PGT Transporter



% R101 (PGT)
% PGF2A y(4) <-> exPGF2A y(23)
r101=PGT*PGTKcat*((y(4)/PGTKmR101)*(1-((y(23)/(y(4)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(4)/PGTKmR101)+(y
(23)/PGTKmR101)+(y(7)/PGTKmR106)+(y(8)/PGTKmR109)+(y(12)/PGTKmR102)+(y(11
)/PGTKmR111)+(y(5)/PGTKmR110)+(y(6)/PGTKmR103)+(y(10)/PGTKmR104)+(y(9)/PG
TKmR105)+(y(44)/PGTKmR108)+(y(46)/PGTKmR107)));



% R102 (PGT)
% PGE2 y(12)<-> exPGE2 y(26)
r102=          PGT*PGTKcat*((y(12)/PGTKmR102)*(1-((y(26)/(y(12)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(4)/PGTKmR102)+(y
(23)/PGTKmR102)+(y(4)/PGTKmR101)+(y(7)/PGTKmR106)+(y(8)/PGTKmR109)+(y(11)
/PGTKmR111)+(y(5)/PGTKmR110)+(y(6)/PGTKmR103)+(y(10)/PGTKmR104)+(y(9)/PGT
KmR105)+(y(44)/PGTKmR108)+(y(46)/PGTKmR107)));



% R103 (PGT)
% PGI2 y(6)<-> exPGI2 y(34)
r103=             PGT*PGTKcat*((y(6)/PGTKmR103)*(1-((y(34)/(y(6)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(6)/PGTKmR103)+(y
(34)/PGTKmR103)+(y(4)/PGTKmR101)+(y(7)/PGTKmR106)+(y(8)/PGTKmR109)+(y(12)
/PGTKmR102)+(y(11)/PGTKmR111)+(y(5)/PGTKmR110)+(y(10)/PGTKmR104)+(y(9)/PG
TKmR105)+(y(44)/PGTKmR108)+(y(46)/PGTKmR107)));



% R104 (PGT)
% PGD2 y(10)<-> exPGD2 y(36)
r104=          PGT*PGTKcat*((y(10)/PGTKmR104)*(1-((y(36)/(y(10)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(10)/PGTKmR104)+(
y(36)/PGTKmR104)+(y(4)/PGTKmR101)+(y(7)/PGTKmR106)+(y(8)/PGTKmR109)+(y(12
)/PGTKmR102)+(y(11)/PGTKmR111)+(y(5)/PGTKmR110)+(y(6)/PGTKmR103)+(y(9)/PG
TKmR105)+(y(44)/PGTKmR108)+(y(46)/PGTKmR107)));



% R105(PGT)
% PGJ2 y(9)<-> exPGJ2 y(37)
r105=             PGT*PGTKcat*((y(9)/PGTKmR105)*(1-((y(37)/(y(9)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(9)/PGTKmR105)+(y
(37)/PGTKmR105)+(y(4)/PGTKmR101)+(y(7)/PGTKmR106)+(y(8)/PGTKmR109)+(y(12)
```

```
/PGTKmR102)+(y(11)/PGTKmR111)+(y(5)/PGTKmR110)+(y(6)/PGTKmR103)+(y(10)/PG
TKmR104)+(y(44)/PGTKmR108)+(y(46)/PGTKmR107)));


% R106 (PGT)
% TXB2  y(7)<-> exTXB2 y(24)
r106=             PGT*PGTKcat*((y(7)/PGTKmR106)*(1-((y(24)/(y(7)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(7)/PGTKmR106)+(y
(24)/PGTKmR106)+(y(4)/PGTKmR101)+(y(8)/PGTKmR109)+(y(12)/PGTKmR102)+(y(11
)/PGTKmR111)+(y(5)/PGTKmR110)+(y(6)/PGTKmR103)+(y(10)/PGTKmR104)+(y(9)/PG
TKmR105)+(y(44)/PGTKmR108)+(y(46)/PGTKmR107)));


% R107 (PGT)
% 13,14-DIHYDRO-15-KETO-PGE2  y(46) <-> ex13,14-DIHYDRO-15-KETO-PGE2 y(47)
r107=             PGT*PGTKcat*((y(46)/PGTKmR107)*(1-((y(47)/(y(46)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(46)/PGTKmR107)+(
y(47)/PGTKmR107)+(y(4)/PGTKmR101)+(y(7)/PGTKmR106)+(y(8)/PGTKmR109)+(y(12
)/PGTKmR102)+(y(11)/PGTKmR111)+(y(5)/PGTKmR110)+(y(6)/PGTKmR103)+(y(10)/P
GTKmR104)+(y(9)/PGTKmR105)+(y(44)/PGTKmR108)));


% R108 (PGT)
% 15-KETO-PGE2 y(44) <-> ex15-KETO-PGE2 y(45)
r108=             PGT*PGTKcat*((y(44)/PGTKmR108)*(1-((y(45)/(y(44)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(44)/PGTKmR108)+(
y(45)/PGTKmR108)+(y(4)/PGTKmR101)+(y(7)/PGTKmR106)+(y(8)/PGTKmR109)+(y(12
)/PGTKmR102)+(y(11)/PGTKmR111)+(y(5)/PGTKmR110)+(y(6)/PGTKmR103)+(y(10)/P
GTKmR104)+(y(9)/PGTKmR105)+(y(46)/PGTKmR107)));


% R109 (PGT)
% 6-KETO-PGF1A y(8)<-> ex6-KETO-PGF1A y(25)
r109=             PGT*PGTKcat*((y(8)/PGTKmR109)*(1-((y(25)/(y(8)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(8)/PGTKmR109)+(y
(25)/PGTKmR109)+(y(4)/PGTKmR101)+(y(7)/PGTKmR106)+(y(12)/PGTKmR102)+(y(11
)/PGTKmR111)+(y(5)/PGTKmR110)+(y(6)/PGTKmR103)+(y(10)/PGTKmR104)+(y(9)/PG
TKmR105)+(y(44)/PGTKmR108)+(y(46)/PGTKmR107)));


% R110 (PGT)
% TXA2 y(5)<-> exTXA2 y(33)
r110=             PGT*PGTKcat*((y(5)/PGTKmR110)*(1-((y(33)/(y(5)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP))))))/(1+(y(5)/PGTKmR110)+(y
(33)/PGTKmR110)+(y(4)/PGTKmR101)+(y(7)/PGTKmR106)+(y(8)/PGTKmR109)+(y(12)
/PGTKmR102)+(y(11)/PGTKmR111)+(y(6)/PGTKmR103)+(y(10)/PGTKmR104)+(y(9)/PG
TKmR105)+(y(44)/PGTKmR108)+(y(46)/PGTKmR107)));


% R111 (PGT)
% 15-DEOXY-PGJ2 y(11)<-> ex15-DEOXY-PGJ2 y(27)
```

```matlab
r111=           PGT*PGTKcat*((y(11)/PGTKmR111)*(1-((y(27)/(y(11)*exp((((-
0.5*(ABCdG+(R*TEMP*log(ATP/ADP))))))/(R*TEMP)))))/(1+(y(11)/PGTKmR111)+(
y(27)/PGTKmR111)+(y(4)/PGTKmR101)+(y(7)/PGTKmR106)+(y(8)/PGTKmR109)+(y(12
)/PGTKmR102)+(y(5)/PGTKmR110)+(y(6)/PGTKmR103)+(y(10)/PGTKmR104)+(y(9)/PG
TKmR105)+(y(44)/PGTKmR108)+(y(46)/PGTKmR107)));


% COX2 Induction event
% -> COX2 (y(48)
r112= (c3/COX2DT)-((c4*log(2)*y(48))/COX2HL);


%% Section 5: ODE


%BAA y(1)
%dydt(1)=r100-r1;


%AA y(2)
%dydt(2)=r95+r1-r2-r11-r17-r19-r42-r65-r92-r100;


%PGH2 y(3)
%dydt(3)=r2+r65-r3-r4-r5-r10-r21-r81-r34;


%PGF2A y(4)
%dydt(4)=r3-r22-r72-r101;


%TXA2 y(5)
%dydt(5)=r4-r6-r32-r74-r110;


%PGI2 y(6)
%dydt(6)=r5-r7-r33-r76-r103;


%TXB2 y(7)
%dydt(7)=r6-r106-r73-r23;


%6-KETO-PGF1A y(8)
%dydt(8)=r7-r24-r75-r109;


%PGJ2 y(9)
%dydt(9)=r8-r9-r36-r79-r105;
```

```matlab
%PGD2 = y(10)
%dydt(10)=r21-r8-r35-r80-r104;


%15-DEOXY-PGJ2 = y(11)
%dydt(11)=r9-r26-r78-r111;


%PGE2 = y(12)
%dydt(12)=r10-r25-r66-r77-r102;


%5-HPETE
%dydt(13)=r11-r12-r13-r39-r87;


%5-HETE =y(14)
%dydt(14)=r12-r14-r40-r83;


%LTA4 = y(15)
%dydt(15)=r13-r15-r16-r41-r86;


%5-OXO-ETE  = y(16)
%dydt(16)=r14-r27-r82;


%LTB4 = y(17)
%dydt(17)=r15-r29-r84;


%LTC4  = y(18)
%dydt(18)=r16-r30-r85;


%15-HPETE  = y(19)
%dydt(19)=r17-r18-r38-r89;


%15-HETE = y(20)
%dydt(20)=r18-r28-r88;


%12-HPETE = y(21)
%dydt(21)=r19-r20-r37-r91;


%12-HETE = y(22)
```

```
%dydt(22)=r20-r31-r90;


%exPGF2A  = y(23)
%dydt(23)=r22+r101-r44;


%exTXB2 = y(24)
%dydt(24)=r23+r106-r45+r96;


%ex6-KETO-PGF1A = y(25)
%dydt(25)=r24+r109-r47+r97;


%exPGE2 = y(26)
%dydt(26)=r25+r102-r49;


%ex15-DEOXY-PGJ2 = y(27)
%dydt(27)=r26+r111-r50+r99;


%ex5-OXO-ETE = y(28)
%dydt(28)=r27-r54;


%ex15-HETE =y(29)
%dydt(29)=r28-r60;


%exLTB4 = y(30)
%dydt(30)=r29-r56;


%exLTC4 = y(31)
%dydt(31)=r30-r57;


%exHETE12 = y(32)
%dydt(32)=r31-r62;


%exTXA2 = y(33)
%dydt(33)=r32+r110-r46-r96;


%exPGI2 = y(34)
%dydt(34)=r33+r103-r48-r97;
```

```
%exPGH2 = y(35)
%dydt(35)=-r53;


%exPGD2 = y(36)
%dydt(36)=r35+r104-r52-r98;


%exPGJ2 = y(37)
%dydt(37)=r36+r105-r51+r98-r99;


%ex12-HPETE = y(38)
%dydt(38)=r37-r63;


%ex15-HPETE = y(39)
%dydt(39)=r38-r61;


%ex5-HPETE = y(40)
%dydt(40)=r39-r59;


%ex5-HETE = y(41)
%dydt(41)=r40-r55;


%exLTA4 = y(42)
%dydt(42)=r41-r58;


%exAA = y(43)
%dydt(43)=-r64;


%15-KETO-PGE2 = y(44)
%dydt(44)=r66-r67-r69-r94-r108;


%ex15-KETO-PGE2 = y(45)
%dydt(45)=r67+r108-r68;


%13,14-DIHYDRO-15-KETO-PGE2 = y(46)
%dydt(46)=r69-r70-r93-r107;
```

```
%ex13,14-DIHYDRO-15-KETO-PGE2  = y(47)
%dydt(47)=r70+r107-r71;


% COX2 = y(48)
%dydt(48)=r112-r2;


% Mischellanous species = y(49)
%dydt(49)=r44+r45+r46+r47+r48+r49+r50+r51+r52+r53+r54+r55+r56+r57+r58+r59
+r60+r61+r62+r63+r64+r68+r71+r72+r73+r74+r75+r76+r77+r78+r79+r80+r81+r82+
r83+r84+r85+r86+r87+r88+r89+r90+r91+r92


dydt=[r100-r1;r95+r1-r2-r11-r17-r19-r42-r65-r92-r100;r2+r65-r3-r4-r5-r10-
r21-r81-r34;r3-r22-r72-r101;r4-r6-r32-r74-r110;r5-r7-r33-r76-r103;r6-r23-
r73-r106;r7-r24-r75-r109;r8-r9-r36-r79-r105;r21-r8-r35-r80-r104;r9-r26-
r78-r111;r10-r25-r66-r77;r11-r12-r13-r39-r87;r12-r14-r40-r83;r13-r15-r16-
r41-r86;r14-r27-r82;r15-r29-r84;r16-r30-r85;r17-r18-r38-r89;r18-r28-
r88;r19-r20-r37-r91;r20-r31-r90;r22+r101-r44;r23+r106-r45+r96;r24+r109-
r47+r97;r25+r102-r49;r26+r111-r50+r99;r27-r54;r28-r60;r29-r56;r30-
r57;r31-r62;r32+r110-r46-r96;r33+r103-r48-r97;r34-r53;r35+r104-r52-
r98;r36+r105-r51+r98-r99;r37-r63;r38-r61;r39-r59;r40-r55;r41-r58;r42-
r64;r66-r67-r69-r94-r108;r67+r108-r68;r69-r70-r93-r107;r70+r107-r71;
r112-r2;
r44+r45+r46+r47+r48+r49+r50+r51+r52+r53+r54+r55+r56+r57+r58+r59+r60+r61+r
62+r63+r64+r68+r71+r72+r73+r74+r75+r76+r77+r78+r79+r80+r81+r82+r83+r84+r8
5+r86+r87+r88+r89+r90+r91+r92];
end
```

Script A. Error! No text of specified style in document.**.1 – The model script. This script defines the structural framework of the model.**

Solver Script

The "Solver script" described the log-normal distributions of uncertain parameters and solves the ODEs. To begin the script, the number of model variants were defined (section 1). For each uncertain parameter, a parameter distribution was generated based upon the μ and σ defined in section * (section 3). For parameters which were thermodynamically connected, multivariate distributions were created (section 4). From these distributions, parameter values were randomly selected to generate unique parameter sets for every model variant (section 5). In the latter half of the "Solver script", the event parameters are assigned a value and a

time at which it changes, and the initial concentration of every metabolite is set (section 6). The ODEs are then solved using MATLABs inbuilt stiff ordinary differential equation solver, ode15 (section 5). The result of these models was then defined as failed if the numerical values cannot be calculated by the solver, as abnormal if the concentration of certain metabolites went below zero, and normal if not (section 6). The choice of metabolite is user defined and for the purposes of this model was arbitrarily set as PGE_2. The models which were classified as normal were then analysed.

```matlab
% Solver Script

tic;


%% Section 1: Define number of model variants
ParamNo = 2;


%% Section 2: Assignment of parameters as global
global  KmsR1     KmpR1    PLA2Kcat    KeqR1    KmsR2    KmpR2    COX2Kcat
KeqR2    KmsR3    KmpR3    PGFSKcat    KeqR3    KmsR4    KmpR4    TXASKcat
KeqR4    KmsR5    KmpR5    PGISKcat    KeqR5    KfR6    KrR6    KfR7    KrR7
KfR8    KrR8    KfR9    KrR9    KmsR10    KmpR10    PGESKcat    KeqR10
KmsR11    KmpR11    LOX5Kcat    KeqR11    KmsR12    KmpR12    PHGPxKcatR12
KeqR12    KmsR13    KmpR13    LOX5FLAPKcat    KeqR13    KmsR14    KmpR14
HEDH5Kcat    KeqR14    KmsR15    KmpR15    LTA4HKcat    KeqR15    KmsR16
KmpR16    LTC4SKcat    KeqR16    KmsR17    KmpR17    LOX15Kcat    KeqR17
KmsR19    KmpR19    LOX12Kcat    KeqR19    KmsR21    KmpR21    PGDSKcat
KeqR21    KmsR65    KmpR65    COX1Kcat    KeqR65    KmsR66    KmpR66
PGDH15Kcat    KeqR66    KmsR69    KmpR69    PTGR2Kcat    KeqR69
ABCKcat    KfR44    KfR45    KfR46    KfR47    KfR48    KfR49    KfR50    KfR51
KfR52    KfR53    KfR54    KfR55    KfR56    KfR57    KfR58    KfR59    KfR60
KfR61    KfR62    KfR63    KfR64    KfR68    KfR71    KmsR100    KmpR100
LATKcat    KeqR100    ABCKmR22    ABCKmR23    ABCKmR24    ABCKmR25
ABCKmR26    ABCKmR27    ABCKmR28    ABCKmR29    ABCKmR30    ABCKmR31
ABCKmR32    ABCKmR33    ABCKmR34    ABCKmR35    ABCKmR36    ABCKmR37
ABCKmR38    ABCKmR39    ABCKmR40    ABCKmR41    ABCKmR42    ABCKmR67
ABCKmR70    c c2 c3 c4    PGTKcat    PGTKmR101    PGTKmR102    PGTKmR103
PGTKmR104    PGTKmR105    PGTKmR106    PGTKmR107    PGTKmR108    PGTKmR109
PGTKmR110    PGTKmR111    KmsR18    KmpR18    PHGPxKcatR18    KeqR18    KmsR20
KmpR20    PHGPxKcatR20    KeqR20    PGDH15    ABC    COX1    HEDH5    LOX12
LOX15    LOX5    LTA4H    LTC4S    PGDS    PGES    PGFS    PGIS    PGT    PHGPX
PLA2    PTGR2    TXAS


%% Section 3: Description of the parameter distributions
```

```matlab
% KmsR1
KmsR1_mu =-2.414 ;
KmsR1_sigma= 0.73487;


% KmpR1
KmpR1_mu = -2.414;
KmpR1_sigma =0.73487;


% PLA2Kcat
PLA2Kcat_mu =8.6294;
PLA2Kcat_sigma=0.76932;


% KeqR1
KeqR1_mu=22.83;
KeqR1_sigma =0.89;


% KmsR2
KmsR2_mu=-4.7218;
KmsR2_sigma=0.77682;


% KmpR2
KmpR2_mu=-4.7218;
KmpR2_sigma=0.77682;


% COX2Kcat
COX2Kcat_mu=8.6976;
COX2Kcat_sigma=1.1445;


% KeqR2
KeqR2_mu=66.70;
KeqR2_sigma=0.89;


% KmsR3
KmsR3_mu=-2.8238;
KmsR3_sigma=1.1815;


% KmpR3
KmpR3_mu=-2.8238;
```

```matlab
KmpR3_sigma=1.1815;


% PGFSKcat
PGFSKcat_mu=3.4597;
PGFSKcat_sigma=0.8715;


% KeqR3
KeqR3_mu=12.01;
KeqR3_sigma=0.89;


% KmsR4
KmsR4_mu=-3.9721;
KmsR4_sigma=0.78374;


% KmpR4
KmpR4_mu=-3.9721;
KmpR4_sigma=0.78374;


% TXASKcat
TXASKcat_mu=8.0056;
TXASKcat_sigma=0.76923;


% KeqR4
KeqR4_mu=0.73;
KeqR4_sigma=0.89;


% KmsR5
KmsR5_mu=-4.22;
KmsR5_sigma= 0.42;


% KmpR5
KmpR5_mu=-4.22;
KmpR5_sigma= 0.42;


% PGISKcat
PGISKcat_mu=5.5206;
PGISKcat_sigma=0.7783;
```

```matlab
% KeqR5
KeqR5_mu=0.73;
KeqR5_sigma=0.89;


% KfR6
KfR6_mu=5.598;
KfR6_sigma=1.2535;


% KrR6
KrR6_mu=5.598;
KrR6_sigma=1.27;


% KfR7
KfR7_mu=5.598;
KfR7_sigma=1.2535;


% KrR7
KrR7_mu= 5.598;
KrR7_sigma=1.27;


% KfR8
KfR8_mu=1.573;
KfR8_sigma=0.9131;


% KrR8
KrR8_mu=1.573;
KrR8_sigma=0.93;


% KfR9
KfR9_mu=1.573;
KfR9_sigma=0.9131;


% KrR9
KrR9_mu=1.573;
KrR9_sigma=0.93;


% KmsR10
KmsR10_mu=-1.1569;
```

```matlab
KmsR10_sigma=0.69253;


% KmpR10
KmpR10_mu=-1.1569;
KmpR10_sigma=0.69253;


% PGESKcat
PGESKcat_mu=8.7371;
PGESKcat_sigma=0.87137;


% KeqR10
KeqR10_mu=12.01;
KeqR10_sigma=0.89;


% KmsR11
KmsR11_mu=-3.6362;
KmsR11_sigma=0.85032;


% KmpR11
KmpR11_mu=-3.6362;
KmpR11_sigma=0.85032;


% LOX5Kcat
LOX5Kcat_mu=7.8959;
LOX5Kcat_sigma=0.76891;


% KeqR11
KeqR11_mu=119.05;
KeqR11_sigma=0.89;


% KmsR12
KmsR12_mu=2.5397;
KmsR12_sigma=1.9193;


% KmpR12
KmpR12_mu=2.5397;
KmpR12_sigma=1.9193;
```

```matlab
% PHGPxKcatR12
PHGPxKcatR12_mu=11.348;
PHGPxKcatR12_sigma=1.1171;


% KeqR12
KeqR12_mu=46.32;
KeqR12_sigma=0.89;


% KmsR13
KmsR13_mu=-3.6362;
KmsR13_sigma=0.85032;


% KmpR13
KmpR13_mu=-3.6362;
KmpR13_sigma=0.85032;


% LOX5FLAPKcat
LOX5FLAPKcat_mu=7.8959;
LOX5FLAPKcat_sigma=0.76891;


% KeqR13
KeqR13_mu=146.13;
KeqR13_sigma=0.89;


% KmsR14
KmsR14_mu=-6.3091;
KmsR14_sigma=1.027;


% KmpR14
KmpR14_mu=-6.3091;
KmpR14_sigma=1.027;


% HEDH5Kcat
HEDH5Kcat_mu=10.92;
HEDH5Kcat_sigma=1.2544;


% KeqR14
KeqR14_mu=-1.3917;
```

```
KeqR14_sigma=0.89;


% KmsR15
KmsR15_mu=-5.51;
KmsR15_sigma=0.6994;


% KmpR15
KmpR15_mu=-5.51;
KmpR15_sigma=0.72;


% LTA4HKcat
LTA4HKcat_mu=3.8938;
LTA4HKcat_sigma=0.7364;


% KeqR15
KeqR15_mu=6.93;
KeqR15_sigma=0.89;


% KmsR16
KmsR16_mu=-2.83;
KmsR16_sigma=0.79;


% KmpR16
KmpR16_mu=-2.83;
KmpR16_sigma=0.79;


% LTC4SKcat
LTC4SKcat_mu=7.4011;
LTC4SKcat_sigma=0.3294;


% KeqR16
KeqR16_mu=-15.99;
KeqR16_sigma=0.89;


% KmsR17
KmsR17_mu=-4.42;
KmsR17_sigma=0.41;
```

```matlab
% KmpR17
KmpR17_mu=-4.42;
KmpR17_sigma=0.41;


% LOX15Kcat
LOX15Kcat_mu=4.6;
LOX15Kcat_sigma=0.65;


% KeqR17
KeqR17_mu=119.05;
KeqR17_sigma=0.89;


% KmsR19
KmsR19_mu=-4.48;
KmsR19_sigma=0.63;


% KmpR19
KmpR19_mu=-4.48;
KmpR19_sigma=0.63;


% LOX12Kcat
LOX12Kcat_mu=6.2203;
LOX12Kcat_sigma=0.1796;


% KeqR19
KeqR19_mu=119.05;
KeqR19_sigma=0.89;


% % KmsR21 previous PGDS Km
% KmsR21_mu=-5.0503;
% KmsR21_sigma=0.68523;
%
% % KmpR21   previous PGDS Km
% KmpR21_mu=-5.0503;
% KmpR21_sigma=0.68523;


% KmsR21
KmsR21_mu=-3.97;
```

```matlab
KmsR21_sigma=0.58;


% KmpR21
KmpR21_mu=-3.97;
KmpR21_sigma=0.58;


% PGDSKcat
PGDSKcat_mu=5.1;
PGDSKcat_sigma=0.2;


% KeqR21
KeqR21_mu=12.01;
KeqR21_sigma=0.89;


% KmsR65
KmsR65_mu=-4.59;
KmsR65_sigma=0.45;


% KmpR65
KmpR65_mu=-4.59;
KmpR65_sigma=0.45;


% COX1Kcat
COX1Kcat_mu=9.0856;
COX1Kcat_sigma=0.0408;


% KeqR65
KeqR65_mu=66.7;
KeqR65_sigma=0.89;


% KmsR66
KmsR66_mu=-4.4125;
KmsR66_sigma=0.68004;


% KmpR66
KmpR66_mu=-4.4125;
KmpR66_sigma=0.68004;
```

```matlab
% PGDH15Kcat
PGDH15Kcat_mu=7.1911;
PGDH15Kcat_sigma=0.70075;


% KeqR66
KeqR66_mu=1.5825;
KeqR66_sigma=0.8911;


% KmsR69
KmsR69_mu=-3.9721;
KmsR69_sigma=0.6709;


% KmpR69
KmpR69_mu=-3.9721;
KmpR69_sigma=0.6709;


% PTGR2Kcat
PTGR2Kcat_mu=3.2194;
PTGR2Kcat_sigma=0.88713;


% KeqR69
KeqR69_mu=-5.2902;
KeqR69_sigma=0.8911;


% ABCKcat
ABCKcat_mu=0.92;
ABCKcat_sigma=0.8;


% KfR44
KfR44_mu=-6.1137;
KfR44_sigma=0.89;


% KfR45
KfR45_mu=-2.5583;
KfR45_sigma=0.89;


% KfR46
KfR46_mu=1.526;
```

```
KfR46_sigma=0.89;


% KfR47
KfR47_mu=-0.6713;
KfR47_sigma=0.89;


% KfR48
KfR48_mu=0.784;
KfR48_sigma=0.89;


% KfR49
KfR49_mu=-6.1137;
KfR49_sigma=0.89;


% KfR50
KfR50_mu=-6.1137;
KfR50_sigma=0.89;


% KfR51
KfR51_mu=-6.1137;
KfR51_sigma=0.89;


% KfR52
KfR52_mu=0.0219;
KfR52_sigma=0.89;


% KfR53 - check
KfR53_mu=-1.1792;
KfR53_sigma=0.89;


% KfR54
KfR54_mu=-1.9548;
KfR54_sigma=0.89;


% KfR55
KfR55_mu=-2.6172;
KfR55_sigma=0.89;
```

```matlab
% KfR56
KfR56_mu=1.1827;
KfR56_sigma=0.89;


% KfR57
KfR57_mu=1.1827;
KfR57_sigma=0.89;


% KfR58
KfR58_mu=3.4233;
KfR58_sigma=0.89;


% KfR59
KfR59_mu=1.1205;
KfR59_sigma=0.89;


% KfR60
KfR60_mu=-2.6172;
KfR60_sigma=0.89;


% KfR61
KfR61_mu=1.1205;
KfR61_sigma=0.89;


% KfR62
KfR62_mu=-4.7274;
KfR62_sigma=0.89;


% KfR63
KfR63_mu=1.1205;
KfR63_sigma=0.89;


% KfR64
KfR64_mu=-5.0151;
KfR64_sigma=0.89;


% KfR68
KfR68_mu=-4.1678;
```

```matlab
KfR68_sigma=0.89;


% KfR71
KfR71_mu=-4.1678;
KfR71_sigma=0.89;


% KmsR100
KmsR100_mu=1.30;
KmsR100_sigma=1.30;


% KmpR100
KmpR100_mu=1.30;
KmpR100_sigma=1.30;


% LATKcat
LATKcat_mu=3.31;
LATKcat_sigma=0.94;


% KeqR100
KeqR100_mu=24.4512;
KeqR100_sigma=0.89;


% ABCKmR22
ABCKmR22_mu=-2.6011;
ABCKmR22_sigma=1.1244;


% ABCKmR23
ABCKmR23_mu=-2.6011;
ABCKmR23_sigma=1.1244;


% ABCKmR24
ABCKmR24_mu=-2.6011;
ABCKmR24_sigma=1.1244;


% ABCKmR25
ABCKmR25_mu=-2.6011;
ABCKmR25_sigma=1.1244;
```

```matlab
% ABCKmR26
ABCKmR26_mu=-2.6011;
ABCKmR26_sigma=1.1244;


% ABCKmR27
ABCKmR27_mu=-2.6011;
ABCKmR27_sigma=1.1244;


% ABCKmR28
ABCKmR28_mu=-2.6011;
ABCKmR28_sigma=1.1244;


% ABCKmR29
ABCKmR29_mu=-2.6011;
ABCKmR29_sigma=1.1244;


% ABCKmR30
ABCKmR30_mu=-2.6011;
ABCKmR30_sigma=1.1244;


% ABCKmR31
ABCKmR31_mu=-2.6011;
ABCKmR31_sigma=1.1244;


% ABCKmR32
ABCKmR32_mu=-2.6011;
ABCKmR32_sigma=1.1244;


% ABCKmR33
ABCKmR33_mu=-2.6011;
ABCKmR33_sigma=1.1244;


% ABCKmR34
ABCKmR34_mu=4.0130;
ABCKmR34_sigma=0.89;


% ABCKmR35
ABCKmR35_mu=-2.6011;
```

```
ABCKmR35_sigma=1.1244;


% ABCKmR36
ABCKmR36_mu=-2.6011;
ABCKmR36_sigma=1.1244;


% ABCKmR37
ABCKmR37_mu=-2.6011;
ABCKmR37_sigma=1.1244;


% ABCKmR38
ABCKmR38_mu=-2.6011;
ABCKmR38_sigma=1.1244;


% ABCKmR39
ABCKmR39_mu=-2.6011;
ABCKmR39_sigma=1.1244;


% ABCKmR40
ABCKmR40_mu=-2.6011;
ABCKmR40_sigma=1.1244;


% ABCKmR41
ABCKmR41_mu=-2.6011;
ABCKmR41_sigma=1.1244;


% ABCKmR42
ABCKmR42_mu=4.0130;
ABCKmR42_sigma=0.89;


% ABCKmR67
ABCKmR67_mu=-2.6011;
ABCKmR67_sigma=1.1244;


% ABCKmR70
ABCKmR70_mu=-2.6011;
ABCKmR70_sigma=1.1244;
```

```matlab
% PGTKcat
PGTKcat_mu=0.92;
PGTKcat_sigma=0.8;


% PGTKmR101
PGTKmR101_mu=-4.67;
PGTKmR101_sigma=1.45;


% PGTKmR102
PGTKmR102_mu=-4.67;
PGTKmR102_sigma=1.45;


% PGTKmR103
PGTKmR103_mu=-4.67;
PGTKmR103_sigma=1.45;


% PGTKmR104
PGTKmR104_mu=-4.67;
PGTKmR104_sigma=1.45;


% PGTKmR105
PGTKmR105_mu=-4.67;
PGTKmR105_sigma=1.45;


% PGTKmR106
PGTKmR106_mu=-4.67;
PGTKmR106_sigma=1.45;


% PGTKmR107
PGTKmR107_mu=-4.67;
PGTKmR107_sigma=1.45;


% PGTKmR108
PGTKmR108_mu=-4.67;
PGTKmR108_sigma=1.45;


% PGTKmR109
PGTKmR109_mu=-4.67;
```

```matlab
PGTKmR109_sigma=1.45;


% PGTKmR110
PGTKmR110_mu=-4.67;
PGTKmR110_sigma=1.45;


% PGTKmR111
PGTKmR111_mu=-4.67;
PGTKmR111_sigma=1.45;


% KmsR18
KmsR18_mu=2.54;
KmsR18_sigma=1.92;


% KmpR18
KmpR18_mu=2.54;
KmpR18_sigma=1.92;


% PHGPxKcatR18
PHGPxKcatR18_mu=11.2;
PHGPxKcatR18_sigma=1.05;


% KeqR18
KeqR18_mu=46.32;
KeqR18_sigma=0.89;


% KmsR20
KmsR20_mu=2.54;
KmsR20_sigma=1.92;


% KmpR20
KmpR20_mu=2.54;
KmpR20_sigma=1.92;


% PHGPxKcatR20
PHGPxKcatR20_mu=11.2;
PHGPxKcatR20_sigma=1.05;
```

```matlab
% KeqR20
KeqR20_mu=46.32;
KeqR20_sigma=0.89;


% PGDH15
PGDH15_mu=-9.2304;
PGDH15_sigma=6.77E-01;


% ABC
ABC_mu=0.498;
ABC_sigma=3.32E-01;


% COX1 Original
COX1_mu=-6.4411;
COX1_sigma=8.92E-01;


% COX1 Inhibitor
% COX1_mu=-8.7442;
% COX1_sigma=8.92E-01;


% % COX1 Inhibitor v2 1e-28
% COX1_mu= -64.4634;
% COX1_sigma=0.0949;
% %
%
% HEDH5
HEDH5_mu=-5.3937;
HEDH5_sigma=5.88E-01;


% LOX12
LOX12_mu=-11.1002;
LOX12_sigma=1.19E+00;


% LOX15
LOX15_mu=-9.8003;
LOX15_sigma=9.46E-01;


% LOX5 Original
```

```
LOX5_mu=-8.0196;
LOX5_sigma=4.21E-01;


% % LOX5  Inhibitor
% LOX5_mu=-10.3227;
% LOX5_sigma=4.21E-01;


% LTA4H
LTA4H_mu=-5.8727;
LTA4H_sigma=1.99E-01;


% LTC4S
LTC4S_mu=-8.5995;
LTC4S_sigma=3.36E-01;


% PGDS
PGDS_mu=-7.7018;
PGDS_sigma=4.30E-01;


% % PGES - Generic
% PGES_mu=-6.458;
% PGES_sigma=9.67E-01;


% PGES - HaCaT
PGES_mu=-6.9944;
PGES_sigma= 0.0949;


% % PGES  46BR.1N
% PGES_mu=-7.762559512;
% PGES_sigma=0.66975987;


% PGFS
PGFS_mu=-7.5675;
PGFS_sigma=6.02E-01;


% PGIS
PGIS_mu=-6.4411;
PGIS_sigma=8.92E-01;
```

```matlab
% PGT
PGT_mu=-8.202;
PGT_sigma=1.02E+00;


% PHGPX
PHGPX_mu=-6.2899;
PHGPX_sigma=2.96E-01;


% PLA2
PLA2_mu=-7.712;
PLA2_sigma=1.27E+00;


% PTGR2
PTGR2_mu=-6.6178;
PTGR2_sigma=1.09E+00;


% TXAS
TXAS_mu=-6.4427;
TXAS_sigma=1.16E+00;


%% Section 4: Generate distributions/multivariate distributions for each
parameter/parameter sets


% Reaction 1
[KeqR1, KmsR1, KmpR1, PLA2Kcat] = Multikcat5f(KeqR1_mu, KeqR1_sigma,
KmsR1_mu, KmsR1_sigma, KmpR1_mu, KmpR1_sigma, PLA2Kcat_mu, PLA2Kcat_sigma,
ParamNo, 4.57E-05);


% Reaction 2
[KeqR2, KmsR2, KmpR2, COX2Kcat] = Multikcat5f(KeqR2_mu, KeqR2_sigma,
KmsR2_mu, KmsR2_sigma, KmpR2_mu, KmpR2_sigma, COX2Kcat_mu, COX2Kcat_sigma,
ParamNo, 2.27E-05);


% REACTION 3
[KeqR3, KmsR3, KmpR3, PGFSKcat] = Multikcat5f(KeqR3_mu, KeqR3_sigma,
KmsR3_mu, KmsR3_sigma, KmpR3_mu, KmpR3_sigma, PGFSKcat_mu, PGFSKcat_sigma,
ParamNo, 4.02E-04);


% REACTION 4
```

```matlab
[KeqR4, KmsR4, KmpR4, TXASKcat] = Multikcat5f(KeqR4_mu, KeqR4_sigma,
KmsR4_mu, KmsR4_sigma, KmpR4_mu, KmpR4_sigma, TXASKcat_mu, TXASKcat_sigma,
ParamNo, 4.35E-04);



% REACTION 5

[KeqR5, KmsR5, KmpR5, PGISKcat] = Multikcat5f(KeqR5_mu, KeqR5_sigma,
KmsR5_mu, KmsR5_sigma, KmpR5_mu, KmpR5_sigma, PGISKcat_mu, PGISKcat_sigma,
ParamNo, 7.36E-04);



% REACTION 6

[KdR6, KfR6, KrR6] = Multivariate3f(-10.8133, 2.1222, KfR6_mu, KfR6_sigma,
KrR6_mu, KrR6_sigma, ParamNo );



% REACTION 7

[KdR7, KfR7, KrR7] = Multivariate3f(-10.8133, 2.1222, KfR7_mu, KfR7_sigma,
KrR7_mu, KrR7_sigma, ParamNo );



% REACTION 8

[KdR8, KfR8, KrR8] = Multivariate3f(-7.6136, 0.3073, KfR8_mu, KfR8_sigma,
KrR8_mu, KrR8_sigma, ParamNo );



% REACTION 9

[KdR9, KfR9, KrR9] = Multivariate3f(-7.6136, 0.3073, KfR9_mu, KfR9_sigma,
KrR9_mu, KrR9_sigma, ParamNo );



% REACTION 10

[KeqR10, KmsR10, KmpR10, PGESKcat] = Multikcat5f( KeqR10_mu, KeqR10_sigma,
KmsR10_mu,    KmsR10_sigma,    KmpR10_mu,    KmpR10_sigma,    PGESKcat_mu,
PGESKcat_sigma,  ParamNo, 4.17E-04);



% REACTION 11

[KeqR11, KmsR11, KmpR11, LOX5Kcat] = Multikcat5f(KeqR11_mu, KeqR11_sigma,
KmsR11_mu,    KmsR11_sigma,    KmpR11_mu,    KmpR11_sigma,    LOX5Kcat_mu,
LOX5Kcat_sigma,  ParamNo, 2.76E-04);



% REACTION 12,18 AND 20

[KeqR12,   KmsR12,   KmpR12,   PHGPxKcatR12]   =   Multikcat5f(KeqR12_mu,
KeqR12_sigma,   KmsR12_mu,   KmsR12_sigma,   KmpR12_mu,   KmpR12_sigma,
PHGPxKcatR12_mu, PHGPxKcatR12_sigma,  ParamNo, 1.70E-03);



[KeqR18,   KmsR18,   KmpR18,   PHGPxKcatR18]   =   Multikcat5f(KeqR18_mu,
KeqR18_sigma,   KmsR18_mu,   KmsR18_sigma,   KmpR18_mu,   KmpR18_sigma,
PHGPxKcatR18_mu, PHGPxKcatR18_sigma,  ParamNo, 1.70E-03);
```

```matlab
[KeqR20,    KmsR20,    KmpR20,    PHGPxKcatR20]    =    Multikcat5f(KeqR20_mu,
KeqR20_sigma,    KmsR20_mu,    KmsR20_sigma,    KmpR20_mu,    KmpR20_sigma,
PHGPxKcatR20_mu, PHGPxKcatR20_sigma,  ParamNo, 1.70E-03);


% REACTION 13

[KeqR13,    KmsR13,    KmpR13,    LOX5FLAPKcat]    =    Multikcat5f(KeqR13_mu,
KeqR13_sigma,    KmsR13_mu,    KmsR13_sigma,    KmpR13_mu,    KmpR13_sigma,
LOX5FLAPKcat_mu, LOX5FLAPKcat_sigma,  ParamNo, 2.76E-04);


% REACTION 14

[KeqR14, KmsR14, KmpR14, HEDH5Kcat] = Multikcat5f(KeqR14_mu, KeqR14_sigma,
KmsR14_mu,    KmsR14_sigma,    KmpR14_mu,    KmpR14_sigma,    HEDH5Kcat_mu,
HEDH5Kcat_sigma,  ParamNo, 2.71E-03);


% REACTION 15

[KeqR15, KmsR15, KmpR15, LTA4HKcat] = Multikcat5f(KeqR15_mu, KeqR15_sigma,
KmsR15_mu,    KmsR15_sigma,    KmpR15_mu,    KmpR15_sigma,    LTA4HKcat_mu,
LTA4HKcat_sigma,  ParamNo, 2.71E-03);


% R16 (LTC4S)

[KeqR16, KmsR16, KmpR16, LTC4SKcat] = Multikcat5f(KeqR16_mu, KeqR16_sigma,
KmsR16_mu,    KmsR16_sigma,    KmpR16_mu,    KmpR16_sigma,    LTC4SKcat_mu,
LTC4SKcat_sigma,  ParamNo, 1.65E-04);


% R17 (LOX15)

[KeqR17, KmsR17, KmpR17, LOX15Kcat] = Multikcat5f(KeqR17_mu, KeqR17_sigma,
KmsR17_mu,    KmsR17_sigma  ,    KmpR17_mu,    KmpR17_sigma,    LOX15Kcat_mu,
LOX15Kcat_sigma,  ParamNo, 2.26E-05);


% R19 (LOX12)

[KeqR19, KmsR19, KmpR19, LOX12Kcat] = Multikcat5f(KeqR19_mu, KeqR19_sigma,
KmsR19_mu,    KmsR19_sigma,    KmpR19_mu,    KmpR19_sigma,    LOX12Kcat_mu,
LOX12Kcat_sigma,  ParamNo, 5.20E-06);


% R21 (PGDS)

[KeqR21, KmsR21, KmpR21, PGDSKcat] = Multikcat5f(KeqR21_mu, KeqR21_sigma,
KmsR21_mu,    KmsR21_sigma,    KmpR21_mu,    KmpR21_sigma,    PGDSKcat_mu,
PGDSKcat_sigma,  ParamNo, 3.76E-04);


% R65

[KeqR65, KmsR65, KmpR65, COX1Kcat] = Multikcat5f(KeqR65_mu, KeqR65_sigma,
KmsR65_mu,    KmsR65_sigma,    KmpR65_mu,    KmpR65_sigma,    COX1Kcat_mu,
COX1Kcat_sigma,  ParamNo, 7.19E-04);
```

```matlab
% R66 (PGDH15)

[KeqR66,    KmsR66,    KmpR66,    PGDH15Kcat]    =    Multikcat5f(KeqR66_mu,
KeqR66_sigma,    KmsR66_mu,    KmsR66_sigma,    KmpR66_mu,    KmpR66_sigma,
PGDH15Kcat_mu, PGDH15Kcat_sigma,  ParamNo, 5.22E-05);


% R69 (PTGR2)

[KeqR69, KmsR69, KmpR69, PTGR2Kcat] = Multikcat5f(KeqR69_mu, KeqR69_sigma,
KmsR69_mu,    KmsR69_sigma,    KmpR69_mu,    KmpR69_sigma,    PTGR2Kcat_mu,
PTGR2Kcat_sigma,  ParamNo, 6.72E-04);


% REACTION 100

[KeqR100,    KmsR100,    KmpR100,    LATKcat]    =    Multikcat5f(KeqR100_mu,
KeqR100_sigma,  KmsR100_mu,  KmsR100_sigma,  KmpR100_mu,  KmpR100_sigma,
LATKcat_mu, LATKcat_sigma,  ParamNo, 8.81E-05);


% INTRACELLULAR EICOSANOID EXPORT(ABC)
% R22-42, 67, 70


% ABCKmR22 PGF2A
% Mode: 0.021   CIF:23.6964
pd81=makedist('Lognormal', ABCKmR22_mu, ABCKmR22_sigma);
ABCKmR22=random(pd81,ParamNo,1);


% ABCKmR23 TXB2
% Mode: 0.021   CIF:23.6964
pd106=makedist('Lognormal', ABCKmR23_mu, ABCKmR23_sigma);
ABCKmR23=random(pd106,ParamNo,1);


% ABCKmR24 K6PGF1A
% Mode: 0.021   CIF:23.6964
pd107=makedist('Lognormal', ABCKmR24_mu, ABCKmR24_sigma);
ABCKmR24=random(pd107,ParamNo,1);


% ABCKmR25 PGE2
% Mode: 0.021   CIF:23.6964
pd108=makedist('Lognormal', ABCKmR25_mu, ABCKmR25_sigma);
ABCKmR25 =random(pd108,ParamNo,1);


% ABCKmR26 D15PGJ2
```

```matlab
% Mode: 0.021   CIF:23.6964
pd109=makedist('Lognormal', ABCKmR26_mu, ABCKmR26_sigma);
ABCKmR26=random(pd109,ParamNo,1);


% ABCKmR27 OETE5
% Mode: 0.021   CIF:23.6964
pd110=makedist('Lognormal', ABCKmR27_mu, ABCKmR27_sigma);
ABCKmR27=random(pd110,ParamNo,1);


% ABCKmR28 HETE15
% Mode: 0.021   CIF:23.6964
pd111=makedist('Lognormal', ABCKmR28_mu, ABCKmR28_sigma);
ABCKmR28=random(pd111,ParamNo,1);


% ABCKmR29 LTB4
% Mode: 0.021   CIF:23.6964
pd112=makedist('Lognormal', ABCKmR29_mu, ABCKmR29_sigma);
ABCKmR29=random(pd112,ParamNo,1);


% ABCKmR30 LTC4
% Mode: 0.021   CIF:23.6964
pd113=makedist('Lognormal', ABCKmR30_mu, ABCKmR30_sigma);
ABCKmR30=random(pd113,ParamNo,1);


% ABCKmR31 HETE12
% Mode: 0.021   CIF:23.6964
pd114=makedist('Lognormal', ABCKmR31_mu, ABCKmR31_sigma);
ABCKmR31=random(pd114,ParamNo,1);


% ABCKmR32  TXA2
% Mode: 0.021   CIF:23.6964
pd115=makedist('Lognormal', ABCKmR32_mu, ABCKmR32_sigma);
ABCKmR32=random(pd115,ParamNo,1);


% ABCKmR33 PGI2
% Mode: 0.021   CIF:23.6964
pd116=makedist('Lognormal', ABCKmR33_mu, ABCKmR33_sigma);
ABCKmR33=random(pd116,ParamNo,1);
```

```matlab
% ABCKmR34 PGH2
% Mode: 25, CI: 10
pd117=makedist('Lognormal', ABCKmR34_mu, ABCKmR34_sigma);
ABCKmR34=random(pd117,ParamNo,1);


% ABCKmR35 PGD2
% Mode: 0.021   CIF:23.6964
pd118=makedist('Lognormal', ABCKmR35_mu, ABCKmR35_sigma);
ABCKmR35=random(pd118,ParamNo,1);


% ABCKmR36  PGJ2
% Mode: 0.021   CIF:23.6964
pd119=makedist('Lognormal', ABCKmR36_mu, ABCKmR36_sigma);
ABCKmR36=random(pd119,ParamNo,1);


% ABCKmR37 12HPETE
% Mode: 0.021   CIF:23.6964
pd120=makedist('Lognormal', ABCKmR37_mu, ABCKmR37_sigma);
ABCKmR37=random(pd120,ParamNo,1);


% ABCKmR38 15HPETE
% Mode: 0.021   CIF:23.6964
pd121=makedist('Lognormal', ABCKmR38_mu, ABCKmR38_sigma);
ABCKmR38=random(pd121,ParamNo,1);


% ABCKmR39 5HPETE
% Mode: 0.021   CIF:23.6964
pd122=makedist('Lognormal', ABCKmR39_mu, ABCKmR39_sigma);
ABCKmR39=random(pd122,ParamNo,1);


% ABCKmR40 HETE5
% Mode: 0.021   CIF:23.6964
pd123=makedist('Lognormal', ABCKmR40_mu, ABCKmR40_sigma);
ABCKmR40=random(pd123,ParamNo,1);


% ABCKmR41 LTA4
% Mode: 0.021   CIF:23.6964
```

```matlab
pd124=makedist('Lognormal', ABCKmR41_mu, ABCKmR41_sigma);
ABCKmR41=random(pd124,ParamNo,1);


% ABCKmR42 AA
% Mode: 25, CI: 10
pd125=makedist('Lognormal', ABCKmR42_mu, ABCKmR42_sigma);
ABCKmR42=random(pd125,ParamNo,1);


% ABCKmR67 KPGE215
% Mode: 0.021   CIF:23.6964
pd126=makedist('Lognormal', ABCKmR67_mu, ABCKmR67_sigma);
ABCKmR67=random(pd126,ParamNo,1);


% ABCKmR70 DHKPGE215
% Mode: 0.021   CIF:23.6964
pd127=makedist('Lognormal', ABCKmR70_mu, ABCKmR70_sigma);
ABCKmR70=random(pd127,ParamNo,1);


% ABCKcat
% Mode: 1.33 CI:7.30
pd82=makedist('Lognormal', ABCKcat_mu, ABCKcat_sigma); %
ABCKcat=random(pd82,ParamNo,1);



% DECAY PARAMETERS

% KfR44
% Mode: 0.001, CI: 10
pd83=makedist('Lognormal', KfR44_mu, KfR44_sigma);
KfR44=random(pd83,ParamNo,1);


% KfR45
% Mode:0.035 , CI:  10
pd84=makedist('Lognormal', KfR45_mu, KfR45_sigma);
KfR45=random(pd84,ParamNo,1);


% KfR46
% Mode: 2.079, CI: 10
```

```matlab
pd85=makedist('Lognormal', KfR46_mu, KfR46_sigma);
KfR46=random(pd85,ParamNo,1);


% KfR47
% Mode:0.231 , CI:  10
pd86=makedist('Lognormal', KfR47_mu, KfR47_sigma);
KfR47=random(pd86,ParamNo,1);


% KfR48
% Mode:0.99 , CI:  10
pd87=makedist('Lognormal', KfR48_mu, KfR48_sigma);
KfR48=random(pd87,ParamNo,1);


% KfR49
% Mode: 0.001, CI:  10
pd88=makedist('Lognormal', KfR49_mu, KfR49_sigma);
KfR49=random(pd88,ParamNo,1);


% KfR50
% Mode: 0.001, CI:  10
pd89=makedist('Lognormal', KfR50_mu, KfR50_sigma);
KfR50=random(pd89,ParamNo,1);


% KfR51
% Mode: 0.001, CI:  10
pd90=makedist('Lognormal', KfR51_mu, KfR51_sigma);
KfR51=random(pd90,ParamNo,1);


% KfR52
% Mode: 0.462, CI:  10
pd91=makedist('Lognormal', KfR52_mu, KfR52_sigma);
KfR52=random(pd91,ParamNo,1);


% KfR53
% Mode:0.139, CI:  10
pd92=makedist('Lognormal', KfR53_mu, KfR53_sigma);
KfR53=random(pd92,ParamNo,1);
```

```matlab
% KfR54
% Mode: 0.064, CI:  10
pd93=makedist('Lognormal', KfR54_mu, KfR54_sigma);
KfR54=random(pd93,ParamNo,1);


% KfR55
% Mode: 0.033, CI:  10
pd94=makedist('Lognormal', KfR55_mu, KfR55_sigma);
KfR55=random(pd94,ParamNo,1);


% KfR56
% Mode: 1.475, CI:  10
pd95=makedist('Lognormal', KfR56_mu, KfR56_sigma);
KfR56=random(pd95,ParamNo,1);


% KfR57
% Mode:1.475 , CI:  10
pd96=makedist('Lognormal', KfR57_mu, KfR57_sigma);
KfR57=random(pd96,ParamNo,1);


% KfR58
% Mode: 13.863, CI:  10
pd97=makedist('Lognormal', KfR58_mu, KfR58_sigma);
KfR58=random(pd97,ParamNo,1);


% KfR59
% Mode:1.386 , CI:  10
pd98=makedist('Lognormal', KfR59_mu, KfR59_sigma);
KfR59=random(pd98,ParamNo,1);


% KfR60
% Mode: 0.033, CI:  10
pd99=makedist('Lognormal', KfR60_mu, KfR60_sigma);
KfR60=random(pd99,ParamNo,1);


% KfR61
% Mode: 1.386, CI:  10
pd100=makedist('Lognormal', KfR61_mu, KfR61_sigma);
```

```matlab
KfR61=random(pd100,ParamNo,1);


% KfR62
% Mode: 0.004, CI:  10
pd101=makedist('Lognormal', KfR62_mu, KfR62_sigma);
KfR62=random(pd101,ParamNo,1);


% KfR63
% Mode: 1.386, CI:  10
pd102=makedist('Lognormal', KfR63_mu, KfR63_sigma);
KfR63=random(pd102,ParamNo,1);


% KfR64
% Mode:0.003 , CI:  10
pd103=makedist('Lognormal', KfR64_mu, KfR64_sigma);
KfR64=random(pd103,ParamNo,1);


% KfR68
% Mode: 0.007, CI:  10
pd104=makedist('Lognormal', KfR68_mu, KfR68_sigma);
KfR68=random(pd104,ParamNo,1);


% KfR71
% Mode: 0.007, CI:  10
pd105=makedist('Lognormal', KfR71_mu, KfR71_sigma);
KfR71=random(pd105,ParamNo,1);


% PGT Transporter Paramters

%PGTKcat
% Mode: 1.33    CIF:7.30
pd106=makedist('Lognormal', PGTKcat_mu, PGTKcat_sigma);
PGTKcat=random(pd106,ParamNo,1);


%PGTKmR101 PGF2a
%Mode: 4.79E-04 CIF:96.9951
pd107=makedist('Lognormal', PGTKmR101_mu, PGTKmR101_sigma);
PGTKmR101=random(pd107,ParamNo,1);
```

```matlab
%PGTKmR102 PGE2
%Mode: 4.15E-04 CIF:90.3325
pd108=makedist('Lognormal', PGTKmR102_mu, PGTKmR102_sigma);
PGTKmR102=random(pd108,ParamNo,1);


%PGTKmR103 PGI2
%Mode: 1.10E-03 CIF: 94.21
pd109=makedist('Lognormal', PGTKmR103_mu, PGTKmR103_sigma);
PGTKmR103=random(pd109,ParamNo,1);


%PGTKmR104 PGD2
%Mode: 1.10E-03 CIF: 94.21
pd110=makedist('Lognormal', PGTKmR104_mu, PGTKmR104_sigma);
PGTKmR104=random(pd110,ParamNo,1);


%PGTKmR105 PGJ2
%Mode: 1.10E-03 CIF: 94.21
pd111=makedist('Lognormal', PGTKmR105_mu, PGTKmR105_sigma);
PGTKmR105=random(pd111,ParamNo,1);


%PGTKmR106 TXB2
%Mode:4.95E-04  CIF:79.5062
pd112=makedist('Lognormal', PGTKmR106_mu, PGTKmR106_sigma);
PGTKmR106=random(pd112,ParamNo,1);


%PGTKmR107 DHKPGE215
%Mode:0.0045    CIF:107.2898
pd113=makedist('Lognormal', PGTKmR107_mu, PGTKmR107_sigma);
PGTKmR107=random(pd113,ParamNo,1);


%PGTKmR108 KPGE215
%Mode:0.0045    CIF:107.2898
pd114=makedist('Lognormal', PGTKmR108_mu, PGTKmR108_sigma);
PGTKmR108=random(pd114,ParamNo,1);


%PGTKmR109 K6PGF1a
%Mode:0.0013    CIF:95.5996
```

```matlab
pd115=makedist('Lognormal', PGTKmR109_mu, PGTKmR109_sigma);
PGTKmR109=random(pd115,ParamNo,1);


%PGTKmR110 TXA2
%Mode: 1.10E-03 CIF: 94.21
pd116=makedist('Lognormal', PGTKmR110_mu, PGTKmR110_sigma);
PGTKmR110=random(pd116,ParamNo,1);


%PGTKmR111 D15PGJ2
%Mode: 1.10E-03 CIF: 94.21
pd117=makedist('Lognormal', PGTKmR111_mu, PGTKmR111_sigma);
PGTKmR111=random(pd117,ParamNo,1);


% Enzyme concentrations


%15-PGDH
%Mode: 6.20E-05 CIF: 2.30E+00
pd118=makedist('Lognormal', PGDH15_mu, PGDH15_sigma);
PGDH15=random(pd118,ParamNo,1);


%ABC
%Mode: 1.45E+00 CIF:1.42E+00
pd119=makedist('Lognormal', ABC_mu, ABC_sigma);
ABC=random(pd119,ParamNo,1);


%COX1
%Mode: 7.19E-04 CIF: 3.48E+00
pd120=makedist('Lognormal', COX1_mu, COX1_sigma); %Normal concentration
% pd120=makedist('Lognormal',-8.7442,8.92E-01); %NSAID treated cell with
10% of COX
COX1=random(pd120,ParamNo,1);


%HEDH5
%Mode: 2.71E-03 CIF:2.00E+00
pd122=makedist('Lognormal', HEDH5_mu, HEDH5_sigma);
HEDH5=random(pd122,ParamNo,1);


%LOX12
```

```matlab
%Mode: 3.70E-06 CIF:7.22E+00
pd123=makedist('Lognormal', LOX12_mu, LOX12_sigma);
LOX12=random(pd123,ParamNo,1);


%LOX15
%Mode: 2.26E-05 CIF:3.93E+00
pd124=makedist('Lognormal', LOX15_mu, LOX15_sigma);
LOX15=random(pd124,ParamNo,1);


%LOX5
%Mode: 2.76E-04 CIF:1.58E+00
pd125=makedist('Lognormal', LOX5_mu, LOX5_sigma);
LOX5=random(pd125,ParamNo,1);


%LTA4H
%Mode: 2.71E-03 CIF:1.22E+00
pd126=makedist('Lognormal', LTA4H_mu, LTA4H_sigma);
LTA4H=random(pd126,ParamNo,1);


%LTC4S
%Mode:1.65E-04  CIF:1.43E+00
pd127=makedist('Lognormal', LTC4S_mu, LTC4S_sigma);
LTC4S=random(pd127,ParamNo,1);


%PGDS
%Mode:3.76E-04  CIF:1.62E+00
pd128=makedist('Lognormal', PGDS_mu, PGDS_sigma);
PGDS=random(pd128,ParamNo,1);


%PGES
%Mode:6.16E-04  CIF:4.12E+00
pd129=makedist('Lognormal', PGES_mu, PGES_sigma);
PGES=random(pd129,ParamNo,1);


%PGFS
%Mode:3.60E-04  CIF:2.04E+00
pd130=makedist('Lognormal', PGFS_mu, PGFS_sigma);
PGFS=random(pd130,ParamNo,1);
```

```matlab
%PGIS
%Mode:7.19E-04  CIF:3.48E+00
pd131=makedist('Lognormal', PGIS_mu, PGIS_sigma);
PGIS=random(pd131,ParamNo,1);


%PGT
%Mode:9.63E-05  CIF:4.70E+00
pd132=makedist('Lognormal', PGT_mu, PGT_sigma);
PGT=random(pd132,ParamNo,1);


%PHGPX
%Mode:1.70E-03  CIF:1.36E+00
pd133=makedist('Lognormal', PHGPX_mu, PHGPX_sigma);
PHGPX=random(pd133,ParamNo,1);


%PLA2
%Mode:8.83E-05  CIF:9.33E+00
pd134=makedist('Lognormal', PLA2_mu, PLA2_sigma);
PLA2=random(pd134,ParamNo,1);


%PTGR2
%Mode:4.10E-04  CIF:5.53E+00
pd135=makedist('Lognormal', PTGR2_mu, PTGR2_sigma);
PTGR2=random(pd135,ParamNo,1);


%TXAS
%Mode:4.17E-04  CIF:6.67E+00
pd136=makedist('Lognormal', TXAS_mu, TXAS_sigma);
TXAS=random(pd136,ParamNo,1);



%% Section 5: Sampling of log-normal distribution and simulation details


ParamSets=[KmsR1 KmpR1 PLA2Kcat KeqR1 KmsR2 KmpR2 COX2Kcat KeqR2 KmsR3
KmpR3 PGFSKcat KeqR3 KmsR4 KmpR4  TXASKcat KeqR4  KmsR5 KmpR5 PGISKcat
KeqR5  KfR6  KrR6 KfR7 KrR7 KfR8 KrR8 KfR9  KrR9  KmsR10 KmpR10 PGESKcat
KeqR10 KmsR11 KmpR11 LOX5Kcat KeqR11 KmsR12 KmpR12 PHGPxKcatR12 KeqR12
KmsR13 KmpR13 LOX5FLAPKcat KeqR13 KmsR14 KmpR14 HEDH5Kcat KeqR14 KmsR15
```

```
KmpR15  LTA4HKcat  KeqR15  KmsR16 KmpR16  LTC4SKcat  KeqR16  KmsR17 KmpR17
LOX15Kcat KeqR17  KmsR19  KmpR19 LOX12Kcat  KeqR19  KmsR21 KmpR21  PGDSKcat
KeqR21  KmsR65 KmpR65  COX1Kcat KeqR65  KmsR66 KmpR66  PGDH15Kcat KeqR66
KmsR69  KmpR69 PTGR2Kcat  KeqR69 ABCKcat  KfR44  KfR45  KfR46  KfR47  KfR48
KfR49  KfR50  KfR51  KfR52  KfR53  KfR54  KfR55  KfR56  KfR57  KfR58  KfR59
KfR60  KfR61  KfR62  KfR63 KfR64  KfR68 KfR71  KmsR100 KmpR100 LATKcat
KeqR100 ABCKmR22 ABCKmR23 ABCKmR24 ABCKmR25 ABCKmR26 ABCKmR27 ABCKmR28
ABCKmR29 ABCKmR30 ABCKmR31 ABCKmR32 ABCKmR33 ABCKmR34 ABCKmR35 ABCKmR36
ABCKmR37 ABCKmR38 ABCKmR39 ABCKmR40 ABCKmR41 ABCKmR42 ABCKmR67 ABCKmR70
PGTKcat  PGTKmR101 PGTKmR102 PGTKmR103 PGTKmR104 PGTKmR105 PGTKmR106
PGTKmR107  PGTKmR108  PGTKmR109  PGTKmR110  PGTKmR111  KmsR18  KmpR18
PHGPxKcatR18 KeqR18 KmsR20 KmpR20 PHGPxKcatR20 KeqR20 PGDH15  ABC COX1
HEDH5  LOX12  LOX15  LOX5  LTA4H  LTC4S  PGDS  PGES  PGFS  PGIS
PGT PHGPX  PLA2  PTGR2  TXAS];


options = odeset('RelTol',1e-15,'AbsTol',1e-14,'NormControl','on');
iter = ParamNo;


countFailed = 0;
countNormal = 0;
countAbnormal = 0;
j=0;
z=0;
m=0;


for i=1:iter
CF1=0;CF2=0;CF3=0;
CN1=0;CN2=0;CN3=0;
CA1=0;CA2=0;CA3=0;
   KmsR1 = ParamSets(i,1);
   KmpR1 = ParamSets(i,2);
   PLA2Kcat = ParamSets(i,3);
   KeqR1 = ParamSets(i,4);
   KmsR2 = ParamSets(i,5);
   KmpR2 = ParamSets(i,6);
   COX2Kcat  = ParamSets(i,7);
   KeqR2  = ParamSets(i,8);
   KmsR3  = ParamSets(i,9);
   KmpR3  = ParamSets(i,10);
   PGFSKcat  = ParamSets(i,11);
   KeqR3  = ParamSets(i,12);
   KmsR4  = ParamSets(i,13);
   KmpR4   = ParamSets(i,14);
```

```
TXASKcat  = ParamSets(i,15);
KeqR4   = ParamSets(i,16);
KmsR5  = ParamSets(i,17);
KmpR5  = ParamSets(i,18);
PGISKcat  = ParamSets(i,19);
KeqR5   = ParamSets(i,20);
KfR6  = ParamSets(i,21);
KrR6  = ParamSets(i,22);
KfR7  = ParamSets(i,23);
KrR7  = ParamSets(i,24);
KfR8  = ParamSets(i,25);
KrR8  = ParamSets(i,26);
KfR9   = ParamSets(i,27);
KrR9   = ParamSets(i,28);
KmsR10  = ParamSets(i,29);
KmpR10  = ParamSets(i,30);
PGESKcat   = ParamSets(i,31);
KeqR10   = ParamSets(i,32);
KmsR11   = ParamSets(i,33);
KmpR11   = ParamSets(i,34);
LOX5Kcat   = ParamSets(i,35);
KeqR11   = ParamSets(i,36);
KmsR12  = ParamSets(i,37);
KmpR12  = ParamSets(i,38);
PHGPxKcatR12  = ParamSets(i,39);
KeqR12   = ParamSets(i,40);
KmsR13  = ParamSets(i,41);
KmpR13  = ParamSets(i,42);
LOX5FLAPKcat   = ParamSets(i,43);
KeqR13   = ParamSets(i,44);
KmsR14  = ParamSets(i,45);
KmpR14   = ParamSets(i,46);
HEDH5Kcat   = ParamSets(i,47);
KeqR14   = ParamSets(i,48);
KmsR15  = ParamSets(i,49);
KmpR15   = ParamSets(i,50);
LTA4HKcat  = ParamSets(i,51);
KeqR15 = ParamSets(i,52);
KmsR16  = ParamSets(i,53);
```

```
KmpR16    = ParamSets(i,54);

LTC4SKcat  = ParamSets(i,55);

KeqR16    = ParamSets(i,56);

KmsR17   = ParamSets(i,57);

KmpR17   = ParamSets(i,58);

LOX15Kcat  = ParamSets(i,59);

KeqR17   = ParamSets(i,60);

KmsR19   = ParamSets(i,61);

KmpR19   = ParamSets(i,62);

LOX12Kcat   = ParamSets(i,63);

KeqR19   = ParamSets(i,64);

KmsR21   = ParamSets(i,65);

KmpR21   = ParamSets(i,66);

PGDSKcat  = ParamSets(i,67);

KeqR21   = ParamSets(i,68);

KmsR65   = ParamSets(i,69);

KmpR65   = ParamSets(i,70);

COX1Kcat  = ParamSets(i,71);

KeqR65   = ParamSets(i,72);

KmsR66   = ParamSets(i,73);

KmpR66    = ParamSets(i,74);

PGDH15Kcat  = ParamSets(i,75);

KeqR66   = ParamSets(i,76);

KmsR69   = ParamSets(i,77);

KmpR69   = ParamSets(i,78);

PTGR2Kcat   = ParamSets(i,79);

KeqR69   = ParamSets(i,80);

ABCKcat   = ParamSets(i,81);

KfR44   = ParamSets(i,82);

KfR45   = ParamSets(i,83);

KfR46   = ParamSets(i,84);

KfR47   = ParamSets(i,85);

KfR48   = ParamSets(i,86);

KfR49   = ParamSets(i,87);

KfR50   = ParamSets(i,88);

KfR51   = ParamSets(i,89);

KfR52   = ParamSets(i,90);

KfR53   = ParamSets(i,91);

KfR54   = ParamSets(i,92);
```

```
KfR55    = ParamSets(i,93);
KfR56    = ParamSets(i,94);
KfR57    = ParamSets(i,95);
KfR58    = ParamSets(i,96);
KfR59    = ParamSets(i,97);
KfR60    = ParamSets(i,98);
KfR61    = ParamSets(i,99);
KfR62    = ParamSets(i,100);
KfR63    = ParamSets(i,101);
KfR64    = ParamSets(i,102);
KfR68    = ParamSets(i,103);
KfR71 = ParamSets(i,104);
KmsR100 = ParamSets(i,105);
KmpR100 = ParamSets(i,106);
LATKcat = ParamSets(i,107);
KeqR100 = ParamSets(i,108);
ABCKmR22 = ParamSets(i,109);
ABCKmR23 = ParamSets(i,110);
ABCKmR24 = ParamSets(i,111);
ABCKmR25 = ParamSets(i,112);
ABCKmR26 = ParamSets(i,113);
ABCKmR27 = ParamSets(i,114);
ABCKmR28 = ParamSets(i,115);
ABCKmR29 = ParamSets(i,116);
ABCKmR30 = ParamSets(i,117);
ABCKmR31 = ParamSets(i,118);
ABCKmR32 = ParamSets(i,119);
ABCKmR33 = ParamSets(i,120);
ABCKmR34 = ParamSets(i,121);
ABCKmR35 = ParamSets(i,122);
ABCKmR36 = ParamSets(i,123);
ABCKmR37 = ParamSets(i,124);
ABCKmR38 = ParamSets(i,125);
ABCKmR39 = ParamSets(i,126);
ABCKmR40 = ParamSets(i,127);
ABCKmR41 = ParamSets(i,128);
ABCKmR42 = ParamSets(i,129);
ABCKmR67 = ParamSets(i,130);
ABCKmR70 = ParamSets(i,131);
```

```
PGTKcat = ParamSets(i,132);

PGTKmR101 = ParamSets(i,133);

PGTKmR102 = ParamSets(i,134);

PGTKmR103 = ParamSets(i,135);

PGTKmR104 = ParamSets(i,136);

PGTKmR105 = ParamSets(i,137);

PGTKmR106 = ParamSets(i,138);

PGTKmR107 = ParamSets(i,139);

PGTKmR108 = ParamSets(i,140);

PGTKmR109 = ParamSets(i,141);

PGTKmR110 = ParamSets(i,142);

PGTKmR111 = ParamSets(i,143);

KmsR18 = ParamSets(i,144);

KmpR18 = ParamSets(i,145);

PHGPxKcatR18 = ParamSets(i,146);

KeqR18 = ParamSets(i,147);

KmsR20 = ParamSets(i,148);

KmpR20 = ParamSets(i,149);

PHGPxKcatR20 = ParamSets(i,150);

KeqR20 = ParamSets(i,151);

PGDH15 = ParamSets(i,152);

ABC = ParamSets(i,153);

COX1 = ParamSets(i,154);

HEDH5 = ParamSets(i,155);

LOX12 = ParamSets(i,156);

LOX15 = ParamSets(i,157);

LOX5 = ParamSets(i,158);

LTA4H = ParamSets(i,159);

LTC4S = ParamSets(i,160);

PGDS = ParamSets(i,161);

PGES = ParamSets(i,162);

PGFS = ParamSets(i,163);

PGIS = ParamSets(i,164);

PGT = ParamSets(i,165);

PHGPX = ParamSets(i,166);

PLA2 = ParamSets(i,167);

PTGR2 = ParamSets(i,168);

TXAS = ParamSets(i,169);
```

```matlab
%% Section 6: Initial metabolite concentrations, event triggers and
classification of simulations as normal/abnormal/failed


time=60; %Activation time

tspan=0:0.5:time; %Length of simulation and step size

y0=ones(49,1)*1E-28; %Initial metabolite concentration


c=0; % Maximum concentration of AA(mM)

c2=0; %Decay switch for AA

c3= 0; % Maximum concentration of COX-2 (mM): 2.27E-2 mM

c4=0; % Decay switch for COX-2


[t,y] = ode15s(@Model,tspan,y0);


   if (max(t)<time)
       display(i);
       countFailed = countFailed + 1;
       CF1 = CF1 +1;


   else if (min(y(:,26))<= 0) %Classifies the simulation as abnormal if
the concentration of PGE2 goes equal or below zero.
           countAbnormal = countAbnormal + 1;
           CA1 = CA1 +1;
       else
           countNormal = countNormal + 1;
           CN1 = CN1 +1;
       end
    end
test{1,1} = [i];
test{1,2} = t;
test{1,3} = y;



Endvalues=y(length(t),:);
y2=Endvalues;
y2=y2';
time2=240; %Second activation time
tspan2=time:0.5:time2;
```

```matlab
c=5.77E-04; % Maximum concentration of AA(mM)
% In silico experiment values for c:   H + A23187: 5.77E-04, H + ATP:
2.40E-04, H + UVR: 5.11E-04, H + Indomethacin + A23187: 4.65E-04, F +
UVR:1.22E-04, F + A23187:1.54E-04, F+ATP:9.36E-06, F + Indo:6.00E-05


c2=0; %Decay switch for AA
c3= 0; % Maximum concentration of COX-2 (mM): 2.27E-2 mM
c4=0; % Decay switch for COX-2


[t,y] = ode15s(@Model,tspan2,y2,options);


if (max(t)<time2)
        display(i);
        countFailed = countFailed + 1;
        CF2 = CF2 +1;
    else if (min(y(:,26))<= 0)
            countAbnormal = countAbnormal + 1;
            CA2 = CA2 +1;
        else
            countNormal = countNormal + 1;
            CN2 = CN2 +1;
        end
end
 test{2,1} = [i];
 test{2,2} = t;
 test{2,3} = y;


Endvalues2=y(length(t),:);
y3=[Endvalues2];
y3=y3';
time3=420; % Final time point of the simulation
tspan3=time2:0.5:time3;


c=5.77E-04; % Maximum concentration of AA(mM)
% In silico experiment values for c:   H + A23187: 5.77E-04, H + ATP:
2.40E-04, H + UVR: 5.11E-04, H + Indomethacin + A23187: 4.65E-04, F +
UVR:1.22E-04, F + A23187:1.54E-04, F+ATP:9.36E-06, F + Indo:6.00E-05
```

```matlab
c2=0; %Decay switch for AA
c3= 0; % Maximum concentration of COX-2 (mM): 2.27E-2 mM
c4=0; % Decay switch for COX-2


    [t,y] = ode15s(@Model,tspan3,y3,options);


    if (max(t)<time3)
        display(i);
        countFailed = countFailed + 1;
        CF3 = CF3 +1;
    else if (min(y(:,26))<= 0)
            countAbnormal = countAbnormal + 1;
        else
            countNormal = countNormal + 1;
            CN3 = CN3 +1;
        end
end
test{3,1} = [i];
test{3,2} = t;
test{3,3} = y;


if CN1 == 1 && CN2 == 1 && CN3 ==1 %1
    normal{i,1}=test{1,1};
    normal{i,2}=[test{1,2}; test{2,2}; test{3,2}];
    normal{i,3}=[test{1,3}; test{2,3}; test{3,3}];


elseif CN1 == 1 && CN2 == 1 && CA3 ==1 || CN1 == 1 && CA2 == 1 && CA3 ==1
|| CN1 == 1 && CA2 == 1 && CN3 ==1  || CA1 == 1 && CA2 == 1 && CA3 ==1 ||
CA1 == 1 && CA2 == 1 && CN3 ==1 || CA1 == 1 && CN2 == 1 && CN3 ==1 || CA1
== 1 && CN2 == 1 && CA3 ==1
    abnormal{i,1}=test{1,1};
    abnormal{i,2}=[test{1,2}; test{2,2}; test{3,2}];
    abnormal{i,3}=[test{1,3}; test{2,3}; test{3,3}];


elseif CN1 == 1 && CN2 == 1 && CF3 ==1 || CN1 == 1 && CA2 == 1 && CF3 ==1
||CN1 == 1 && CF2 == 1 && CA3 ==1 || CN1 == 1 && CF2 == 1 && CF3 ==1 ||CN1
== 1 && CF2 == 1 && CN3 ==1 || CA1 == 1 && CA2 == 1 && CF3 ==1 ||CA1 == 1
&& CN2 == 1 && CF3 ==1 || CA1 == 1 && CF2 == 1 && CN3 ==1 ||CA1 == 1 &&
CF2 == 1 && CF3 ==1 || CA1 == 1 && CF2 == 1 && CA3 ==1 ||CF1 == 1 && CF2
== 1 && CF3 ==1 ||CF1 == 1 && CF2 == 1 && CN3 ==1 ||CF1 == 1 && CF2 == 1
&& CA3 ==1 ||CF1 == 1 && CN2 == 1 && CN3 ==1 ||CF1 == 1 && CN2 == 1 && CA3
```

```
==1 ||CF1 == 1 && CN2 == 1 && CF3 ==1 ||CF1 == 1 && CA2 == 1 && CN3 ==1
||CF1 == 1 && CA2 == 1 && CA3 ==1 ||CF1 == 1 && CA2 == 1 && CF3 ==1

    failed{i,1}=test{1,1};

    failed{i,2}=[test{1,2}; test{2,2}; test{3,2}];

    failed{i,3}=[test{1,3}; test{2,3}; test{3,3}];


end


FinalcountFailed = countFailed/3;

FinalcountNormal = countNormal/3;

FinalcountAbnormal = countAbnormal/3;




end


toc;
```

Script A. Error! No text of specified style in document.**.2 – The solver script. This script was used to define and sample parameter distributions and solve ODEs.**