

## Original model of rat liver beta oxidation

```
function [output] = liver_Karen_fulldata(varargin)
time = varargin{1};
statevector = varargin{2};

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% STATES
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
C16AcylCarCYT = statevector(1);
C16AcylCarMAT = statevector(2);
C16AcylCoAMAT = statevector(3);
C16EnoylCoAMAT = statevector(4);
C16HydroxyacylCoAMAT = statevector(5);
C16KetoacylCoAMAT = statevector(6);
C14AcylCarCYT = statevector(7);
C14AcylCarMAT = statevector(8);
C14AcylCoAMAT = statevector(9);
C14EnoylCoAMAT = statevector(10);
C14HydroxyacylCoAMAT = statevector(11);
C14KetoacylCoAMAT = statevector(12);
C12AcylCarCYT = statevector(13);
C12AcylCarMAT = statevector(14);
C12AcylCoAMAT = statevector(15);
C12EnoylCoAMAT = statevector(16);
C12HydroxyacylCoAMAT = statevector(17);
C12KetoacylCoAMAT = statevector(18);
C10AcylCarCYT = statevector(19);
C10AcylCarMAT = statevector(20);
C10AcylCoAMAT = statevector(21);
C10EnoylCoAMAT = statevector(22);
C10HydroxyacylCoAMAT = statevector(23);
C10KetoacylCoAMAT = statevector(24);
C8AcylCarCYT = statevector(25);
C8AcylCarMAT = statevector(26);
C8AcylCoAMAT = statevector(27);
C8EnoylCoAMAT = statevector(28);
C8HydroxyacylCoAMAT = statevector(29);
C8KetoacylCoAMAT = statevector(30);
C6AcylCarCYT = statevector(31);
C6AcylCarMAT = statevector(32);
C6AcylCoAMAT = statevector(33);
C6EnoylCoAMAT = statevector(34);
C6HydroxyacylCoAMAT = statevector(35);
C6KetoacylCoAMAT = statevector(36);
C4AcylCarCYT = statevector(37);
C4AcylCarMAT = statevector(38);
C4AcylCoAMAT = statevector(39);
C4EnoylCoAMAT = statevector(40);
C4HydroxyacylCoAMAT = statevector(41);
C4AcetoacylCoAMAT = statevector(42);
AcetylCoAMAT = statevector(43);
FADHMAT = statevector(44);
NADHMAT = statevector(45);
```

```

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% PARAMETERS
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
C16AcylCoACYT = 26.8*exp(-0.18*time);
sfcpt1C16 = 1;
Vcpt1 = 0.012;
Kmcpt1C16AcylCoACYT = 13.8;
Kmcpt1CarCYT = 125;
Kmcpt1C16AcylCarCYT = 136;
Kmcpt1CoACYT = 40.7;
Kicpt1MalCoACYT = 9.1;
Keqcpt1 = 0.45;
ncpt1 = 2.4799;
Vfcact = 0.42;
Vrcact = 0.42;
KmcactC16AcylCarCYT = 15;
KmcactC14AcylCarCYT = 15;
KmcactC12AcylCarCYT = 15;
KmcactC10AcylCarCYT = 15;
KmcactC8AcylCarCYT = 15;
KmcactC6AcylCarCYT = 15;
KmcactC4AcylCarCYT = 15;
KmcactCarMAT = 130;
KmcactC16AcylCarMAT = 15;
KmcactC14AcylCarMAT = 15;
KmcactC12AcylCarMAT = 15;
KmcactC10AcylCarMAT = 15;
KmcactC8AcylCarMAT = 15;
KmcactC6AcylCarMAT = 15;
KmcactC4AcylCarMAT = 15;
KmcactCarCYT = 130;
KicactC16AcylCarCYT = 56;
KicactC14AcylCarCYT = 56;
KicactC12AcylCarCYT = 56;
KicactC10AcylCarCYT = 56;
KicactC8AcylCarCYT = 56;
KicactC6AcylCarCYT = 56;
KicactC4AcylCarCYT = 56;
KicactCarCYT = 200;
Keqcact = 1;
sfcpt2C16 = 0.85;
sfcpt2C14 = 1;
sfcpt2C12 = 0.95;
sfcpt2C10 = 0.95;
sfcpt2C8 = 0.35;
sfcpt2C6 = 0.15;
sfcpt2C4 = 0.01;
Vcpt2 = 0.391;
Kmcpt2C16AcylCarMAT = 51;
Kmcpt2C14AcylCarMAT = 51;
Kmcpt2C12AcylCarMAT = 51;
Kmcpt2C10AcylCarMAT = 51;
Kmcpt2C8AcylCarMAT = 51;
Kmcpt2C6AcylCarMAT = 51;
Kmcpt2C4AcylCarMAT = 51;
Kmcpt2CoAMAT = 30;

```

Kmcpt2C16AcylCoAMAT = 38;  
Kmcpt2C14AcylCoAMAT = 38;  
Kmcpt2C12AcylCoAMAT = 38;  
Kmcpt2C10AcylCoAMAT = 38;  
Kmcpt2C8AcylCoAMAT = 38;  
Kmcpt2C6AcylCoAMAT = 1000;  
Kmcpt2C4AcylCoAMAT = 1000000;  
Kmcpt2CarMAT = 350;  
Keqcpt2 = 2.22;  
sfvlcadC16 = 1;  
sfvlcadC14 = 0.42;  
sfvlcadC12 = 0.11;  
Vvlcad = 0.008;  
KmvlcadC16AcylCoAMAT = 6.5;  
KmvlcadC14AcylCoAMAT = 4;  
KmvlcadC12AcylCoAMAT = 2.7;  
KmvlcadFAD = 0.12;  
KmvlcadC16EnoylCoAMAT = 1.08;  
KmvlcadC14EnoylCoAMAT = 1.08;  
KmvlcadC12EnoylCoAMAT = 1.08;  
KmvlcadFADH = 24.2;  
Keqvlcad = 6;  
sflcadC16 = 0.9;  
sflcadC14 = 1;  
sflcadC12 = 0.9;  
sflcadC10 = 0.75;  
sflcadC8 = 0.4;  
Vlcad = 0.01;  
KmlcadC16AcylCoAMAT = 2.5;  
KmlcadC14AcylCoAMAT = 7.4;  
KmlcadC12AcylCoAMAT = 9;  
KmlcadC10AcylCoAMAT = 24.3;  
KmlcadC8AcylCoAMAT = 123;  
KmlcadFAD = 0.12;  
KmlcadC16EnoylCoAMAT = 1.08;  
KmlcadC14EnoylCoAMAT = 1.08;  
KmlcadC12EnoylCoAMAT = 1.08;  
KmlcadC10EnoylCoAMAT = 1.08;  
KmlcadC8EnoylCoAMAT = 1.08;  
KmlcadFADH = 24.2;  
Keqlcad = 6;  
sfmcadC12 = 0.38;  
sfmcadC10 = 0.8;  
sfmcadC8 = 0.87;  
sfmcadC6 = 1;  
sfmcadC4 = 0.12;  
Vmcad = 0.081;  
KmmcadC12AcylCoAMAT = 5.7;  
KmmcadC10AcylCoAMAT = 5.4;  
KmmcadC8AcylCoAMAT = 4;  
KmmcadC6AcylCoAMAT = 9.4;  
KmmcadC4AcylCoAMAT = 135;  
KmmcadFAD = 0.12;  
KmmcadC12EnoylCoAMAT = 1.08;  
KmmcadC10EnoylCoAMAT = 1.08;  
KmmcadC8EnoylCoAMAT = 1.08;  
KmmcadC6EnoylCoAMAT = 1.08;

KmmcadC4EnoylCoAMAT = 1.08;  
KmmcadFADH = 24.2;  
Keqmcad = 6;  
sfscadC6 = 0.3;  
sfscadC4 = 1;  
Vscad = 0.081;  
KmscadC6AcylCoAMAT = 285;  
KmscadC4AcylCoAMAT = 10.7;  
KmscadFAD = 0.12;  
KmscadC6EnoylCoAMAT = 1.08;  
KmscadC4EnoylCoAMAT = 1.08;  
KmscadFADH = 24.2;  
Keqscad = 6;  
sfrcrotC16 = 0.13;  
sfrcrotC14 = 0.2;  
sfrcrotC12 = 0.25;  
sfrcrotC10 = 0.33;  
sfrcrotC8 = 0.58;  
sfrcrotC6 = 0.83;  
sfrcrotC4 = 1;  
Vrcrot = 3.6;  
KmcrotC16EnoylCoAMAT = 150;  
KmcrotC14EnoylCoAMAT = 100;  
KmcrotC12EnoylCoAMAT = 25;  
KmcrotC10EnoylCoAMAT = 25;  
KmcrotC8EnoylCoAMAT = 25;  
KmcrotC6EnoylCoAMAT = 25;  
KmcrotC4EnoylCoAMAT = 40;  
KmcrotC16HydroxyacylCoAMAT = 45;  
KmcrotC14HydroxyacylCoAMAT = 45;  
KmcrotC12HydroxyacylCoAMAT = 45;  
KmcrotC10HydroxyacylCoAMAT = 45;  
KmcrotC8HydroxyacylCoAMAT = 45;  
KmcrotC6HydroxyacylCoAMAT = 45;  
KmcrotC4HydroxyacylCoAMAT = 45;  
KicrotC4AcetoacylCoA = 1.6;  
Keqcrot = 3.13;  
sfmschadC16 = 0.6;  
sfmschadC14 = 0.5;  
sfmschadC12 = 0.43;  
sfmschadC10 = 0.64;  
sfmschadC8 = 0.89;  
sfmschadC6 = 1;  
sfmschadC4 = 0.67;  
Vmschad = 1;  
KmmschadC16HydroxyacylCoAMAT = 1.5;  
KmmschadC14HydroxyacylCoAMAT = 1.8;  
KmmschadC12HydroxyacylCoAMAT = 3.7;  
KmmschadC10HydroxyacylCoAMAT = 8.8;  
KmmschadC8HydroxyacylCoAMAT = 16.3;  
KmmschadC6HydroxyacylCoAMAT = 28.6;  
KmmschadC4HydroxyacylCoAMAT = 69.9;  
KmmschadNADMAT = 58.5;  
KmmschadC16KetoacylCoAMAT = 1.4;  
KmmschadC14KetoacylCoAMAT = 1.4;  
KmmschadC12KetoacylCoAMAT = 1.6;  
KmmschadC10KetoacylCoAMAT = 2.3;

KmmschadC8KetoacylCoAMAT = 4.1;  
KmmschadC6KetoacylCoAMAT = 5.8;  
KmmschadC4AcetoacylCoAMAT = 16.9;  
KmmschadNADHMAT = 5.4;  
Kegmschad = 2.17/10<sup>4</sup>;  
sfmckatC16 = 0.197;  
sfmckatC14 = 0.2;  
sfmckatC12 = 0.38;  
sfmckatC10 = 0.65;  
sfmckatC8 = 0.81;  
sfmckatC6 = 1;  
sfmckatC4 = 0.49;  
Vmckat = 0.377;  
KmmckatC16KetoacylCoAMAT = 1.1;  
KmmckatC14KetoacylCoAMAT = 1.2;  
KmmckatC12KetoacylCoAMAT = 1.3;  
KmmckatC10KetoacylCoAMAT = 2.1;  
KmmckatC8KetoacylCoAMAT = 3.2;  
KmmckatC6KetoacylCoAMAT = 6.7;  
KmmckatC4AcetoacylCoAMAT = 12.4;  
KmmckatCoAMAT = 26.6;  
KmmckatC14AcylCoAMAT = 13.83;  
KmmckatC16AcylCoAMAT = 13.83;  
KmmckatC12AcylCoAMAT = 13.83;  
KmmckatC10AcylCoAMAT = 13.83;  
KmmckatC8AcylCoAMAT = 13.83;  
KmmckatC6AcylCoAMAT = 13.83;  
KmmckatC4AcylCoAMAT = 13.83;  
KmmckatAcetylCoAMAT = 30;  
Kegmckat = 1051;  
sfmtpC16 = 1;  
sfmtpC14 = 0.9;  
sfmtpC12 = 0.81;  
sfmtpC10 = 0.73;  
sfmtpC8 = 0.34;  
Vmtp = 2.84;  
KmmtpC16EnoylCoAMAT = 25;  
KmmtpC14EnoylCoAMAT = 25;  
KmmtpC12EnoylCoAMAT = 25;  
KmmtpC10EnoylCoAMAT = 25;  
KmmtpC8EnoylCoAMAT = 25;  
KmmtpNADMAT = 60;  
KmmtpCoAMAT = 30;  
KmmtpC14AcylCoAMAT = 13.83;  
KmmtpC16AcylCoAMAT = 13.83;  
KmmtpC12AcylCoAMAT = 13.83;  
KmmtpC10AcylCoAMAT = 13.83;  
KmmtpC8AcylCoAMAT = 13.83;  
KmmtpC6AcylCoAMAT = 13.83;  
KmmtpNADHMAT = 50;  
KmmtpAcetylCoAMAT = 30;  
Kegmtp = 7138.4971/10<sup>4</sup>;  
Ksacesink = 6000000;  
Klacesink = 30;  
Ksfadhsink = 6000000;  
Klfadhsink = 0.46;  
Ksnadhsink = 6000000;

```
Klnadhsink = 16;
%C16AcylCoACYT = 25;
CarCYT = 400;
CoACYT = 140;
MalCoACYT = 0;
CarMAT = 950;
FADtMAT = 0.77;
NADtMAT = 250;
CoAMATt = 5000;
VCYT = 0.01;
VMAT = 1.8/10^6;
```

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% REACTION KINETICS
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

```
CoAMAT = CoAMATt - C16AcylCoAMAT - C16EnoylCoAMAT - C16HydroxyacylCoAMAT -
C16KetoacylCoAMAT - C14AcylCoAMAT - C14EnoylCoAMAT - C14HydroxyacylCoAMAT -
C14KetoacylCoAMAT - C12AcylCoAMAT - C12EnoylCoAMAT - C12HydroxyacylCoAMAT -
C12KetoacylCoAMAT - C10AcylCoAMAT - C10EnoylCoAMAT - C10HydroxyacylCoAMAT -
C10KetoacylCoAMAT - C8AcylCoAMAT - C8EnoylCoAMAT - C8HydroxyacylCoAMAT -
C8KetoacylCoAMAT - C6AcylCoAMAT - C6EnoylCoAMAT - C6HydroxyacylCoAMAT -
C6KetoacylCoAMAT - C4AcylCoAMAT - C4EnoylCoAMAT - C4HydroxyacylCoAMAT -
C4AcetoacylCoAMAT - AcetylCoAMAT;
```

```
vept1C16 = CPT1([sfcpt1C16, Vcpt1, Kmcpt1C16AcylCoACYT, Kmcpt1CarCYT,
Kmcpt1C16AcylCarCYT, Kmcpt1CoACYT, Kicpt1MalCoACYT, Keqcpt1, C16AcylCoACYT,
CarCYT, C16AcylCarCYT, CoACYT, MalCoACYT, ncpt1]);
vcactC16 = CACT([Vfcact, Vrcact, KmcactC16AcylCarCYT, KmcactCarMAT,
KmcactC16AcylCarMAT, KmcactCarCYT, KicactC16AcylCarCYT, KicactCarCYT,
Keqcact, C16AcylCarCYT, CarMAT, C16AcylCarMAT, CarCYT]);
vcactC14 = CACT([Vfcact, Vrcact, KmcactC14AcylCarCYT, KmcactCarMAT,
KmcactC14AcylCarMAT, KmcactCarCYT, KicactC14AcylCarCYT, KicactCarCYT,
Keqcact, C14AcylCarCYT, CarMAT, C14AcylCarMAT, CarCYT]);
vcactC12 = CACT([Vfcact, Vrcact, KmcactC12AcylCarCYT, KmcactCarMAT,
KmcactC12AcylCarMAT, KmcactCarCYT, KicactC12AcylCarCYT, KicactCarCYT,
Keqcact, C12AcylCarCYT, CarMAT, C12AcylCarMAT, CarCYT]);
vcactC10 = CACT([Vfcact, Vrcact, KmcactC10AcylCarCYT, KmcactCarMAT,
KmcactC10AcylCarMAT, KmcactCarCYT, KicactC10AcylCarCYT, KicactCarCYT,
Keqcact, C10AcylCarCYT, CarMAT, C10AcylCarMAT, CarCYT]);
vcactC8 = CACT([Vfcact, Vrcact, KmcactC8AcylCarCYT, KmcactCarMAT,
KmcactC8AcylCarMAT, KmcactCarCYT, KicactC8AcylCarCYT, KicactCarCYT, Keqcact,
C8AcylCarCYT, CarMAT, C8AcylCarMAT, CarCYT]);
vcactC6 = CACT([Vfcact, Vrcact, KmcactC6AcylCarCYT, KmcactCarMAT,
KmcactC6AcylCarMAT, KmcactCarCYT, KicactC6AcylCarCYT, KicactCarCYT, Keqcact,
C6AcylCarCYT, CarMAT, C6AcylCarMAT, CarCYT]);
vcactC4 = CACT([Vfcact, Vrcact, KmcactC4AcylCarCYT, KmcactCarMAT,
KmcactC4AcylCarMAT, KmcactCarCYT, KicactC4AcylCarCYT, KicactCarCYT, Keqcact,
C4AcylCarCYT, CarMAT, C4AcylCarMAT, CarCYT]);
vept2C16 = CPT2([sfcpt2C16, Vcpt2, Kmcpt2C16AcylCarMAT, Kmcpt2C14AcylCarMAT,
Kmcpt2C12AcylCarMAT, Kmcpt2C10AcylCarMAT, Kmcpt2C8AcylCarMAT,
Kmcpt2C6AcylCarMAT, Kmcpt2C4AcylCarMAT, Kmcpt2CoAMAT, Kmcpt2C16AcylCoAMAT,
Kmcpt2C14AcylCoAMAT, Kmcpt2C12AcylCoAMAT, Kmcpt2C10AcylCoAMAT,
Kmcpt2C8AcylCoAMAT, Kmcpt2C6AcylCoAMAT, Kmcpt2C4AcylCoAMAT, Kmcpt2CarMAT,
Keqcpt2, C16AcylCarMAT, C14AcylCarMAT, C12AcylCarMAT, C10AcylCarMAT,
C8AcylCarMAT, C6AcylCarMAT, C4AcylCarMAT, CoAMAT, C16AcylCoAMAT,
```



```

vvlcadC16 = VLCAD([sfvlcadC16, Vvlcad, KmvlcadC16AcylCoAMAT,
KmvlcadC14AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadFAD,
KmvlcadC16EnoylCoAMAT, KmvlcadC14EnoylCoAMAT, KmvlcadC12EnoylCoAMAT,
KmvlcadFADH, Keqvlcad, C16AcylCoAMAT, C14AcylCoAMAT, C12AcylCoAMAT, FADtMAT,
C16EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, FADHMAT]);
vvlcadC14 = VLCAD([sfvlcadC14, Vvlcad, KmvlcadC14AcylCoAMAT,
KmvlcadC16AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadFAD,
KmvlcadC14EnoylCoAMAT, KmvlcadC16EnoylCoAMAT, KmvlcadC12EnoylCoAMAT,
KmvlcadFADH, Keqvlcad, C14AcylCoAMAT, C16AcylCoAMAT, C12AcylCoAMAT, FADtMAT,
C14EnoylCoAMAT, C16EnoylCoAMAT, C12EnoylCoAMAT, FADHMAT]);
vvlcadC12 = VLCAD([sfvlcadC12, Vvlcad, KmvlcadC12AcylCoAMAT,
KmvlcadC16AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadFAD,
KmvlcadC12EnoylCoAMAT, KmvlcadC16EnoylCoAMAT, KmvlcadC14EnoylCoAMAT,
KmvlcadFADH, Keqvlcad, C12AcylCoAMAT, C16AcylCoAMAT, C14AcylCoAMAT, FADtMAT,
C12EnoylCoAMAT, C16EnoylCoAMAT, C14EnoylCoAMAT, FADHMAT]);
vlcadC16 = LCAD([sflcadC16, Vlcad, KmlcadC16AcylCoAMAT, KmlcadC14AcylCoAMAT,
KmlcadC12AcylCoAMAT, KmlcadC10AcylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadFAD,
KmlcadC16EnoylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC12EnoylCoAMAT,
KmlcadC10EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, Keqlcad,
C16AcylCoAMAT, C14AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT,
FADtMAT, C16EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT,
C8EnoylCoAMAT, FADHMAT]);
vlcadC14 = LCAD([sflcadC14, Vlcad, KmlcadC14AcylCoAMAT, KmlcadC16AcylCoAMAT,
KmlcadC12AcylCoAMAT, KmlcadC10AcylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadFAD,
KmlcadC14EnoylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC12EnoylCoAMAT,
KmlcadC10EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, Keqlcad,
C14AcylCoAMAT, C16AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT,
FADtMAT, C14EnoylCoAMAT, C16EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT,
C8EnoylCoAMAT, FADHMAT]);
vlcadC12 = LCAD([sflcadC12, Vlcad, KmlcadC12AcylCoAMAT, KmlcadC16AcylCoAMAT,
KmlcadC14AcylCoAMAT, KmlcadC10AcylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadFAD,
KmlcadC12EnoylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC14EnoylCoAMAT,
KmlcadC10EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, Keqlcad,
C12AcylCoAMAT, C16AcylCoAMAT, C14AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT,
FADtMAT, C14EnoylCoAMAT, C16EnoylCoAMAT, C14EnoylCoAMAT, C10EnoylCoAMAT,
C8EnoylCoAMAT, FADHMAT]);
vlcadC10 = LCAD([sflcadC10, Vlcad, KmlcadC10AcylCoAMAT, KmlcadC16AcylCoAMAT,
KmlcadC14AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadFAD,
KmlcadC10EnoylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC14EnoylCoAMAT,
KmlcadC12EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, Keqlcad,
C10AcylCoAMAT, C16AcylCoAMAT, C14AcylCoAMAT, C12AcylCoAMAT, C8AcylCoAMAT,
FADtMAT, C10EnoylCoAMAT, C16EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT,
C8EnoylCoAMAT, FADHMAT]);
vlcadC8 = LCAD([sflcadC8, Vlcad, KmlcadC8AcylCoAMAT, KmlcadC16AcylCoAMAT,
KmlcadC14AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC10AcylCoAMAT, KmlcadFAD,
KmlcadC8EnoylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC14EnoylCoAMAT,
KmlcadC12EnoylCoAMAT, KmlcadC10EnoylCoAMAT, KmlcadFADH, Keqlcad,
C8AcylCoAMAT, C16AcylCoAMAT, C14AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT,
FADtMAT, C8EnoylCoAMAT, C16EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT,
C10EnoylCoAMAT, FADHMAT]);
vmcadC12 = MCAD([sfmcadC12, Vmcad, KmmcadC12AcylCoAMAT, KmmcadC10AcylCoAMAT,
KmmcadC8AcylCoAMAT, KmmcadC6AcylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadFAD,
KmmcadC12EnoylCoAMAT, KmmcadC10EnoylCoAMAT, KmmcadC8EnoylCoAMAT,
KmmcadC6EnoylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadFADH, Keqmcad, C12AcylCoAMAT,
C10AcylCoAMAT, C8AcylCoAMAT, C6AcylCoAMAT, C4AcylCoAMAT, FADtMAT,
C12EnoylCoAMAT, C10EnoylCoAMAT, C8EnoylCoAMAT, C6EnoylCoAMAT, C4EnoylCoAMAT,
FADHMAT]);

```



```

vmcadC10 = MCAD([sfmcadC10, Vmcad, KmmcadC10AcylCoAMAT, KmmcadC12AcylCoAMAT,
KmmcadC8AcylCoAMAT, KmmcadC6AcylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadFAD,
KmmcadC10EnoylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC8EnoylCoAMAT,
KmmcadC6EnoylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadFADH, Keqmcad, C10AcylCoAMAT,
C12AcylCoAMAT, C8AcylCoAMAT, C6AcylCoAMAT, C4AcylCoAMAT, FADtMAT,
C10EnoylCoAMAT, C12EnoylCoAMAT, C8EnoylCoAMAT, C6EnoylCoAMAT, C4EnoylCoAMAT,
FADHMAT]);
vmcadC8 = MCAD([sfmcadC8, Vmcad, KmmcadC8AcylCoAMAT, KmmcadC12AcylCoAMAT,
KmmcadC10AcylCoAMAT, KmmcadC6AcylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadFAD,
KmmcadC8EnoylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC10EnoylCoAMAT,
KmmcadC6EnoylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadFADH, Keqmcad, C8AcylCoAMAT,
C12AcylCoAMAT, C10AcylCoAMAT, C6AcylCoAMAT, C4AcylCoAMAT, FADtMAT,
C8EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C6EnoylCoAMAT, C4EnoylCoAMAT,
FADHMAT]);
vmcadC6 = MCAD([sfmcadC6, Vmcad, KmmcadC6AcylCoAMAT, KmmcadC12AcylCoAMAT,
KmmcadC10AcylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadFAD,
KmmcadC8EnoylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC10EnoylCoAMAT,
KmmcadC6EnoylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadFADH, Keqmcad, C6AcylCoAMAT,
C12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, C4AcylCoAMAT, FADtMAT,
C6EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C8EnoylCoAMAT, C4EnoylCoAMAT,
FADHMAT]);
vmcadC4 = MCAD([sfmcadC4, Vmcad, KmmcadC4AcylCoAMAT, KmmcadC12AcylCoAMAT,
KmmcadC10AcylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC6AcylCoAMAT, KmmcadFAD,
KmmcadC4EnoylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC10EnoylCoAMAT,
KmmcadC8EnoylCoAMAT, KmmcadC6EnoylCoAMAT, KmmcadFADH, Keqmcad, C4AcylCoAMAT,
C12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, C6AcylCoAMAT, FADtMAT,
C4EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C8EnoylCoAMAT, C6EnoylCoAMAT,
FADHMAT]);
vscadC6 = SCAD([sfscadC6, Vscad, KmscadC6AcylCoAMAT, KmscadC4AcylCoAMAT,
KmscadFAD, KmscadC6EnoylCoAMAT, KmscadC4EnoylCoAMAT, KmscadFADH, Keqscad,
C6AcylCoAMAT, C4AcylCoAMAT, FADtMAT, C6EnoylCoAMAT, C4EnoylCoAMAT, FADHMAT]);
vscadC4 = SCAD([sfscadC4, Vscad, KmscadC4AcylCoAMAT, KmscadC6AcylCoAMAT,
KmscadFAD, KmscadC4EnoylCoAMAT, KmscadC6EnoylCoAMAT, KmscadFADH, Keqscad,
C4AcylCoAMAT, C6AcylCoAMAT, FADtMAT, C4EnoylCoAMAT, C6EnoylCoAMAT, FADHMAT]);
vcrotC16 = CROT([sfrcrotC16, Vcrot, KmcrotC16EnoylCoAMAT,
KmcrotC14EnoylCoAMAT, KmcrotC12EnoylCoAMAT, KmcrotC10EnoylCoAMAT,
KmcrotC8EnoylCoAMAT, KmcrotC6EnoylCoAMAT, KmcrotC4EnoylCoAMAT,
KmcrotC16HydroxyacylCoAMAT, KmcrotC14HydroxyacylCoAMAT,
KmcrotC12HydroxyacylCoAMAT, KmcrotC10HydroxyacylCoAMAT,
KmcrotC8HydroxyacylCoAMAT, KmcrotC6HydroxyacylCoAMAT,
KmcrotC4HydroxyacylCoAMAT, KicrotC4AcetoacylCoA, Keqcrot, C16EnoylCoAMAT,
C14EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C8EnoylCoAMAT, C6EnoylCoAMAT,
C4EnoylCoAMAT, C16HydroxyacylCoAMAT, C14HydroxyacylCoAMAT,
C12HydroxyacylCoAMAT, C10HydroxyacylCoAMAT, C8HydroxyacylCoAMAT,
C6HydroxyacylCoAMAT, C4HydroxyacylCoAMAT, C4AcetoacylCoAMAT]);
vcrotC14 = CROT([sfrcrotC14, Vcrot, KmcrotC14EnoylCoAMAT,
KmcrotC16EnoylCoAMAT, KmcrotC12EnoylCoAMAT, KmcrotC10EnoylCoAMAT,
KmcrotC8EnoylCoAMAT, KmcrotC6EnoylCoAMAT, KmcrotC4EnoylCoAMAT,
KmcrotC14HydroxyacylCoAMAT, KmcrotC16HydroxyacylCoAMAT,
KmcrotC12HydroxyacylCoAMAT, KmcrotC10HydroxyacylCoAMAT,
KmcrotC8HydroxyacylCoAMAT, KmcrotC6HydroxyacylCoAMAT,
KmcrotC4HydroxyacylCoAMAT, KicrotC4AcetoacylCoA, Keqcrot, C14EnoylCoAMAT,
C16EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C8EnoylCoAMAT, C6EnoylCoAMAT,
C4EnoylCoAMAT, C14HydroxyacylCoAMAT, C16HydroxyacylCoAMAT,
C12HydroxyacylCoAMAT, C10HydroxyacylCoAMAT, C8HydroxyacylCoAMAT,
C6HydroxyacylCoAMAT, C4HydroxyacylCoAMAT, C4AcetoacylCoAMAT]);

```





C8KetoacylCoAMAT, C16KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCoAMAT, C10KetoacylCoAMAT, C6KetoacylCoAMAT, C4AcetoacylCoAMAT, NADHMAT]);  
vmschadC6 = MSCHAD([sfmschadC6, Vmschad, KmmschadC6HydroxyacylCoAMAT, KmmschadC16HydroxyacylCoAMAT, KmmschadC14HydroxyacylCoAMAT, KmmschadC12HydroxyacylCoAMAT, KmmschadC10HydroxyacylCoAMAT, KmmschadC8HydroxyacylCoAMAT, KmmschadC4HydroxyacylCoAMAT, KmmschadNADMAT, KmmschadC6KetoacylCoAMAT, KmmschadC16KetoacylCoAMAT, KmmschadC14KetoacylCoAMAT, KmmschadC12KetoacylCoAMAT, KmmschadC10KetoacylCoAMAT, KmmschadC8KetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT, KmmschadNADHMAT, Keqmschad, C6HydroxyacylCoAMAT, C16HydroxyacylCoAMAT, C14HydroxyacylCoAMAT, C12HydroxyacylCoAMAT, C10HydroxyacylCoAMAT, C8HydroxyacylCoAMAT, C4HydroxyacylCoAMAT, NADtMAT, C6KetoacylCoAMAT, C16KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCoAMAT, C10KetoacylCoAMAT, C8KetoacylCoAMAT, C4AcetoacylCoAMAT, NADHMAT]);  
vmschadC4 = MSCHAD([sfmschadC4, Vmschad, KmmschadC4HydroxyacylCoAMAT, KmmschadC16HydroxyacylCoAMAT, KmmschadC14HydroxyacylCoAMAT, KmmschadC12HydroxyacylCoAMAT, KmmschadC10HydroxyacylCoAMAT, KmmschadC8HydroxyacylCoAMAT, KmmschadC6HydroxyacylCoAMAT, KmmschadNADMAT, KmmschadC4AcetoacylCoAMAT, KmmschadC16KetoacylCoAMAT, KmmschadC14KetoacylCoAMAT, KmmschadC12KetoacylCoAMAT, KmmschadC10KetoacylCoAMAT, KmmschadC8KetoacylCoAMAT, KmmschadC6KetoacylCoAMAT, KmmschadNADHMAT, Keqmschad, C4HydroxyacylCoAMAT, C16HydroxyacylCoAMAT, C14HydroxyacylCoAMAT, C12HydroxyacylCoAMAT, C10HydroxyacylCoAMAT, C8HydroxyacylCoAMAT, C6HydroxyacylCoAMAT, NADtMAT, C4AcetoacylCoAMAT, C16KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCoAMAT, C10KetoacylCoAMAT, C8KetoacylCoAMAT, C6KetoacylCoAMAT, NADHMAT]);  
vmckatC16 = MCKATA([sfmckatC16, Vmckat, KmmckatC16KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT, KmmckatC12KetoacylCoAMAT, KmmckatC10KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC6KetoacylCoAMAT, KmmckatC4AcetoacylCoAMAT, KmmckatCoAMAT, KmmckatC14AcylCoAMAT, KmmckatC16AcylCoAMAT, KmmckatC12AcylCoAMAT, KmmckatC10AcylCoAMAT, KmmckatC8AcylCoAMAT, KmmckatC6AcylCoAMAT, KmmckatC4AcylCoAMAT, KmmckatAcetylCoAMAT, Keqmckat, C16KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCoAMAT, C10KetoacylCoAMAT, C8KetoacylCoAMAT, C6KetoacylCoAMAT, C4AcetoacylCoAMAT, CoAMAT, C14AcylCoAMAT, C16AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, C6AcylCoAMAT, C4AcylCoAMAT, AcetylCoAMAT]);  
vmckatC14 = MCKATA([sfmckatC14, Vmckat, KmmckatC14KetoacylCoAMAT, KmmckatC16KetoacylCoAMAT, KmmckatC12KetoacylCoAMAT, KmmckatC10KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC6KetoacylCoAMAT, KmmckatC4AcetoacylCoAMAT, KmmckatCoAMAT, KmmckatC12AcylCoAMAT, KmmckatC16AcylCoAMAT, KmmckatC14AcylCoAMAT, KmmckatC10AcylCoAMAT, KmmckatC8AcylCoAMAT, KmmckatC6AcylCoAMAT, KmmckatC4AcylCoAMAT, KmmckatAcetylCoAMAT, Keqmckat, C14KetoacylCoAMAT, C16KetoacylCoAMAT, C12KetoacylCoAMAT, C10KetoacylCoAMAT, C8KetoacylCoAMAT, C6KetoacylCoAMAT, C4AcetoacylCoAMAT, CoAMAT, C12AcylCoAMAT, C16AcylCoAMAT, C14AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, C6AcylCoAMAT, C4AcylCoAMAT, AcetylCoAMAT]);  
vmckatC12 = MCKATA([sfmckatC12, Vmckat, KmmckatC12KetoacylCoAMAT, KmmckatC16KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT, KmmckatC10KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC6KetoacylCoAMAT, KmmckatC4AcetoacylCoAMAT, KmmckatCoAMAT, KmmckatC10AcylCoAMAT, KmmckatC16AcylCoAMAT, KmmckatC14AcylCoAMAT, KmmckatC12AcylCoAMAT, KmmckatC8AcylCoAMAT, KmmckatC6AcylCoAMAT, KmmckatC4AcylCoAMAT, KmmckatAcetylCoAMAT, Keqmckat, C12KetoacylCoAMAT, C16KetoacylCoAMAT, C14KetoacylCoAMAT, C10KetoacylCoAMAT, C8KetoacylCoAMAT, C6KetoacylCoAMAT, C4AcetoacylCoAMAT, CoAMAT, C10AcylCoAMAT, C16AcylCoAMAT, C14AcylCoAMAT, C12AcylCoAMAT, C8AcylCoAMAT, C6AcylCoAMAT, C4AcylCoAMAT, AcetylCoAMAT]);

```

vmckatC10 = MCKATA([sfmckatC10, Vmckat, KmmckatC10KetoacylCoAMAT,
KmmckatC16KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT, KmmckatC12KetoacylCoAMAT,
KmmckatC8KetoacylCoAMAT, KmmckatC6KetoacylCoAMAT, KmmckatC4AcetoacylCoAMAT,
KmmckatCoAMAT, KmmckatC8AcylCoAMAT, KmmckatC16AcylCoAMAT,
KmmckatC14AcylCoAMAT, KmmckatC12AcylCoAMAT, KmmckatC10AcylCoAMAT,
KmmckatC6AcylCoAMAT, KmmckatC4AcylCoAMAT, KmmckatAcetylCoAMAT, Keqmckat,
C10KetoacylCoAMAT, C16KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCoAMAT,
C8KetoacylCoAMAT, C6KetoacylCoAMAT, C4AcetoacylCoAMAT, CoAMAT, C8AcylCoAMAT,
C16AcylCoAMAT, C14AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT, C6AcylCoAMAT,
C4AcylCoAMAT, AcetylCoAMAT]);
vmckatC8 = MCKATA([sfmckatC8, Vmckat, KmmckatC8KetoacylCoAMAT,
KmmckatC16KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT, KmmckatC12KetoacylCoAMAT,
KmmckatC10KetoacylCoAMAT, KmmckatC6KetoacylCoAMAT, KmmckatC4AcetoacylCoAMAT,
KmmckatCoAMAT, KmmckatC6AcylCoAMAT, KmmckatC16AcylCoAMAT,
KmmckatC14AcylCoAMAT, KmmckatC12AcylCoAMAT, KmmckatC10AcylCoAMAT,
KmmckatC8AcylCoAMAT, KmmckatC4AcylCoAMAT, KmmckatAcetylCoAMAT, Keqmckat,
C8KetoacylCoAMAT, C16KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCoAMAT,
C10KetoacylCoAMAT, C6KetoacylCoAMAT, C4AcetoacylCoAMAT, CoAMAT, C6AcylCoAMAT,
C16AcylCoAMAT, C14AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT,
C4AcylCoAMAT, AcetylCoAMAT]);
vmckatC6 = MCKATA([sfmckatC6, Vmckat, KmmckatC6KetoacylCoAMAT,
KmmckatC16KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT, KmmckatC12KetoacylCoAMAT,
KmmckatC10KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC4AcetoacylCoAMAT,
KmmckatCoAMAT, KmmckatC4AcylCoAMAT, KmmckatC16AcylCoAMAT,
KmmckatC14AcylCoAMAT, KmmckatC12AcylCoAMAT, KmmckatC10AcylCoAMAT,
KmmckatC8AcylCoAMAT, KmmckatC6AcylCoAMAT, KmmckatAcetylCoAMAT, Keqmckat,
C6KetoacylCoAMAT, C16KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCoAMAT,
C10KetoacylCoAMAT, C8KetoacylCoAMAT, C4AcetoacylCoAMAT, CoAMAT, C4AcylCoAMAT,
C16AcylCoAMAT, C14AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT,
C6AcylCoAMAT, AcetylCoAMAT]);
vmckatC4 = MCKATB([sfmckatC4, Vmckat, KmmckatC4AcetoacylCoAMAT,
KmmckatC16KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT, KmmckatC12KetoacylCoAMAT,
KmmckatC10KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC6KetoacylCoAMAT,
KmmckatCoAMAT, KmmckatC4AcylCoAMAT, KmmckatC16AcylCoAMAT,
KmmckatC14AcylCoAMAT, KmmckatC12AcylCoAMAT, KmmckatC10AcylCoAMAT,
KmmckatC8AcylCoAMAT, KmmckatC6AcylCoAMAT, KmmckatAcetylCoAMAT, Keqmckat,
C4AcetoacylCoAMAT, C16KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCoAMAT,
C10KetoacylCoAMAT, C8KetoacylCoAMAT, C6KetoacylCoAMAT, CoAMAT, C4AcylCoAMAT,
C16AcylCoAMAT, C14AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT,
C6AcylCoAMAT, AcetylCoAMAT]);
vmtpC16 = MTP([sfmtpC16, Vmtp, KmmtP16EnoylCoAMAT, KmmtP14EnoylCoAMAT,
KmmtP12EnoylCoAMAT, KmmtP10EnoylCoAMAT, KmmtP8EnoylCoAMAT, KmmtPNADMAT,
KmmtPCoAMAT, KmmtP14AcylCoAMAT, KmmtP16AcylCoAMAT, KmmtP12AcylCoAMAT,
KmmtP10AcylCoAMAT, KmmtP8AcylCoAMAT, KmmtP6AcylCoAMAT, KmmtPNADHMAT,
KmmtPAcetylCoAMAT, KeqmtP, C16EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT,
C10EnoylCoAMAT, C8EnoylCoAMAT, NADtMAT, CoAMAT, C14AcylCoAMAT, C16AcylCoAMAT,
C12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, C6AcylCoAMAT, NADHMAT,
AcetylCoAMAT]);
vmtpC14 = MTP([sfmtpC14, Vmtp, KmmtP14EnoylCoAMAT, KmmtP16EnoylCoAMAT,
KmmtP12EnoylCoAMAT, KmmtP10EnoylCoAMAT, KmmtP8EnoylCoAMAT, KmmtPNADMAT,
KmmtPCoAMAT, KmmtP12AcylCoAMAT, KmmtP16AcylCoAMAT, KmmtP14AcylCoAMAT,
KmmtP10AcylCoAMAT, KmmtP8AcylCoAMAT, KmmtP6AcylCoAMAT, KmmtPNADHMAT,
KmmtPAcetylCoAMAT, KeqmtP, C14EnoylCoAMAT, C16EnoylCoAMAT, C12EnoylCoAMAT,
C10EnoylCoAMAT, C8EnoylCoAMAT, NADtMAT, CoAMAT, C12AcylCoAMAT, C16AcylCoAMAT,
C14AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, C6AcylCoAMAT, NADHMAT,
AcetylCoAMAT]);

```

```

vmtpc12 = MTP([sfmtpC12, Vmtp, Kmmtpc12EnoylCoAMAT, Kmmtpc16EnoylCoAMAT,
Kmmtpc14EnoylCoAMAT, Kmmtpc10EnoylCoAMAT, Kmmtpc8EnoylCoAMAT, KmmtpnADMAT,
KmmtpcCoAMAT, Kmmtpc10AcylCoAMAT, Kmmtpc16AcylCoAMAT, Kmmtpc14AcylCoAMAT,
Kmmtpc12AcylCoAMAT, Kmmtpc8AcylCoAMAT, Kmmtpc6AcylCoAMAT, KmmtpnADHMAT,
KmmtpcAcetylCoAMAT, Keqmtpc, C12EnoylCoAMAT, C16EnoylCoAMAT, C14EnoylCoAMAT,
C10EnoylCoAMAT, C8EnoylCoAMAT, NADtMAT, CoAMAT, C10AcylCoAMAT, C16AcylCoAMAT,
C14AcylCoAMAT, C12AcylCoAMAT, C8AcylCoAMAT, C6AcylCoAMAT, NADHMAT,
AcetylCoAMAT]);
vmtpc10 = MTP([sfmtpC10, Vmtp, Kmmtpc10EnoylCoAMAT, Kmmtpc16EnoylCoAMAT,
Kmmtpc14EnoylCoAMAT, Kmmtpc12EnoylCoAMAT, Kmmtpc8EnoylCoAMAT, KmmtpnADMAT,
KmmtpcCoAMAT, Kmmtpc8AcylCoAMAT, Kmmtpc16AcylCoAMAT, Kmmtpc14AcylCoAMAT,
Kmmtpc12AcylCoAMAT, Kmmtpc10AcylCoAMAT, Kmmtpc6AcylCoAMAT, KmmtpnADHMAT,
KmmtpcAcetylCoAMAT, Keqmtpc, C10EnoylCoAMAT, C16EnoylCoAMAT, C14EnoylCoAMAT,
C12EnoylCoAMAT, C8EnoylCoAMAT, NADtMAT, CoAMAT, C8AcylCoAMAT, C16AcylCoAMAT,
C14AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT, C6AcylCoAMAT, NADHMAT,
AcetylCoAMAT]);
vmtpc8 = MTP([sfmtpC8, Vmtp, Kmmtpc8EnoylCoAMAT, Kmmtpc16EnoylCoAMAT,
Kmmtpc14EnoylCoAMAT, Kmmtpc12EnoylCoAMAT, Kmmtpc10EnoylCoAMAT, KmmtpnADMAT,
KmmtpcCoAMAT, Kmmtpc6AcylCoAMAT, Kmmtpc16AcylCoAMAT, Kmmtpc14AcylCoAMAT,
Kmmtpc12AcylCoAMAT, Kmmtpc10AcylCoAMAT, Kmmtpc8AcylCoAMAT, KmmtpnADHMAT,
KmmtpcAcetylCoAMAT, Keqmtpc, C8EnoylCoAMAT, C16EnoylCoAMAT, C14EnoylCoAMAT,
C12EnoylCoAMAT, C10EnoylCoAMAT, NADtMAT, CoAMAT, C6AcylCoAMAT, C16AcylCoAMAT,
C14AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, NADHMAT,
AcetylCoAMAT]);
vacesink = RES([Ksacesink, AcetylCoAMAT, Klacesink]);
vfadhsink = RES([Ksfadhsink, FADHMAT, Klfadhsink]);
vnadhsink = RES([Ksnadhsink, NADHMAT, Klnadhsink]);

```

```

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% DIFFERENTIAL EQUATIONS
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

```

```

output(1) = (vcpt1C16 - vactC16)/VCYT;
output(2) = (vactC16 - vcpt2C16)/VMAT;
output(3) = (vcpt2C16 - vvlcadC16 - vlcadC16)/VMAT;
output(4) = (vvlcadC16 + vlcadC16 - vcrotC16 - vmtpc16)/VMAT;
output(5) = (vcrotC16 - vmschadC16)/VMAT;
output(6) = (vmschadC16 - vmckatC16)/VMAT;
output(7) = - vactC14/VCYT;
output(8) = (vactC14 - vcpt2C14)/VMAT;
output(9) = (vcpt2C14 + vmtpc16 + vmckatC16 - vvlcadC14 - vlcadC14)/VMAT;
output(10) = (vvlcadC14 + vlcadC14 - vcrotC14 - vmtpc14)/VMAT;
output(11) = (vcrotC14 - vmschadC14)/VMAT;
output(12) = (vmschadC14 - vmckatC14)/VMAT;
output(13) = - vactC12/VCYT;
output(14) = (vactC12 - vcpt2C12)/VMAT;
output(15) = (vcpt2C12 + vmtpc14 + vmckatC14 - vvlcadC12 - vlcadC12 -
vmcadC12)/VMAT;
output(16) = (vvlcadC12 + vlcadC12 + vmcadC12 - vcrotC12 - vmtpc12)/VMAT;
output(17) = (vcrotC12 - vmschadC12)/VMAT;
output(18) = (vmschadC12 - vmckatC12)/VMAT;
output(19) = - vactC10/VCYT;
output(20) = (vactC10 - vcpt2C10)/VMAT;
output(21) = (vcpt2C10 + vmtpc12 + vmckatC12 - vlcadC10 - vmcadC10)/VMAT;
output(22) = (vlcadC10 + vmcadC10 - vcrotC10 - vmtpc10)/VMAT;
output(23) = (vcrotC10 - vmschadC10)/VMAT;
output(24) = (vmschadC10 - vmckatC10)/VMAT;
output(25) = - vactC8/VCYT;

```

```

output(26) = (vcactC8 - vcpt2C8)/VMAT;
output(27) = (vcpt2C8 + vmtpC10 + vmckatC10 - vlcadC8 - vmcadC8)/VMAT;
output(28) = (vlcadC8 + vmcadC8 - vcrotC8 - vmtpC8)/VMAT;
output(29) = (vcrotC8 - vmschadC8)/VMAT;
output(30) = (vmschadC8 - vmckatC8)/VMAT;
output(31) = - vcactC6/VCYT;
output(32) = (vcactC6 - vcpt2C6)/VMAT;
output(33) = (vcpt2C6 + vmtpC8 + vmckatC8 - vmcadC6 - vscadC6)/VMAT;
output(34) = (vmcadC6 + vscadC6 - vcrotC6)/VMAT;
output(35) = (vcrotC6 - vmschadC6)/VMAT;
output(36) = (vmschadC6 - vmckatC6)/VMAT;
output(37) = - vcactC4/VCYT;
output(38) = (vcactC4 - vcpt2C4)/VMAT;
output(39) = (vcpt2C4 + vmckatC6 - vmcadC4 - vscadC4)/VMAT;
output(40) = (vmcadC4 + vscadC4 - vcrotC4)/VMAT;
output(41) = (vcrotC4 - vmschadC4)/VMAT;
output(42) = (vmschadC4 - vmckatC4)/VMAT;
output(43) = (1/VMAT)*(vmtpC16 + vmckatC16 + vmtpC14 + vmckatC14 + vmtpC12 +
vmckatC12 + vmtpC10 + vmckatC10 + vmtpC8 + vmckatC8 + vmckatC6 + 2*vmckatC4 -
vacesink);
output(44) = (1/VMAT)*(vvlcadc16 + vvlcadc14 + vvlcadc12 + vlcadC16 +
vlcadc14 + vlcadc12 + vlcadc10 + vlcadc8 + vmcadC12 + vmcadC10 + vmcadC8 +
vmcadC6 + vmcadC4 + vscadC6 + vscadC4 - vfadhsink);
output(45) = (1/VMAT)*(vmtpC16 + vmtpC14 + vmtpC12 + vmtpC10 + vmtpC8 +
vmschadC16 + vmschadC14 + vmschadC12 + vmschadC10 + vmschadC8 + vmschadC6 +
vmschadC4 - vнадhsink);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% RETURN VALUES
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% return a column vector
output = output(:);
%end;

function output = CPT1(input)

sf = input(1);
V = input(2);
Kms1 = input(3);
Kms2 = input(4);
Kmp1 = input(5);
Kmp2 = input(6);
Kil = input(7);
Keq = input(8);
S1 = input(9);
S2 = input(10);
P1 = input(11);
P2 = input(12);
I1 = input(13);
n = input(14);

output = (sf*V*((S1*S2)/(Kms1*Kms2) - (P1*P2)/(Kms1*Kms2*Keq)))/((1 + S1/Kms1
+ P1/Kmp1 + (I1/Kil)^n)*(1 + S2/Kms2 + P2/Kmp2));
%end;

function output = CACT(input)

```

```

Vf = input(1);
Vr = input(2);
Kms1 = input(3);
Kms2 = input(4);
Kmp1 = input(5);
Kmp2 = input(6);
Kis1 = input(7);
Kip2 = input(8);
Keq = input(9);
S1 = input(10);
S2 = input(11);
P1 = input(12);
P2 = input(13);

output = (Vf*(S1*S2 - (P1*P2)/Keq))/(S1*S2 + Kms2*S1 + Kms1*S2*(1 + P2/Kip2)
+ (Vf/(Vr*Keq))*(Kmp2*P1*(1 + S1/Kis1) + P2*(Kmp1 + P1)));
%end;

```

```

function output = CPT2(input)

```

```

sf = input(1);
V = input(2);
Kms1 = input(3);
Kms2 = input(4);
Kms3 = input(5);
Kms4 = input(6);
Kms5 = input(7);
Kms6 = input(8);
Kms7 = input(9);
Kms8 = input(10);
Kmp1 = input(11);
Kmp2 = input(12);
Kmp3 = input(13);
Kmp4 = input(14);
Kmp5 = input(15);
Kmp6 = input(16);
Kmp7 = input(17);
Kmp8 = input(18);
Keq = input(19);
S1 = input(20);
S2 = input(21);
S3 = input(22);
S4 = input(23);
S5 = input(24);
S6 = input(25);
S7 = input(26);
S8 = input(27);
P1 = input(28);
P2 = input(29);
P3 = input(30);
P4 = input(31);
P5 = input(32);
P6 = input(33);
P7 = input(34);
P8 = input(35);

```



```

output = (sf*V*((S1*S8)/(Kms1*Kms8) - (P1*P8)/(Kms1*Kms8*Keq)))/((1 + S1/Kms1
+ P1/Kmp1 + S2/Kms2 + P2/Kmp2 + S3/Kms3 + P3/Kmp3 + S4/Kms4 + P4/Kmp4 +
S5/Kms5 + P5/Kmp5 + S6/Kms6 + P6/Kmp6 + S7/Kms7 + P7/Kmp7)*(1 + S8/Kms8 +
P8/Kmp8));
%end;

```

```

function output = VLCAD(input)

```

```

sf = input(1);
V = input(2);
Kms1 = input(3);
Kms2 = input(4);
Kms3 = input(5);
Kms4 = input(6);
Kmp1 = input(7);
Kmp2 = input(8);
Kmp3 = input(9);
Kmp4 = input(10);
Keq = input(11);
S1 = input(12);
S2 = input(13);
S3 = input(14);
S4 = input(15);
P1 = input(16);
P2 = input(17);
P3 = input(18);
P4 = input(19);

```

```

output = (sf*V*((S1*(S4 - P4))/(Kms1*Kms4) - (P1*P4)/(Kms1*Kms4*Keq)))/((1 +
S1/Kms1 + P1/Kmp1 + S2/Kms2 + P2/Kmp2 + S3/Kms3 + P3/Kmp3)*(1 + (S4 -
P4)/Kms4 + P4/Kmp4));
%end;

```

```

function output = LCAD(input)

```

```

sf = input(1);
V = input(2);
Kms1 = input(3);
Kms2 = input(4);
Kms3 = input(5);
Kms4 = input(6);
Kms5 = input(7);
Kms6 = input(8);
Kmp1 = input(9);
Kmp2 = input(10);
Kmp3 = input(11);
Kmp4 = input(12);
Kmp5 = input(13);
Kmp6 = input(14);
Keq = input(15);
S1 = input(16);
S2 = input(17);
S3 = input(18);
S4 = input(19);
S5 = input(20);
S6 = input(21);

```

```

P1 = input(22);
P2 = input(23);
P3 = input(24);
P4 = input(25);
P5 = input(26);
P6 = input(27);

output = (sf*V*((S1*(S6 - P6))/(Kms1*Kms6) - (P1*P6)/(Kms1*Kms6*Keq)))/((1 +
S1/Kms1 + P1/Kmp1 + S2/Kms2 + P2/Kmp2 + S3/Kms3 + P3/Kmp3 + S4/Kms4 + P4/Kmp4
+ S5/Kms5 + P5/Kmp5)*(1 + (S6 - P6)/Kms6 + P6/Kmp6));
%end;

```

```
function output = MCAD(input)
```

```

sf = input(1);
V = input(2);
Kms1 = input(3);
Kms2 = input(4);
Kms3 = input(5);
Kms4 = input(6);
Kms5 = input(7);
Kms6 = input(8);
Kmp1 = input(9);
Kmp2 = input(10);
Kmp3 = input(11);
Kmp4 = input(12);
Kmp5 = input(13);
Kmp6 = input(14);
Keq = input(15);
S1 = input(16);
S2 = input(17);
S3 = input(18);
S4 = input(19);
S5 = input(20);
S6 = input(21);
P1 = input(22);
P2 = input(23);
P3 = input(24);
P4 = input(25);
P5 = input(26);
P6 = input(27);

output = (sf*V*((S1*(S6 - P6))/(Kms1*Kms6) - (P1*P6)/(Kms1*Kms6*Keq)))/((1 +
S1/Kms1 + P1/Kmp1 + S2/Kms2 + P2/Kmp2 + S3/Kms3 + P3/Kmp3 + S4/Kms4 + P4/Kmp4
+ S5/Kms5 + P5/Kmp5)*(1 + (S6 - P6)/Kms6 + P6/Kmp6));
%end;

```

```
function output = SCAD(input)
```

```

sf = input(1);
V = input(2);
Kms1 = input(3);
Kms2 = input(4);
Kms3 = input(5);
Kmp1 = input(6);
Kmp2 = input(7);

```

```

Kmp3 = input(8);
Keq = input(9);
S1 = input(10);
S2 = input(11);
S3 = input(12);
P1 = input(13);
P2 = input(14);
P3 = input(15);

output = (sf*V*((S1*(S3 - P3))/(Kms1*Kms3) - (P1*P3)/(Kms1*Kms3*Keq)))/((1 +
S1/Kms1 + P1/Kmp1 + S2/Kms2 + P2/Kmp2)*(1 + (S3 - P3)/Kms3 + P3/Kmp3));

%end;

function output = CROT(input)

sf = input(1);
V = input(2);
Kms1 = input(3);
Kms2 = input(4);
Kms3 = input(5);
Kms4 = input(6);
Kms5 = input(7);
Kms6 = input(8);
Kms7 = input(9);
Kmp1 = input(10);
Kmp2 = input(11);
Kmp3 = input(12);
Kmp4 = input(13);
Kmp5 = input(14);
Kmp6 = input(15);
Kmp7 = input(16);
Ki = input(17);
Keq = input(18);
S1 = input(19);
S2 = input(20);
S3 = input(21);
S4 = input(22);
S5 = input(23);
S6 = input(24);
S7 = input(25);
P1 = input(26);
P2 = input(27);
P3 = input(28);
P4 = input(29);
P5 = input(30);
P6 = input(31);
P7 = input(32);
I1 = input(33);

output = (sf*V*(S1/Kms1 - P1/(Kms1*Keq)))/((1 + S1/Kms1 + P1/Kmp1 + S2/Kms2 +
P2/Kmp2 + S3/Kms3 + P3/Kmp3 + S4/Kms4 + P4/Kmp4 + S5/Kms5 + P5/Kmp5 + S6/Kms6
+ P6/Kmp6 + S7/Kms7 + P7/Kmp7 + I1/Ki);
%end;

function output = MSCHAD(input)

```

```

sf = input(1);
V = input(2);
Kms1 = input(3);
Kms2 = input(4);
Kms3 = input(5);
Kms4 = input(6);
Kms5 = input(7);
Kms6 = input(8);
Kms7 = input(9);
Kms8 = input(10);
Kmp1 = input(11);
Kmp2 = input(12);
Kmp3 = input(13);
Kmp4 = input(14);
Kmp5 = input(15);
Kmp6 = input(16);
Kmp7 = input(17);
Kmp8 = input(18);
Keq = input(19);
S1 = input(20);
S2 = input(21);
S3 = input(22);
S4 = input(23);
S5 = input(24);
S6 = input(25);
S7 = input(26);
S8 = input(27);
P1 = input(28);
P2 = input(29);
P3 = input(30);
P4 = input(31);
P5 = input(32);
P6 = input(33);
P7 = input(34);
P8 = input(35);

output = (sf*V*((S1*(S8 - P8))/(Kms1*Kms8) - (P1*P8)/(Kms1*Kms8*Keq)))/((1 +
S1/Kms1 + P1/Kmp1 + S2/Kms2 + P2/Kmp2 + S3/Kms3 + P3/Kmp3 + S4/Kms4 + P4/Kmp4
+ S5/Kms5 + P5/Kmp5 + S6/Kms6 + P6/Kmp6 + S7/Kms7 + P7/Kmp7)*(1 + (S8 -
P8)/Kms8 + P8/Kmp8));

%end;

function output = MCKATA(input)

sf = input(1);
V = input(2);
Kms1 = input(3);
Kms2 = input(4);
Kms3 = input(5);
Kms4 = input(6);
Kms5 = input(7);
Kms6 = input(8);
Kms7 = input(9);
Kms8 = input(10);

```

```

Kmp1 = input(11);
Kmp2 = input(12);
Kmp3 = input(13);
Kmp4 = input(14);
Kmp5 = input(15);
Kmp6 = input(16);
Kmp7 = input(17);
Kmp8 = input(18);
Keq = input(19);
S1 = input(20);
S2 = input(21);
S3 = input(22);
S4 = input(23);
S5 = input(24);
S6 = input(25);
S7 = input(26);
S8 = input(27);
P1 = input(28);
P2 = input(29);
P3 = input(30);
P4 = input(31);
P5 = input(32);
P6 = input(33);
P7 = input(34);
P8 = input(35);

output = (sf*V*((S1*S8)/(Kms1*Kms8) - (P1*P8)/(Kms1*Kms8*Keq)))/((1 + S1/Kms1
+ P1/Kmp1 + S2/Kms2 + P2/Kmp2 + S3/Kms3 + P3/Kmp3 + S4/Kms4 + P4/Kmp4 +
S5/Kms5 + P5/Kmp5 + S6/Kms6 + P6/Kmp6 + S7/Kms7 + P7/Kmp7 + P8/Kmp8)*(1 +
S8/Kms8 + P8/Kmp8));
%end;

function output = MCKATB(input)

sf = input(1);
V = input(2);
Kms1 = input(3);
Kms2 = input(4);
Kms3 = input(5);
Kms4 = input(6);
Kms5 = input(7);
Kms6 = input(8);
Kms7 = input(9);
Kms8 = input(10);
Kmp1 = input(11);
Kmp2 = input(12);
Kmp3 = input(13);
Kmp4 = input(14);
Kmp5 = input(15);
Kmp6 = input(16);
Kmp7 = input(17);
Kmp8 = input(18);
Keq = input(19);
S1 = input(20);
S2 = input(21);
S3 = input(22);

```

```

S4 = input(23);
S5 = input(24);
S6 = input(25);
S7 = input(26);
S8 = input(27);
P1 = input(28);
P2 = input(29);
P3 = input(30);
P4 = input(31);
P5 = input(32);
P6 = input(33);
P7 = input(34);
P8 = input(35);

output = (sf*v*((S1*S8)/(Kms1*Kms8) - (P8*P8)/(Kms1*Kms8*Keq)))/((1 + S1/Kms1
+ P1/Kmp1 + S2/Kms2 + P2/Kmp2 + S3/Kms3 + P3/Kmp3 + S4/Kms4 + P4/Kmp4 +
S5/Kms5 + P5/Kmp5 + S6/Kms6 + P6/Kmp6 + S7/Kms7 + P7/Kmp7 + P8/Kmp8)*(1 +
S8/Kms8 + P8/Kmp8));
%end;

function output = MTP(input)
sf = input(1);
V = input(2);
Kms1 = input(3);
Kms2 = input(4);
Kms3 = input(5);
Kms4 = input(6);
Kms5 = input(7);
%Kms6 = input(8);
Kms7 = input(8);
Kms8 = input(9);
Kmp1 = input(10);
Kmp2 = input(11);
Kmp3 = input(12);
Kmp4 = input(13);
Kmp5 = input(14);
Kmp6 = input(15);
Kmp7 = input(16);
Kmp8 = input(17);
Keq = input(18);
S1 = input(19);
S2 = input(20);
S3 = input(21);
S4 = input(22);
S5 = input(23);
%S6 = input(25);
S7 = input(24);
S8 = input(25);
P1 = input(26);
P2 = input(27);
P3 = input(28);
P4 = input(29);
P5 = input(30);
P6 = input(31);
P7 = input(32);
P8 = input(33);

```

```
output = (sf*V*((S1*(S7 - P7)*S8)/(Kms1*Kms7*Kms8) -  
(P1*P7*P8)/(Kms1*Kms7*Kms8*Keq)))/((1 + S1/Kms1 + P1/Kmp1 + S2/Kms2 + P2/Kmp2  
+ S3/Kms3 + P3/Kmp3 + S4/Kms4 + P4/Kmp4 + S5/Kms5 + P5/Kmp5 + P6/Kmp6)*(1 +  
(S7 - P7)/Kms7 + P7/Kmp7)*(1 + S8/Kms8 + P8/Kmp8));  
%end;
```

```
function output = RES(input)
```

```
Ks = input(1);
```

```
S = input(2);
```

```
K1 = input(3);
```

```
output = Ks*(S - K1);
```

```
%end;
```