

# Mitochondrial Fatty Acid Oxidation Kinetic model with ACOT Extension

## Definitions of the various functions

$$\ln[=] := \text{CPT1}[\text{sf}_-, \text{V}_-, \text{Kms1}_-, \text{Kms2}_-, \text{Kmp1}_-, \text{Kmp2}_-, \text{Ki1}_-, \text{Keq}_-, \text{S1}_-, \text{S2}_-, \text{P1}_-, \text{P2}_-, \text{I1}_-, \text{n}_-] :=$$

$$\frac{\text{sf} * \text{V} * \left( \frac{\text{S1} * \text{S2}}{\text{Kms1} * \text{Kms2}} - \frac{\text{P1} * \text{P2}}{\text{Kms1} * \text{Kms2} * \text{Keq}} \right)}{\left( 1 + \frac{\text{S1}}{\text{Kms1}} + \frac{\text{P1}}{\text{Kmp1}} + \left( \frac{\text{I1}}{\text{Ki1}} \right)^{\text{n}} \right) * \left( 1 + \frac{\text{S2}}{\text{Kms2}} + \frac{\text{P2}}{\text{Kmp2}} \right)}$$

$$\ln[=] := \text{CACT}[\text{Vf}_-, \text{Vr}_-, \text{Kms1}_-, \text{Kms2}_-, \text{Kmp1}_-, \text{Kmp2}_-, \text{Kis1}_-, \text{Kip2}_-, \text{Keq}_-, \text{S1}_-, \text{S2}_-, \text{P1}_-, \text{P2}_-] :=$$

$$\frac{\text{Vf} * \left( \text{S1} * \text{S2} - \frac{\text{P1} * \text{P2}}{\text{Keq}} \right)}{\text{S1} * \text{S2} + \text{Kms2} * \text{S1} + \text{Kms1} * \text{S2} * \left( 1 + \frac{\text{P2}}{\text{Kip2}} \right) + \frac{\text{Vf}}{\text{Vr} * \text{Keq}} * \left( \text{Kmp2} * \text{P1} * \left( 1 + \frac{\text{S1}}{\text{Kis1}} \right) + \text{P2} * (\text{Kmp1} + \text{P1}) \right)}$$

$$\ln[=] := \text{CPT2}[\text{sf}_-, \text{V}_-, \text{Kms1}_-, \text{Kms2}_-, \text{Kms3}_-, \text{Kms4}_-, \text{Kms5}_-, \text{Kms6}_-, \text{Kms7}_-, \text{Kms8}_-, \text{Kmp1}_-, \text{Kmp2}_-, \text{Kmp3}_-, \text{Kmp4}_-, \text{Kmp5}_-, \text{Kmp6}_-, \text{Kmp7}_-, \text{Kmp8}_-, \text{Keq}_-, \text{S1}_-, \text{S2}_-, \text{S3}_-, \text{S4}_-, \text{S5}_-, \text{S6}_-, \text{S7}_-, \text{S8}_-, \text{P1}_-, \text{P2}_-, \text{P3}_-, \text{P4}_-, \text{P5}_-, \text{P6}_-, \text{P7}_-, \text{P8}_-] :=$$

$$\left( \text{sf} * \text{V} * \left( \frac{\text{S1} * \text{S8}}{\text{Kms1} * \text{Kms8}} - \frac{\text{P1} * \text{P8}}{\text{Kms1} * \text{Kms8} * \text{Keq}} \right) \right) / \left( \left( 1 + \frac{\text{S1}}{\text{Kms1}} + \frac{\text{P1}}{\text{Kmp1}} + \frac{\text{S2}}{\text{Kms2}} + \frac{\text{P2}}{\text{Kmp2}} + \frac{\text{S3}}{\text{Kms3}} + \frac{\text{P3}}{\text{Kmp3}} + \frac{\text{S4}}{\text{Kms4}} + \frac{\text{P4}}{\text{Kmp4}} + \frac{\text{S5}}{\text{Kms5}} + \frac{\text{P5}}{\text{Kmp5}} + \frac{\text{S6}}{\text{Kms6}} + \frac{\text{P6}}{\text{Kmp6}} + \frac{\text{S7}}{\text{Kms7}} + \frac{\text{P7}}{\text{Kmp7}} \right) * \left( 1 + \frac{\text{S8}}{\text{Kms8}} + \frac{\text{P8}}{\text{Kmp8}} \right) \right)$$

$$\ln[=] := \text{VLCAD}[\text{sf}_-, \text{V}_-, \text{Kms1}_-, \text{Kms2}_-, \text{Kms3}_-, \text{Kms4}_-, \text{Kmp1}_-, \text{Kmp2}_-, \text{Kmp3}_-, \text{Kmp4}_-, \text{Keq}_-, \text{S1}_-, \text{S2}_-, \text{S3}_-, \text{S4}_-, \text{P1}_-, \text{P2}_-, \text{P3}_-, \text{P4}_-] :=$$

$$\frac{\text{sf} * \text{V} * \left( \frac{\text{S1} * (\text{S4} - \text{P4})}{\text{Kms1} * \text{Kms4}} - \frac{\text{P1} * \text{P4}}{\text{Kms1} * \text{Kms4} * \text{Keq}} \right)}{\left( 1 + \frac{\text{S1}}{\text{Kms1}} + \frac{\text{P1}}{\text{Kmp1}} + \frac{\text{S2}}{\text{Kms2}} + \frac{\text{P2}}{\text{Kmp2}} + \frac{\text{S3}}{\text{Kms3}} + \frac{\text{P3}}{\text{Kmp3}} \right) * \left( 1 + \frac{(\text{S4} - \text{P4})}{\text{Kms4}} + \frac{\text{P4}}{\text{Kmp4}} \right)}$$

$$\ln[=] := \text{LCAD}[\text{sf}_-, \text{V}_-, \text{Kms1}_-, \text{Kms2}_-, \text{Kms3}_-, \text{Kms4}_-, \text{Kms5}_-, \text{Kms6}_-, \text{Kmp1}_-, \text{Kmp2}_-, \text{Kmp3}_-, \text{Kmp4}_-, \text{Kmp5}_-, \text{Kmp6}_-, \text{Keq}_-, \text{S1}_-, \text{S2}_-, \text{S3}_-, \text{S4}_-, \text{S5}_-, \text{S6}_-, \text{P1}_-, \text{P2}_-, \text{P3}_-, \text{P4}_-, \text{P5}_-, \text{P6}_-] :=$$

$$\frac{\text{sf} * \text{V} * \left( \frac{\text{S1} * (\text{S6} - \text{P6})}{\text{Kms1} * \text{Kms6}} - \frac{\text{P1} * \text{P6}}{\text{Kms1} * \text{Kms6} * \text{Keq}} \right)}{\left( 1 + \frac{\text{S1}}{\text{Kms1}} + \frac{\text{P1}}{\text{Kmp1}} + \frac{\text{S2}}{\text{Kms2}} + \frac{\text{P2}}{\text{Kmp2}} + \frac{\text{S3}}{\text{Kms3}} + \frac{\text{P3}}{\text{Kmp3}} + \frac{\text{S4}}{\text{Kms4}} + \frac{\text{P4}}{\text{Kmp4}} + \frac{\text{S5}}{\text{Kms5}} + \frac{\text{P5}}{\text{Kmp5}} \right) * \left( 1 + \frac{(\text{S6} - \text{P6})}{\text{Kms6}} + \frac{\text{P6}}{\text{Kmp6}} \right)}$$

$$\ln[=] := \text{MCAD}[\text{sf}_-, \text{V}_-, \text{Kms1}_-, \text{Kms2}_-, \text{Kms3}_-, \text{Kms4}_-, \text{Kms5}_-, \text{Kms6}_-, \text{Kmp1}_-, \text{Kmp2}_-, \text{Kmp3}_-, \text{Kmp4}_-, \text{Kmp5}_-, \text{Kmp6}_-, \text{Keq}_-, \text{S1}_-, \text{S2}_-, \text{S3}_-, \text{S4}_-, \text{S5}_-, \text{S6}_-, \text{P1}_-, \text{P2}_-, \text{P3}_-, \text{P4}_-, \text{P5}_-, \text{P6}_-] :=$$

$$\frac{\text{sf} * \text{V} * \left( \frac{\text{S1} * (\text{S6} - \text{P6})}{\text{Kms1} * \text{Kms6}} - \frac{\text{P1} * \text{P6}}{\text{Kms1} * \text{Kms6} * \text{Keq}} \right)}{\left( 1 + \frac{\text{S1}}{\text{Kms1}} + \frac{\text{P1}}{\text{Kmp1}} + \frac{\text{S2}}{\text{Kms2}} + \frac{\text{P2}}{\text{Kmp2}} + \frac{\text{S3}}{\text{Kms3}} + \frac{\text{P3}}{\text{Kmp3}} + \frac{\text{S4}}{\text{Kms4}} + \frac{\text{P4}}{\text{Kmp4}} + \frac{\text{S5}}{\text{Kms5}} + \frac{\text{P5}}{\text{Kmp5}} \right) * \left( 1 + \frac{(\text{S6} - \text{P6})}{\text{Kms6}} + \frac{\text{P6}}{\text{Kmp6}} \right)}$$

$$\ln[=] := \text{SCAD}[\text{sf}_-, \text{V}_-, \text{Kms1}_-, \text{Kms2}_-, \text{Kms3}_-, \text{Kmp1}_-, \text{Kmp2}_-, \text{Kmp3}_-, \text{Keq}_-, \text{S1}_-, \text{S2}_-, \text{S3}_-, \text{P1}_-, \text{P2}_-, \text{P3}_-] :=$$

$$\frac{\text{sf} * \text{V} * \left( \frac{\text{S1} * (\text{S3} - \text{P3})}{\text{Kms1} * \text{Kms3}} - \frac{\text{P1} * \text{P3}}{\text{Kms1} * \text{Kms3} * \text{Keq}} \right)}{\left( 1 + \frac{\text{S1}}{\text{Kms1}} + \frac{\text{P1}}{\text{Kmp1}} + \frac{\text{S2}}{\text{Kms2}} + \frac{\text{P2}}{\text{Kmp2}} \right) * \left( 1 + \frac{(\text{S3} - \text{P3})}{\text{Kms3}} + \frac{\text{P3}}{\text{Kmp3}} \right)}$$

*In[1]:= CROT [sf\_, V\_, Kms1\_, Kms2\_, Kms3\_, Kms4\_, Kms5\_, Kms6\_, Kms7\_, Kmp1\_, Kmp2\_, Kmp3\_, Kmp4\_, Kmp5\_, Kmp6\_, Kmp7\_, Ki1\_, Keq\_, S1\_, S2\_, S3\_, S4\_, S5\_, S6\_, S7\_, P1\_, P2\_, P3\_, P4\_, P5\_, P6\_, P7\_, I1\_] :=*

$$\frac{sf * V * \left( \frac{S1}{Kms1} - \frac{P1}{Kms1 * Keq} \right)}{1 + \frac{S1}{Kms1} + \frac{P1}{Kmp1} + \frac{S2}{Kms2} + \frac{P2}{Kmp2} + \frac{S3}{Kms3} + \frac{P3}{Kmp3} + \frac{S4}{Kms4} + \frac{P4}{Kmp4} + \frac{S5}{Kms5} + \frac{P5}{Kmp5} + \frac{S6}{Kms6} + \frac{P6}{Kmp6} + \frac{S7}{Kms7} + \frac{P7}{Kmp7} + \frac{I1}{Ki1}}$$

*In[2]:= MSCHAD [sf\_, V\_, Kms1\_, Kms2\_, Kms3\_, Kms4\_, Kms5\_, Kms6\_, Kms7\_, Kms8\_, Kmp1\_, Kmp2\_, Kmp3\_, Kmp4\_, Kmp5\_, Kmp6\_, Kmp7\_, Kmp8\_, Keq\_, S1\_, S2\_, S3\_, S4\_, S5\_, S6\_, S7\_, S8\_, P1\_, P2\_, P3\_, P4\_, P5\_, P6\_, P7\_, P8\_] :=*

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

*In[3]:= MCKATA [sf\_, V\_, Kms1\_, Kms2\_, Kms3\_, Kms4\_, Kms5\_, Kms6\_, Kms7\_, Kms8\_, Kmp1\_, Kmp2\_, Kmp3\_, Kmp4\_, Kmp5\_, Kmp6\_, Kmp7\_, Kmp8\_, Keq\_, S1\_, S2\_, S3\_, S4\_, S5\_, S6\_, S7\_, S8\_, P1\_, P2\_, P3\_, P4\_, P5\_, P6\_, P7\_, P8\_, E1\_, KmE1\_, nm\_] :=*

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

*In[4]:= MCKATB [sf\_, V\_, Kms1\_, Kms2\_, Kms3\_, Kms4\_, Kms5\_, Kms6\_, Kms7\_, Kms8\_, Kmp1\_, Kmp2\_, Kmp3\_, Kmp4\_, Kmp5\_, Kmp6\_, Kmp7\_, Kmp8\_, Keq\_, S1\_, S2\_, S3\_, S4\_, S5\_, S6\_, S7\_, S8\_, P1\_, P2\_, P3\_, P4\_, P5\_, P6\_, P7\_, P8\_, E1\_, KmE1\_, nm\_] :=*

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

*In[5]:= MTP [sf\_, V\_, Kms1\_, Kms2\_, Kms3\_, Kms4\_, Kms5\_, Kms7\_, Kms8\_, Kmp1\_, Kmp2\_, Kmp3\_, Kmp4\_, Kmp5\_, Kmp6\_, Kmp7\_, Kmp8\_, Ki1\_, Keq\_, S1\_, S2\_, S3\_, S4\_, S5\_, S7\_, S8\_, P1\_, P2\_, P3\_, P4\_, P5\_, P6\_, P7\_, P8\_, I1\_] :=*

$$\left( sf * V * \left( \frac{S1 * (S7 - P7) * S8}{Kms1 * Kms7 * Kms8} - \frac{P1 * P7 * P8}{Kms1 * Kms7 * Kms8 * Keq} \right) \right) / \left( \left( 1 + \frac{S1}{Kms1} + \frac{P1}{Kmp1} + \frac{S2}{Kms2} + \frac{P2}{Kmp2} + \frac{S3}{Kms3} + \frac{P3}{Kmp3} + \frac{S4}{Kms4} + \frac{P4}{Kmp4} + \frac{S5}{Kms5} + \frac{P5}{Kmp5} + \frac{S6}{Kms6} + \frac{P6}{Kmp6} + \frac{S7}{Kms7} + \frac{P7}{Kmp7} + \frac{I1}{Ki1} \right) * \left( 1 + \frac{(S7 - P7)}{Kms7} + \frac{P7}{Kmp7} \right) * \left( 1 + \frac{S8}{Kms8} + \frac{P8}{Kmp8} \right) \right)$$

*In[6]:= RES [Ks\_, S\_, K1\_] := Ks \* (S - K1)*

*In[7]:= ACOT [sf\_, V\_, Kms1\_, Kms2\_, Kms3\_, Kms4\_, Kms5\_, Kms6\_, Kms7\_, Kmcoa\_, Kmp1\_, Kmp2\_, Kmp3\_, Kmp4\_, Kmp5\_, Kmp6\_, Kmp7\_, Keq\_, S1\_, S2\_, S3\_, S4\_, S5\_, S6\_, S7\_, coa\_, P1\_, P2\_, P3\_, P4\_, P5\_, P6\_, P7\_] :=*

$$\left( sf * V * \left( \frac{S1}{Kms1} - \frac{coa * P1}{Kms1 * Keq} \right) \right) / \left( \left( 1 + \frac{S1}{Kms1} + \frac{P1}{Kmp1} + \frac{S2}{Kms2} + \frac{P2}{Kmp2} + \frac{S3}{Kms3} + \frac{P3}{Kmp3} + \frac{S4}{Kms4} + \frac{P4}{Kmp4} + \frac{S5}{Kms5} + \frac{P5}{Kmp5} + \frac{S6}{Kms6} + \frac{P6}{Kmp6} + \frac{S7}{Kms7} + \frac{P7}{Kmp7} \right) * \left( 1 + \frac{coa}{Kmcoa} \right) \right)$$

*In[*]:= ExportRate[ke\_, S\_] := ke \* S

*In[*]:=

## Define the differential equations

```
In[]:= Odes = {
  C16AcylCarCYT'[t] == (vcpt1C16 - vcactC16) / VCYT,
  C16AcylCarMAT'[t] == (vcactC16 - vcpt2C16) / VMAT,
  C16AcylCoAMAT'[t] == (vcpt2C16 - vvlcadC16 - vlcadC16 - vacotC16) / VMAT,
  C16EnoylCoAMAT'[t] == (vvlcadC16 + vlcadC16 - vcrotC16 - vmtpC16) / VMAT,
  C16HydroxyacylCoAMAT'[t] == (vcrotC16 - vmschadC16) / VMAT,
  C16KetoacylCoAMAT'[t] == (vmschadC16 - vmckatC16) / VMAT,
  C14AcylCarCYT'[t] == (-vcactC14) / VCYT,
  C14AcylCarMAT'[t] == (vcactC14 - vcpt2C14) / VMAT,
  C14AcylCoAMAT'[t] ==
    (vcpt2C14 + vmtpC16 + vmckatC16 - vvlcadC14 - vlcadC14 - vacotC14) / VMAT,
  C14EnoylCoAMAT'[t] == (vvlcadC14 + vlcadC14 - vcrotC14 - vmtpC14) / VMAT,
  C14HydroxyacylCoAMAT'[t] == (vcrotC14 - vmschadC14) / VMAT,
  C14KetoacylCoAMAT'[t] == (vmschadC14 - vmckatC14) / VMAT,
  C12AcylCarCYT'[t] == (-vcactC12) / VCYT,
  C12AcylCarMAT'[t] == (vcactC12 - vcpt2C12) / VMAT,
  C12AcylCoAMAT'[t] ==
    (vcpt2C12 + vmtpC14 + vmckatC14 - vvlcadC12 - vlcadC12 - vmcadC12 - vacotC12) / VMAT,
  C12EnoylCoAMAT'[t] == (vvlcadC12 + vlcadC12 + vmcadC12 - vcrotC12 - vmtpC12) / VMAT,
  C12HydroxyacylCoAMAT'[t] == (vcrotC12 - vmschadC12) / VMAT,
  C12KetoacylCoAMAT'[t] == (vmschadC12 - vmckatC12) / VMAT,
  C10AcylCarCYT'[t] == (-vcactC10) / VCYT,
  C10AcylCarMAT'[t] == (vcactC10 - vcpt2C10) / VMAT,
  C10AcylCoAMAT'[t] ==
    (vcpt2C10 + vmtpC12 + vmckatC12 - vlcadC10 - vmcadC10 - vacotC10) / VMAT,
  C10EnoylCoAMAT'[t] == (vlcadC10 + vmcadC10 - vcrotC10 - vmtpC10) / VMAT,
  C10HydroxyacylCoAMAT'[t] == (vcrotC10 - vmschadC10) / VMAT,
  C10KetoacylCoAMAT'[t] == (vmschadC10 - vmckatC10) / VMAT,
  C8AcylCarCYT'[t] == (-vcactC8) / VCYT,
  C8AcylCarMAT'[t] == (vcactC8 - vcpt2C8) / VMAT,
  C8AcylCoAMAT'[t] ==
    (vcpt2C8 + vmtpC10 + vmckatC10 - vlcadC8 - vmcadC8 - vacotC8) / VMAT,
  C8EnoylCoAMAT'[t] == (vlcadC8 + vmcadC8 - vcrotC8 - vmtpC8) / VMAT,
  C8HydroxyacylCoAMAT'[t] == (vcrotC8 - vmschadC8) / VMAT,
  C8KetoacylCoAMAT'[t] == (vmschadC8 - vmckatC8) / VMAT,
  C6AcylCarCYT'[t] == (-vcactC6) / VCYT,
  C6AcylCarMAT'[t] == (vcactC6 - vcpt2C6) / VMAT,
  C6AcylCoAMAT'[t] == (vcpt2C6 + vmtpC8 + vmckatC8 - vmcadC6 - vscadC6 - vacotC6) / VMAT,
  C6EnoylCoAMAT'[t] == (vmcadC6 + vscadC6 - vcrotC6) / VMAT,
  C6HydroxyacylCoAMAT'[t] == (vcrotC6 - vmschadC6) / VMAT,
  C6KetoacylCoAMAT'[t] == (vmschadC6 - vmckatC6) / VMAT,
  C4AcylCarCYT'[t] == (-vcactC4) / VCYT,
  C4AcylCarMAT'[t] == (vcactC4 - vcpt2C4) / VMAT,
  C4AcylCoAMAT'[t] == (vcpt2C4 + vmckatC6 - vmcadC4 - vscadC4 - vacotC4) / VMAT,
  C4EnoylCoAMAT'[t] == (vmcadC4 + vscadC4 - vcrotC4) / VMAT,
  C4HydroxyacylCoAMAT'[t] == (vcrotC4 - vmschadC4) / VMAT,
  C4AcetoacylCoAMAT'[t] == (vmschadC4 - vmckatC4) / VMAT,
  AcetylCoAMAT'[t] ==
    (1 / VMAT) (vmtpC16 + vmckatC16 + vmtpC14 + vmckatC14 + vmtpC12 + vmckatC12 +
```

```

        vmtcpC10 + vmckatC10 + vmtcpC8 + vmckatC8 + vmckatC6 + 2 * vmckatC4 - vacesink),
FADHMAT'[t] == (1 / VMAT) (vvlcadC16 + vvlcadC14 + vvlcadC12 + vlcadC16 +
    vlcadC14 + vlcadC12 + vlcadC10 + vlcadC8 + vmcadC12 + vmcadC10 +
    vmcadC8 + vmcadC6 + vmcadC4 + vscadC6 + vscadC4 - vfadhsink),
NADHMAT'[t] == (1 / VMAT) (vmtcpC16 + vmtcpC14 + vmtcpC12 + vmtcpC10 +
    vmtcpC8 + vmschadC16 + vmschadC14 + vmschadC12 + vmschadC10 +
    vmschadC8 + vmschadC6 + vmschadC4 - vnadhsink),
C16FFA'[t] == (vacotC16 - vffaC16) / VMAT,
C14FFA'[t] == (vacotC14 - vffaC14) / VMAT,
C12FFA'[t] == (vacotC12 - vffaC12) / VMAT,
C10FFA'[t] == (vacotC10 - vffaC10) / VMAT,
C8FFA'[t] == (vacotC8 - vffaC8) / VMAT,
C6FFA'[t] == (vacotC6 - vffaC6) / VMAT,
C4FFA'[t] == (vacotC4 - vffaC4) / VMAT};

RateEqs = {vcpt1C16 → CPT1[sfcpt1C16, Vcpt1, Kmcp1C16AcylCoACYT,
    Kmcp1CarCYT, Kmcp1C16AcylCarCYT, Kmcp1CoACYT, Kicp1MalCoACYT, Keqcpt1,
    C16AcylCoACYT, CarCYT, C16AcylCarCYT[t], CoACYT, MalCoACYT, ncpt1],
    vcactC16 → CACT[Vfcact, Vrcact, KmcactC16AcylCarCYT, KmcactCarMAT,
    KmcactC16AcylCarMAT, KmcactCarCYT, KicactC16AcylCarCYT, KicactCarCYT,
    Keqcact, C16AcylCarCYT[t], CarMAT, C16AcylCarMAT[t], CarCYT],
    vcactC14 → CACT[Vfcact, Vrcact, KmcactC14AcylCarCYT, KmcactCarMAT,
    KmcactC14AcylCarMAT, KmcactCarCYT, KicactC14AcylCarCYT, KicactCarCYT,
    Keqcact, C14AcylCarCYT[t], CarMAT, C14AcylCarMAT[t], CarCYT],
    vcactC12 → CACT[Vfcact, Vrcact, KmcactC12AcylCarCYT, KmcactCarMAT,
    KmcactC12AcylCarMAT, KmcactCarCYT, KicactC12AcylCarCYT, KicactCarCYT,
    Keqcact, C12AcylCarCYT[t], CarMAT, C12AcylCarMAT[t], CarCYT],
    vcactC10 → CACT[Vfcact, Vrcact, KmcactC10AcylCarCYT, KmcactCarMAT,
    KmcactC10AcylCarMAT, KmcactCarCYT, KicactC10AcylCarCYT, KicactCarCYT,
    Keqcact, C10AcylCarCYT[t], CarMAT, C10AcylCarMAT[t], CarCYT],
    vcactC8 → CACT[Vfcact, Vrcact, KmcactC8AcylCarCYT, KmcactCarMAT,
    KmcactC8AcylCarMAT, KmcactCarCYT, KicactC8AcylCarCYT, KicactCarCYT,
    Keqcact, C8AcylCarCYT[t], CarMAT, C8AcylCarMAT[t], CarCYT],
    vcactC6 → CACT[Vfcact, Vrcact, KmcactC6AcylCarCYT, KmcactCarMAT,
    KmcactC6AcylCarMAT, KmcactCarCYT, KicactC6AcylCarCYT, KicactCarCYT,
    Keqcact, C6AcylCarCYT[t], CarMAT, C6AcylCarMAT[t], CarCYT],
    vcactC4 → CACT[Vfcact, Vrcact, KmcactC4AcylCarCYT, KmcactCarMAT,
    KmcactC4AcylCarMAT, KmcactCarCYT, KicactC4AcylCarCYT, KicactCarCYT,
    Keqcact, C4AcylCarCYT[t], CarMAT, C4AcylCarMAT[t], CarCYT],
    vcpt2C16 → CPT2[sfcpt2C16, Vcpt2, Kmcp2C16AcylCarMAT, Kmcp2C14AcylCarMAT,
    Kmcp2C12AcylCarMAT, Kmcp2C10AcylCarMAT, Kmcp2C8AcylCarMAT, Kmcp2C6AcylCarMAT,
    Kmcp2C4AcylCarMAT, Kmcp2CoAMAT, Kmcp2C16AcylCoAMAT, Kmcp2C14AcylCoAMAT,
    Kmcp2C12AcylCoAMAT, Kmcp2C10AcylCoAMAT, Kmcp2C8AcylCoAMAT, Kmcp2C6AcylCoAMAT,
    Kmcp2C4AcylCoAMAT, Kmcp2CarMAT, Keqcpt2, C16AcylCarMAT[t], C14AcylCarMAT[t],
    C12AcylCarMAT[t], C10AcylCarMAT[t], C8AcylCarMAT[t], C6AcylCarMAT[t],
    C4AcylCarMAT[t], CoAMAT, C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t],
    C10AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t], C4AcylCoAMAT[t], CarMAT],
    vcpt2C14 → CPT2[sfcpt2C14, Vcpt2, Kmcp2C14AcylCarMAT, Kmcp2C16AcylCarMAT,
    Kmcp2C12AcylCarMAT, Kmcp2C10AcylCarMAT, Kmcp2C8AcylCarMAT, Kmcp2C6AcylCarMAT,
    Kmcp2C4AcylCoAMAT, Kmcp2CoAMAT, Kmcp2C14AcylCoAMAT, Kmcp2C16AcylCoAMAT,
    Kmcp2C12AcylCoAMAT, Kmcp2C10AcylCoAMAT, Kmcp2C8AcylCoAMAT, Kmcp2C6AcylCoAMAT,
    Kmcp2C4AcylCoAMAT, Kmcp2CarMAT, Keqcpt2, C14AcylCarMAT[t], C16AcylCarMAT[t],
    C12AcylCarMAT[t], C10AcylCarMAT[t], C8AcylCarMAT[t], C6AcylCarMAT[t],
    C4AcylCarMAT[t], CoAMAT, C14AcylCoAMAT[t], C16AcylCoAMAT[t], C12AcylCoAMAT[t],
    C10AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t], C4AcylCoAMAT[t], CarMAT],
}

```

$v_{cpt2C12} \rightarrow CPT2[sfcpt2C12, Vcpt2, Km cpt2C12AcylCarMAT, Km cpt2C16AcylCarMAT,$   
 $Km cpt2C14AcylCarMAT, Km cpt2C10AcylCarMAT, Km cpt2C8AcylCarMAT, Km cpt2C6AcylCarMAT,$   
 $Km cpt2C4AcylCarMAT, Km cpt2CoAMAT, Km cpt2C12AcylCoAMAT, Km cpt2C16AcylCoAMAT,$   
 $Km cpt2C14AcylCoAMAT, Km cpt2C10AcylCoAMAT, Km cpt2C8AcylCoAMAT, Km cpt2C6AcylCoAMAT,$   
 $Km cpt2C4AcylCoAMAT, Km cpt2CarMAT, Keqcpt2, C12AcylCarMAT[t], C16AcylCarMAT[t],$   
 $C14AcylCarMAT[t], C10AcylCarMAT[t], C8AcylCarMAT[t], C6AcylCarMAT[t],$   
 $C4AcylCarMAT[t], CoAMAT, C12AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t],$   
 $C10AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t], C4AcylCoAMAT[t], CarMAT],$   
 $v_{cpt2C10} \rightarrow CPT2[sfcpt2C10, Vcpt2, Km cpt2C10AcylCarMAT, Km cpt2C16AcylCarMAT,$   
 $Km cpt2C14AcylCarMAT, Km cpt2C12AcylCarMAT, Km cpt2C8AcylCarMAT, Km cpt2C6AcylCarMAT,$   
 $Km cpt2C4AcylCarMAT, Km cpt2CoAMAT, Km cpt2C10AcylCoAMAT, Km cpt2C16AcylCoAMAT,$   
 $Km cpt2C14AcylCoAMAT, Km cpt2C12AcylCoAMAT, Km cpt2C8AcylCoAMAT, Km cpt2C6AcylCoAMAT,$   
 $Km cpt2C4AcylCoAMAT, Km cpt2CarMAT, Keqcpt2, C10AcylCarMAT[t], C16AcylCarMAT[t],$   
 $C14AcylCarMAT[t], C12AcylCarMAT[t], C8AcylCarMAT[t], C6AcylCarMAT[t],$   
 $C4AcylCarMAT[t], CoAMAT, C10AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t],$   
 $C12AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t], C4AcylCoAMAT[t], CarMAT],$   
 $v_{cpt2C8} \rightarrow CPT2[sfcpt2C8, Vcpt2, Km cpt2C8AcylCarMAT, Km cpt2C16AcylCarMAT,$   
 $Km cpt2C14AcylCarMAT, Km cpt2C12AcylCarMAT, Km cpt2C10AcylCarMAT, Km cpt2C6AcylCarMAT,$   
 $Km cpt2C4AcylCarMAT, Km cpt2CoAMAT, Km cpt2C8AcylCoAMAT, Km cpt2C16AcylCoAMAT,$   
 $Km cpt2C14AcylCoAMAT, Km cpt2C12AcylCoAMAT, Km cpt2C10AcylCoAMAT, Km cpt2C6AcylCoAMAT,$   
 $Km cpt2C4AcylCoAMAT, Km cpt2CarMAT, Keqcpt2, C8AcylCarMAT[t], C16AcylCarMAT[t],$   
 $C14AcylCarMAT[t], C12AcylCarMAT[t], C10AcylCarMAT[t], C6AcylCarMAT[t],$   
 $C4AcylCarMAT[t], CoAMAT, C8AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t],$   
 $C12AcylCoAMAT[t], C10AcylCoAMAT[t], C6AcylCoAMAT[t], C4AcylCoAMAT[t], CarMAT],$   
 $v_{cpt2C6} \rightarrow CPT2[sfcpt2C6, Vcpt2, Km cpt2C6AcylCarMAT, Km cpt2C16AcylCarMAT,$   
 $Km cpt2C14AcylCarMAT, Km cpt2C12AcylCarMAT, Km cpt2C10AcylCarMAT, Km cpt2C8AcylCarMAT,$   
 $Km cpt2C4AcylCarMAT, Km cpt2CoAMAT, Km cpt2C6AcylCoAMAT, Km cpt2C16AcylCoAMAT,$   
 $Km cpt2C14AcylCoAMAT, Km cpt2C12AcylCoAMAT, Km cpt2C10AcylCoAMAT, Km cpt2C8AcylCoAMAT,$   
 $Km cpt2C4AcylCoAMAT, Km cpt2CarMAT, Keqcpt2, C6AcylCarMAT[t], C16AcylCarMAT[t],$   
 $C14AcylCarMAT[t], C12AcylCarMAT[t], C10AcylCarMAT[t], C8AcylCarMAT[t],$   
 $C4AcylCarMAT[t], CoAMAT, C6AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t],$   
 $C12AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t], C4AcylCoAMAT[t], CarMAT],$   
 $v_{cpt2C4} \rightarrow CPT2[sfcpt2C4, Vcpt2, Km cpt2C4AcylCarMAT, Km cpt2C16AcylCarMAT,$   
 $Km cpt2C14AcylCarMAT, Km cpt2C12AcylCarMAT, Km cpt2C10AcylCarMAT, Km cpt2C8AcylCarMAT,$   
 $Km cpt2C6AcylCarMAT, Km cpt2CoAMAT, Km cpt2C4AcylCoAMAT, Km cpt2C16AcylCoAMAT,$   
 $Km cpt2C14AcylCoAMAT, Km cpt2C12AcylCoAMAT, Km cpt2C10AcylCoAMAT, Km cpt2C8AcylCoAMAT,$   
 $Km cpt2C6AcylCoAMAT, Km cpt2CarMAT, Keqcpt2, C4AcylCarMAT[t], C16AcylCarMAT[t],$   
 $C14AcylCarMAT[t], C12AcylCarMAT[t], C10AcylCarMAT[t], C8AcylCarMAT[t],$   
 $C6AcylCarMAT[t], CoAMAT, C4AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t],$   
 $C12AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t], CarMAT],$   
 $v_{vlcadC16} \rightarrow VLCAD[sfvlcadC16, Vvlcad, Km vlcadC16AcylCoAMAT, Km vlcadC14AcylCoAMAT,$   
 $Km vlcadC12AcylCoAMAT, Km vlcadFAD, Km vlcadC16EnoylCoAMAT,$   
 $Km vlcadC14EnoylCoAMAT, Km vlcadC12EnoylCoAMAT, Km vlcadFADH, Keqvlcad,$   
 $C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t], FADtMAT,$   
 $C16EnoylCoAMAT[t], C14EnoylCoAMAT[t], C12EnoylCoAMAT[t], FADHMAT[t]],$   
 $v_{vlcadC14} \rightarrow VLCAD[sfvlcadC14, Vvlcad, Km vlcadC14AcylCoAMAT, Km vlcadC16AcylCoAMAT,$   
 $Km vlcadC12AcylCoAMAT, Km vlcadFAD, Km vlcadC14EnoylCoAMAT,$   
 $Km vlcadC16EnoylCoAMAT, Km vlcadC12EnoylCoAMAT, Km vlcadFADH, Keqvlcad,$   
 $C14AcylCoAMAT[t], C16AcylCoAMAT[t], C12AcylCoAMAT[t], FADtMAT,$   
 $C14EnoylCoAMAT[t], C16EnoylCoAMAT[t], C12EnoylCoAMAT[t], FADHMAT[t]],$   
 $v_{vlcadC12} \rightarrow VLCAD[sfvlcadC12, Vvlcad, Km vlcadC12AcylCoAMAT, Km vlcadC16AcylCoAMAT,$   
 $Km vlcadC14AcylCoAMAT, Km vlcadFAD, Km vlcadC12EnoylCoAMAT,$   
 $Km vlcadC16EnoylCoAMAT, Km vlcadC14EnoylCoAMAT, Km vlcadFADH, Keqvlcad,$   
 $C12AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t], FADtMAT,$   
 $C12EnoylCoAMAT[t], C16EnoylCoAMAT[t], C14EnoylCoAMAT[t], FADHMAT[t]],$

$v_{lcadC16} \rightarrow LCAD[sflcadC16, Vlcad, KmlcadC16AcylCoAMAT, KmlcadC14AcylCoAMAT,$   
 $KmlcadC12AcylCoAMAT, KmlcadC10AcylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadFAD,$   
 $KmlcadC16EnoylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC12EnoylCoAMAT,$   
 $KmlcadC10EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, Keqlcad,$   
 $C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t],$   
 $C8AcylCoAMAT[t], FADtMAT, C16EnoylCoAMAT[t], C14EnoylCoAMAT[t],$   
 $C12EnoylCoAMAT[t], C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], FADHMAT[t]],$   
 $v_{lcadC14} \rightarrow LCAD[sflcadC14, Vlcad, KmlcadC14AcylCoAMAT, KmlcadC16AcylCoAMAT,$   
 $KmlcadC12AcylCoAMAT, KmlcadC10AcylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadFAD,$   
 $KmlcadC14EnoylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC12EnoylCoAMAT,$   
 $KmlcadC10EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, Keqlcad,$   
 $C14AcylCoAMAT[t], C16AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t],$   
 $C8AcylCoAMAT[t], FADtMAT, C14EnoylCoAMAT[t], C16EnoylCoAMAT[t],$   
 $C12EnoylCoAMAT[t], C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], FADHMAT[t]],$   
 $v_{lcadC12} \rightarrow LCAD[sflcadC12, Vlcad, KmlcadC12AcylCoAMAT, KmlcadC16AcylCoAMAT,$   
 $KmlcadC14AcylCoAMAT, KmlcadC10AcylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadFAD,$   
 $KmlcadC12EnoylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC14EnoylCoAMAT,$   
 $KmlcadC10EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, Keqlcad,$   
 $C12AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t], C10AcylCoAMAT[t],$   
 $C8AcylCoAMAT[t], FADtMAT, C14EnoylCoAMAT[t], C16EnoylCoAMAT[t],$   
 $C14EnoylCoAMAT[t], C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], FADHMAT[t]],$   
 $v_{lcadC10} \rightarrow LCAD[sflcadC10, Vlcad, KmlcadC10AcylCoAMAT, KmlcadC16AcylCoAMAT,$   
 $KmlcadC14AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadFAD,$   
 $KmlcadC10EnoylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC14EnoylCoAMAT,$   
 $KmlcadC12EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, Keqlcad,$   
 $C10AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t],$   
 $C8AcylCoAMAT[t], FADtMAT, C10EnoylCoAMAT[t], C16EnoylCoAMAT[t],$   
 $C14EnoylCoAMAT[t], C12EnoylCoAMAT[t], C8EnoylCoAMAT[t], FADHMAT[t]],$   
 $v_{lcadC8} \rightarrow LCAD[sflcadC8, Vlcad, KmlcadC8AcylCoAMAT, KmlcadC16AcylCoAMAT,$   
 $KmlcadC14AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC10AcylCoAMAT, KmlcadFAD,$   
 $KmlcadC8EnoylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC14EnoylCoAMAT,$   
 $KmlcadC12EnoylCoAMAT, KmlcadC10EnoylCoAMAT, KmlcadFADH, Keqlcad,$   
 $C8AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t],$   
 $C10AcylCoAMAT[t], FADtMAT, C8EnoylCoAMAT[t], C16EnoylCoAMAT[t],$   
 $C14EnoylCoAMAT[t], C12EnoylCoAMAT[t], C10EnoylCoAMAT[t], FADHMAT[t]],$   
 $v_{mcadC12} \rightarrow MCAD[sfmcadC12, Vmcad, KmmcadC12AcylCoAMAT, KmmcadC10AcylCoAMAT,$   
 $KmmcadC8AcylCoAMAT, KmmcadC6AcylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadFAD,$   
 $KmmcadC12EnoylCoAMAT, KmmcadC10EnoylCoAMAT, KmmcadC8EnoylCoAMAT,$   
 $KmmcadC6EnoylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadFADH, Keqmcad,$   
 $C12AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t],$   
 $C4AcylCoAMAT[t], FADtMAT, C12EnoylCoAMAT[t], C10EnoylCoAMAT[t],$   
 $C8EnoylCoAMAT[t], C6EnoylCoAMAT[t], C4EnoylCoAMAT[t], FADHMAT[t]],$   
 $v_{mcadC10} \rightarrow MCAD[sfmcadC10, Vmcad, KmmcadC10AcylCoAMAT, KmmcadC12AcylCoAMAT,$   
 $KmmcadC8AcylCoAMAT, KmmcadC6AcylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadFAD,$   
 $KmmcadC10EnoylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC8EnoylCoAMAT,$   
 $KmmcadC6EnoylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadFADH, Keqmcad,$   
 $C10AcylCoAMAT[t], C12AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t],$   
 $C4AcylCoAMAT[t], FADtMAT, C10EnoylCoAMAT[t], C12EnoylCoAMAT[t],$   
 $C8EnoylCoAMAT[t], C6EnoylCoAMAT[t], C4EnoylCoAMAT[t], FADHMAT[t]],$   
 $v_{mcadC8} \rightarrow MCAD[sfmcadC8, Vmcad, KmmcadC8AcylCoAMAT, KmmcadC12AcylCoAMAT,$   
 $KmmcadC10AcylCoAMAT, KmmcadC6AcylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadFAD,$   
 $KmmcadC8EnoylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC10EnoylCoAMAT,$   
 $KmmcadC6EnoylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadFADH, Keqmcad,$   
 $C8AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t], C6AcylCoAMAT[t],$   
 $C4AcylCoAMAT[t], FADtMAT, C8EnoylCoAMAT[t], C12EnoylCoAMAT[t],$

C10EnoylCoAMAT[t], C6EnoylCoAMAT[t], C4EnoylCoAMAT[t], FADHMAT[t]],  
 vmcadC6 → MCAD[sfmcadC6, Vmcad, KmmcadC6AcylCoAMAT, KmmcadC12AcylCoAMAT,  
 KmmcadC10AcylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadFAD,  
 KmmcadC6EnoylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC10EnoylCoAMAT,  
 KmmcadC8EnoylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadFADH, Keqmcad,  
 C6AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t],  
 C4AcylCoAMAT[t], FADtMAT, C6EnoylCoAMAT[t], C12EnoylCoAMAT[t],  
 C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], C4EnoylCoAMAT[t], FADHMAT[t]],  
 vmcadC4 → MCAD[sfmcadC4, Vmcad, KmmcadC4AcylCoAMAT, KmmcadC12AcylCoAMAT,  
 KmmcadC10AcylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC6AcylCoAMAT, KmmcadFAD,  
 KmmcadC4EnoylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC10EnoylCoAMAT,  
 KmmcadC8EnoylCoAMAT, KmmcadC6EnoylCoAMAT, KmmcadFADH, Keqmcad,  
 C4AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t],  
 C6AcylCoAMAT[t], FADtMAT, C4EnoylCoAMAT[t], C12EnoylCoAMAT[t],  
 C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], C6EnoylCoAMAT[t], FADHMAT[t]],  
 vscadC6 → SCAD[sfscadC6, Vscad, KmscadC6AcylCoAMAT, KmscadC4AcylCoAMAT, KmscadFAD,  
 KmscadC6EnoylCoAMAT, KmscadC4EnoylCoAMAT, KmscadFADH, Keqscad, C6AcylCoAMAT[t],  
 C4AcylCoAMAT[t], FADtMAT, C6EnoylCoAMAT[t], C4EnoylCoAMAT[t], FADHMAT[t]],  
 vscadC4 → SCAD[sfscadC4, Vscad, KmscadC4AcylCoAMAT, KmscadC6AcylCoAMAT, KmscadFAD,  
 KmscadC4EnoylCoAMAT, KmscadC6EnoylCoAMAT, KmscadFADH, Keqscad, C4AcylCoAMAT[t],  
 C6AcylCoAMAT[t], FADtMAT, C4EnoylCoAMAT[t], C6EnoylCoAMAT[t], FADHMAT[t]],  
 vcrotC16 → CROT[sfcrotC16, Vcrot, KmcrotC16EnoylCoAMAT, KmcrotC14EnoylCoAMAT,  
 KmcrotC12EnoylCoAMAT, KmcrotC10EnoylCoAMAT, KmcrotC8EnoylCoAMAT,  
 KmcrotC6EnoylCoAMAT, KmcrotC4EnoylCoAMAT, KmcrotC16HydroxyacylCoAMAT,  
 KmcrotC14HydroxyacylCoAMAT, KmcrotC12HydroxyacylCoAMAT,  
 KmcrotC10HydroxyacylCoAMAT, KmcrotC8HydroxyacylCoAMAT,  
 KmcrotC6HydroxyacylCoAMAT, KmcrotC4HydroxyacylCoAMAT, KicrotC4AcetoacylCoA,  
 Keqcrot, C16EnoylCoAMAT[t], C14EnoylCoAMAT[t], C12EnoylCoAMAT[t],  
 C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], C6EnoylCoAMAT[t],  
 C4EnoylCoAMAT[t], C16HydroxyacylCoAMAT[t], C14HydroxyacylCoAMAT[t],  
 C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t], C8HydroxyacylCoAMAT[t],  
 C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
 vcrotC14 → CROT[sfcrotC14, Vcrot, KmcrotC14EnoylCoAMAT, KmcrotC16EnoylCoAMAT,  
 KmcrotC12EnoylCoAMAT, KmcrotC10EnoylCoAMAT, KmcrotC8EnoylCoAMAT,  
 KmcrotC6EnoylCoAMAT, KmcrotC4EnoylCoAMAT, KmcrotC14HydroxyacylCoAMAT,  
 KmcrotC16HydroxyacylCoAMAT, KmcrotC12HydroxyacylCoAMAT,  
 KmcrotC10HydroxyacylCoAMAT, KmcrotC8HydroxyacylCoAMAT,  
 KmcrotC6HydroxyacylCoAMAT, KmcrotC4HydroxyacylCoAMAT, KicrotC4AcetoacylCoA,  
 Keqcrot, C14EnoylCoAMAT[t], C16EnoylCoAMAT[t], C12EnoylCoAMAT[t],  
 C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], C6EnoylCoAMAT[t],  
 C4EnoylCoAMAT[t], C14HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t],  
 C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t], C8HydroxyacylCoAMAT[t],  
 C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
 vcrotC12 → CROT[sfcrotC12, Vcrot, KmcrotC12EnoylCoAMAT, KmcrotC16EnoylCoAMAT,  
 KmcrotC14EnoylCoAMAT, KmcrotC10EnoylCoAMAT, KmcrotC8EnoylCoAMAT,  
 KmcrotC6EnoylCoAMAT, KmcrotC4EnoylCoAMAT, KmcrotC12HydroxyacylCoAMAT,  
 KmcrotC16HydroxyacylCoAMAT, KmcrotC14HydroxyacylCoAMAT,  
 KmcrotC10HydroxyacylCoAMAT, KmcrotC8HydroxyacylCoAMAT,  
 KmcrotC6HydroxyacylCoAMAT, KmcrotC4HydroxyacylCoAMAT, KicrotC4AcetoacylCoA,  
 Keqcrot, C12EnoylCoAMAT[t], C16EnoylCoAMAT[t], C14EnoylCoAMAT[t],  
 C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], C6EnoylCoAMAT[t],  
 C4EnoylCoAMAT[t], C12HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t],  
 C14HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t], C8HydroxyacylCoAMAT[t],  
 C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
 vcrotC10 → CROT[sfcrotC10, Vcrot, KmcrotC10EnoylCoAMAT, KmcrotC16EnoylCoAMAT,

KmcrotC14EnoylCoAMAT, KmcrotC12EnoylCoAMAT, KmcrotC8EnoylCoAMAT,  
KmcrotC6EnoylCoAMAT, KmcrotC4EnoylCoAMAT, KmcrotC10HydroxyacylCoAMAT,  
KmcrotC16HydroxyacylCoAMAT, KmcrotC14HydroxyacylCoAMAT,  
KmcrotC12HydroxyacylCoAMAT, KmcrotC8HydroxyacylCoAMAT,  
KmcrotC6HydroxyacylCoAMAT, KmcrotC4HydroxyacylCoAMAT, KicrotC4AcetoacylCoA,  
Keqcrot, C10EnoylCoAMAT[t], C16EnoylCoAMAT[t], C14EnoylCoAMAT[t],  
C12EnoylCoAMAT[t], C8EnoylCoAMAT[t], C6EnoylCoAMAT[t],  
C4EnoylCoAMAT[t], C10HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t],  
C14HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C8HydroxyacylCoAMAT[t],  
C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
vcrotC8 → CROT[sfcrotC8, Vcrot, KmcrotC8EnoylCoAMAT, KmcrotC16EnoylCoAMAT,  
KmcrotC14EnoylCoAMAT, KmcrotC12EnoylCoAMAT, KmcrotC10EnoylCoAMAT,  
KmcrotC6EnoylCoAMAT, KmcrotC4EnoylCoAMAT, KmcrotC8HydroxyacylCoAMAT,  
KmcrotC16HydroxyacylCoAMAT, KmcrotC14HydroxyacylCoAMAT,  
KmcrotC12HydroxyacylCoAMAT, KmcrotC10HydroxyacylCoAMAT,  
KmcrotC6HydroxyacylCoAMAT, KmcrotC4HydroxyacylCoAMAT, KicrotC4AcetoacylCoA,  
Keqcrot, C8EnoylCoAMAT[t], C16EnoylCoAMAT[t], C14EnoylCoAMAT[t],  
C12EnoylCoAMAT[t], C10EnoylCoAMAT[t], C6EnoylCoAMAT[t],  
C4EnoylCoAMAT[t], C8HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t],  
C14HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t],  
C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
vcrotC6 → CROT[sfcrotC6, Vcrot, KmcrotC6EnoylCoAMAT, KmcrotC16EnoylCoAMAT,  
KmcrotC14EnoylCoAMAT, KmcrotC12EnoylCoAMAT, KmcrotC10EnoylCoAMAT,  
KmcrotC8EnoylCoAMAT, KmcrotC4EnoylCoAMAT, KmcrotC6HydroxyacylCoAMAT,  
KmcrotC16HydroxyacylCoAMAT, KmcrotC14HydroxyacylCoAMAT,  
KmcrotC12HydroxyacylCoAMAT, KmcrotC10HydroxyacylCoAMAT,  
KmcrotC8HydroxyacylCoAMAT, KmcrotC4HydroxyacylCoAMAT, KicrotC4AcetoacylCoA,  
Keqcrot, C6EnoylCoAMAT[t], C16EnoylCoAMAT[t], C14EnoylCoAMAT[t],  
C12EnoylCoAMAT[t], C10EnoylCoAMAT[t], C8EnoylCoAMAT[t],  
C4EnoylCoAMAT[t], C6HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t],  
C14HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t],  
C8HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
vcrotC4 → CROT[sfcrotC4, Vcrot, KmcrotC4EnoylCoAMAT, KmcrotC16EnoylCoAMAT,  
KmcrotC14EnoylCoAMAT, KmcrotC12EnoylCoAMAT, KmcrotC10EnoylCoAMAT,  
KmcrotC8EnoylCoAMAT, KmcrotC6EnoylCoAMAT, KmcrotC4HydroxyacylCoAMAT,  
KmcrotC16HydroxyacylCoAMAT, KmcrotC14HydroxyacylCoAMAT,  
KmcrotC12HydroxyacylCoAMAT, KmcrotC10HydroxyacylCoAMAT,  
KmcrotC8HydroxyacylCoAMAT, KmcrotC6HydroxyacylCoAMAT, KicrotC4AcetoacylCoA,  
Keqcrot, C4EnoylCoAMAT[t], C16EnoylCoAMAT[t], C14EnoylCoAMAT[t],  
C12EnoylCoAMAT[t], C10EnoylCoAMAT[t], C8EnoylCoAMAT[t],  
C6EnoylCoAMAT[t], C4HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t],  
C14HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t],  
C8HydroxyacylCoAMAT[t], C6HydroxyacylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
vmschadC16 → MSCHAD[sfmschadC16, Vmschad, KmmschadC16HydroxyacylCoAMAT,  
KmmschadC14HydroxyacylCoAMAT, KmmschadC12HydroxyacylCoAMAT,  
KmmschadC10HydroxyacylCoAMAT, KmmschadC8HydroxyacylCoAMAT,  
KmmschadC6HydroxyacylCoAMAT, KmmschadC4HydroxyacylCoAMAT,  
KmmschadNADMAT, KmmschadC16KetoacylCoAMAT, KmmschadC14KetoacylCoAMAT,  
KmmschadC12KetoacylCoAMAT, KmmschadC10KetoacylCoAMAT, KmmschadC8KetoacylCoAMAT,  
KmmschadC6KetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT, KmmschadNADHMAT,  
Keqmschad, C16HydroxyacylCoAMAT[t], C14HydroxyacylCoAMAT[t],  
C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t], C8HydroxyacylCoAMAT[t],  
C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], NADtMAT, C16KetoacylCoAMAT[t],  
C14KetoacylCoAMAT[t], C12KetoacylCoAMAT[t], C10KetoacylCoAMAT[t],  
C8KetoacylCoAMAT[t], C6KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], NADHMAT[t]],

vmschadC14 → MSCHAD [sfmschadC14, Vmschad, KmmschadC14HydroxyacylCoAMAT, KmmschadC16HydroxyacylCoAMAT, KmmschadC12HydroxyacylCoAMAT, KmmschadC10HydroxyacylCoAMAT, KmmschadC8HydroxyacylCoAMAT, KmmschadC6HydroxyacylCoAMAT, KmmschadC4HydroxyacylCoAMAT, KmmschadNADMAT, KmmschadC14KetoacylCoAMAT, KmmschadC16KetoacylCoAMAT, KmmschadC12KetoacylCoAMAT, KmmschadC10KetoacylCoAMAT, KmmschadC8KetoacylCoAMAT, KmmschadC6KetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT, KmmschadNADHMAT, Keqmschad, C14HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t], C8HydroxyacylCoAMAT[t], C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], NADtMAT, C14KetoacylCoAMAT[t], C16KetoacylCoAMAT[t], C12KetoacylCoAMAT[t], C10KetoacylCoAMAT[t], C8KetoacylCoAMAT[t], C6KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], NADHMAT[t]], vmschadC12 → MSCHAD [sfmschadC12, Vmschad, KmmschadC12HydroxyacylCoAMAT, KmmschadC16HydroxyacylCoAMAT, KmmschadC14HydroxyacylCoAMAT, KmmschadC10HydroxyacylCoAMAT, KmmschadC8HydroxyacylCoAMAT, KmmschadC6HydroxyacylCoAMAT, KmmschadC4HydroxyacylCoAMAT, KmmschadNADMAT, KmmschadC12KetoacylCoAMAT, KmmschadC16KetoacylCoAMAT, KmmschadC14KetoacylCoAMAT, KmmschadC10KetoacylCoAMAT, KmmschadC8KetoacylCoAMAT, KmmschadC6KetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT, KmmschadNADHMAT, Keqmschad, C12HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t], C14HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t], C8HydroxyacylCoAMAT[t], C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], NADtMAT, C12KetoacylCoAMAT[t], C16KetoacylCoAMAT[t], C14KetoacylCoAMAT[t], C10KetoacylCoAMAT[t], C8KetoacylCoAMAT[t], C6KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], NADHMAT[t]], vmschadC10 → MSCHAD [sfmschadC10, Vmschad, KmmschadC10HydroxyacylCoAMAT, KmmschadC16HydroxyacylCoAMAT, KmmschadC12HydroxyacylCoAMAT, KmmschadC8HydroxyacylCoAMAT, KmmschadC6HydroxyacylCoAMAT, KmmschadC4HydroxyacylCoAMAT, KmmschadNADMAT, KmmschadC10KetoacylCoAMAT, KmmschadC16KetoacylCoAMAT, KmmschadC14KetoacylCoAMAT, KmmschadC12KetoacylCoAMAT, KmmschadC8KetoacylCoAMAT, KmmschadC6KetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT, KmmschadNADHMAT, Keqmschad, C10HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t], C14HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C8HydroxyacylCoAMAT[t], C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], NADtMAT, C10KetoacylCoAMAT[t], C16KetoacylCoAMAT[t], C14KetoacylCoAMAT[t], C12KetoacylCoAMAT[t], C8KetoacylCoAMAT[t], C6KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], NADHMAT[t]], vmschadC8 → MSCHAD [sfmschadC8, Vmschad, KmmschadC8HydroxyacylCoAMAT, KmmschadC16HydroxyacylCoAMAT, KmmschadC14HydroxyacylCoAMAT, KmmschadC12HydroxyacylCoAMAT, KmmschadC10HydroxyacylCoAMAT, KmmschadC6HydroxyacylCoAMAT, KmmschadC4HydroxyacylCoAMAT, KmmschadNADMAT, KmmschadC8KetoacylCoAMAT, KmmschadC16KetoacylCoAMAT, KmmschadC14KetoacylCoAMAT, KmmschadC12KetoacylCoAMAT, KmmschadC10KetoacylCoAMAT, KmmschadC6KetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT, KmmschadNADHMAT, Keqmschad, C8HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t], C14HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t], C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], NADtMAT, C8KetoacylCoAMAT[t], C16KetoacylCoAMAT[t], C14KetoacylCoAMAT[t], C12KetoacylCoAMAT[t], C10KetoacylCoAMAT[t], C6KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], NADHMAT[t]], vmschadC6 → MSCHAD [sfmschadC6, Vmschad, KmmschadC6HydroxyacylCoAMAT, KmmschadC16HydroxyacylCoAMAT, KmmschadC12HydroxyacylCoAMAT, KmmschadC10HydroxyacylCoAMAT, KmmschadC8HydroxyacylCoAMAT, KmmschadNADMAT, KmmschadC6KetoacylCoAMAT, KmmschadC16KetoacylCoAMAT, KmmschadC14KetoacylCoAMAT, KmmschadC12KetoacylCoAMAT, KmmschadC10KetoacylCoAMAT, KmmschadC8KetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT, KmmschadNADHMAT,

Keqmschad, C6HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t],  
 C14HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t],  
 C8HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], NADtMAT, C6KetoacylCoAMAT[t],  
 C16KetoacylCoAMAT[t], C14KetoacylCoAMAT[t], C12KetoacylCoAMAT[t],  
 C10KetoacylCoAMAT[t], C8KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], NADHMAT[t]],  
 vmschadC4 → MSCHAD[sfmschadC4, Vmschad, KmmschadC4HydroxyacylCoAMAT,  
 KmmschadC16HydroxyacylCoAMAT, KmmschadC14HydroxyacylCoAMAT,  
 KmmschadC12HydroxyacylCoAMAT, KmmschadC10HydroxyacylCoAMAT,  
 KmmschadC8HydroxyacylCoAMAT, KmmschadC6HydroxyacylCoAMAT,  
 KmmschadNADMAT, KmmschadC4AcetoacylCoAMAT, KmmschadC16KetoacylCoAMAT,  
 KmmschadC14KetoacylCoAMAT, KmmschadC12KetoacylCoAMAT, KmmschadC10KetoacylCoAMAT,  
 KmmschadC8KetoacylCoAMAT, KmmschadC6KetoacylCoAMAT, KmmschadNADHMAT,  
 Keqmschad, C4HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t],  
 C14HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t],  
 C8HydroxyacylCoAMAT[t], C6HydroxyacylCoAMAT[t], NADtMAT, C4AcetoacylCoAMAT[t],  
 C16KetoacylCoAMAT[t], C14KetoacylCoAMAT[t], C12KetoacylCoAMAT[t],  
 C10KetoacylCoAMAT[t], C8KetoacylCoAMAT[t], C6KetoacylCoAMAT[t], NADHMAT[t]],  
 vmckatC16 → MCKATA[sfmckatC16, Vmckat, KmmckatC16KetoacylCoAMAT,  
 KmmckatC14KetoacylCoAMAT, KmmckatC12KetoacylCoAMAT,  
 KmmckatC10KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC6KetoacylCoAMAT,  
 KmmckatC4AcetoacylCoAMAT, KmmckatCoAMAT, KmmckatC14AcylCoAMAT,  
 KmmckatC16AcylCoAMAT, KmmckatC12AcylCoAMAT, KmmckatC10AcylCoAMAT,  
 KmmckatC8AcylCoAMAT, KmmckatC6AcylCoAMAT, KmmckatC4AcylCoAMAT,  
 KmmckatAcetylCoAMAT, Keqmckat, C16KetoacylCoAMAT[t], C14KetoacylCoAMAT[t],  
 C12KetoacylCoAMAT[t], C10KetoacylCoAMAT[t], C8KetoacylCoAMAT[t],  
 C6KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], CoAMAT, C14AcylCoAMAT[t],  
 C16AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t],  
 C6AcylCoAMAT[t], C4AcylCoAMAT[t], AcetylCoAMAT[t], CE1, KmCE1, nE1],  
 vmckatC14 → MCKATA[sfmckatC14, Vmckat, KmmckatC14KetoacylCoAMAT,  
 KmmckatC16KetoacylCoAMAT, KmmckatC12KetoacylCoAMAT,  
 KmmckatC10KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC6KetoacylCoAMAT,  
 KmmckatC4AcetoacylCoAMAT, KmmckatCoAMAT, KmmckatC12AcylCoAMAT,  
 KmmckatC16AcylCoAMAT, KmmckatC14AcylCoAMAT, KmmckatC10AcylCoAMAT,  
 KmmckatC8AcylCoAMAT, KmmckatC6AcylCoAMAT, KmmckatC4AcylCoAMAT,  
 KmmckatAcetylCoAMAT, Keqmckat, C14KetoacylCoAMAT[t], C16KetoacylCoAMAT[t],  
 C12KetoacylCoAMAT[t], C10KetoacylCoAMAT[t], C8KetoacylCoAMAT[t],  
 C6KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], CoAMAT, C12AcylCoAMAT[t],  
 C16AcylCoAMAT[t], C14AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t],  
 C6AcylCoAMAT[t], C4AcylCoAMAT[t], AcetylCoAMAT[t], CE1, KmCE1, nE1],  
 vmckatC12 → MCKATA[sfmckatC12, Vmckat, KmmckatC12KetoacylCoAMAT,  
 KmmckatC16KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT,  
 KmmckatC10KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC6KetoacylCoAMAT,  
 KmmckatC4AcetoacylCoAMAT, KmmckatCoAMAT, KmmckatC10AcylCoAMAT,  
 KmmckatC16AcylCoAMAT, KmmckatC14AcylCoAMAT, KmmckatC12AcylCoAMAT,  
 KmmckatC8AcylCoAMAT, KmmckatC6AcylCoAMAT, KmmckatC4AcylCoAMAT,  
 KmmckatAcetylCoAMAT, Keqmckat, C12KetoacylCoAMAT[t], C16KetoacylCoAMAT[t],  
 C14KetoacylCoAMAT[t], C10KetoacylCoAMAT[t], C8KetoacylCoAMAT[t],  
 C6KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], CoAMAT, C10AcylCoAMAT[t],  
 C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t], C8AcylCoAMAT[t],  
 C6AcylCoAMAT[t], C4AcylCoAMAT[t], AcetylCoAMAT[t], CE1, KmCE1, nE1],  
 vmckatC10 → MCKATA[sfmckatC10, Vmckat, KmmckatC10KetoacylCoAMAT,  
 KmmckatC16KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT,  
 KmmckatC12KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC6KetoacylCoAMAT,  
 KmmckatC4AcetoacylCoAMAT, KmmckatCoAMAT, KmmckatC8AcylCoAMAT,  
 KmmckatC16AcylCoAMAT, KmmckatC14AcylCoAMAT, KmmckatC12AcylCoAMAT,

KmmckatC10AcylCoAMAT, KmmckatC6AcylCoAMAT, KmmckatC4AcylCoAMAT,  
 KmmckatAcetylCoAMAT, Keqmckat, C10KetoacylCoAMAT[t], C16KetoacylCoAMAT[t],  
 C14KetoacylCoAMAT[t], C12KetoacylCoAMAT[t], C8KetoacylCoAMAT[t],  
 C6KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], CoAMAT, C8AcylCoAMAT[t],  
 C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t],  
 C6AcylCoAMAT[t], C4AcylCoAMAT[t], AcetylCoAMAT[t], CE1, KmCE1, nE1],  
 vmckatC8 → MCKATA [sfmckatC8, Vmckat, KmmckatC8KetoacylCoAMAT,  
 KmmckatC16KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT,  
 KmmckatC12KetoacylCoAMAT, KmmckatC10KetoacylCoAMAT, KmmckatC6KetoacylCoAMAT,  
 KmmckatC4AcetoacylCoAMAT, KmmckatCoAMAT, KmmckatC6AcylCoAMAT,  
 KmmckatC16AcylCoAMAT, KmmckatC14AcylCoAMAT, KmmckatC12AcylCoAMAT,  
 KmmckatC10AcylCoAMAT, KmmckatC8AcylCoAMAT, KmmckatC4AcylCoAMAT,  
 KmmckatAcetylCoAMAT, Keqmckat, C8KetoacylCoAMAT[t], C16KetoacylCoAMAT[t],  
 C14KetoacylCoAMAT[t], C12KetoacylCoAMAT[t], C10KetoacylCoAMAT[t],  
 C6KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], CoAMAT, C6AcylCoAMAT[t],  
 C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t],  
 C8AcylCoAMAT[t], C4AcylCoAMAT[t], AcetylCoAMAT[t], CE1, KmCE1, nE1],  
 vmckatC6 → MCKATA [sfmckatC6, Vmckat, KmmckatC6KetoacylCoAMAT,  
 KmmckatC16KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT,  
 KmmckatC12KetoacylCoAMAT, KmmckatC10KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT,  
 KmmckatC4AcetoacylCoAMAT, KmmckatCoAMAT, KmmckatC4AcylCoAMAT,  
 KmmckatC16AcylCoAMAT, KmmckatC14AcylCoAMAT, KmmckatC12AcylCoAMAT,  
 KmmckatC10AcylCoAMAT, KmmckatC8AcylCoAMAT, KmmckatC6AcylCoAMAT,  
 KmmckatAcetylCoAMAT, Keqmckat, C6KetoacylCoAMAT[t], C16KetoacylCoAMAT[t],  
 C14KetoacylCoAMAT[t], C12KetoacylCoAMAT[t], C10KetoacylCoAMAT[t],  
 C8KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], CoAMAT, C4AcylCoAMAT[t],  
 C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t],  
 C8AcylCoAMAT[t], C6AcylCoAMAT[t], AcetylCoAMAT[t], CE1, KmCE1, nE1],  
 vmckatC4 → MCKATB [sfmckatC4, Vmckat, KmmckatC4AcetoacylCoAMAT,  
 KmmckatC16KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT,  
 KmmckatC12KetoacylCoAMAT, KmmckatC10KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT,  
 KmmckatC6KetoacylCoAMAT, KmmckatCoAMAT, KmmckatC4AcylCoAMAT,  
 KmmckatC16AcylCoAMAT, KmmckatC14AcylCoAMAT, KmmckatC12AcylCoAMAT,  
 KmmckatC10AcylCoAMAT, KmmckatC8AcylCoAMAT, KmmckatC6AcylCoAMAT,  
 KmmckatAcetylCoAMAT, Keqmckat, C4AcetoacylCoAMAT[t], C16KetoacylCoAMAT[t],  
 C14KetoacylCoAMAT[t], C12KetoacylCoAMAT[t], C10KetoacylCoAMAT[t],  
 C8KetoacylCoAMAT[t], C6KetoacylCoAMAT[t], CoAMAT, C4AcylCoAMAT[t],  
 C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t],  
 C8AcylCoAMAT[t], C6AcylCoAMAT[t], AcetylCoAMAT[t], CE1, KmCE1, nE1],  
 vmtcpC16 → MTP [sfmtpC16, Vmtp, KmmtpC16EnoylCoAMAT, KmmtpC14EnoylCoAMAT,  
 KmmtpC12EnoylCoAMAT, KmmtpC10EnoylCoAMAT, KmmtpC8EnoylCoAMAT,  
 KmmtpNADMAT, KmmtpCoAMAT, KmmtpC14AcylCoAMAT, KmmtpC16AcylCoAMAT,  
 KmmtpC12AcylCoAMAT, KmmtpC10AcylCoAMAT, KmmtpC8AcylCoAMAT,  
 KmmtpC6AcylCoAMAT, KmmtpNADHMAT, KmmtpAcetylCoAMAT, KicrotC4AcetoacylCoA,  
 Keqntp, C16EnoylCoAMAT[t], C14EnoylCoAMAT[t], C12EnoylCoAMAT[t],  
 C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], NADtMAT, CoAMAT, C14AcylCoAMAT[t],  
 C16AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t],  
 C6AcylCoAMAT[t], NADHMAT[t], AcetylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
 vmtcpC14 → MTP [sfmtpC14, Vmtp, KmmtpC14EnoylCoAMAT, KmmtpC16EnoylCoAMAT,  
 KmmtpC12EnoylCoAMAT, KmmtpC10EnoylCoAMAT, KmmtpC8EnoylCoAMAT,  
 KmmtpNADMAT, KmmtpCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC16AcylCoAMAT,  
 KmmtpC14AcylCoAMAT, KmmtpC10AcylCoAMAT, KmmtpC8AcylCoAMAT,  
 KmmtpC6AcylCoAMAT, KmmtpNADHMAT, KmmtpAcetylCoAMAT, KicrotC4AcetoacylCoA,  
 Keqntp, C14EnoylCoAMAT[t], C16EnoylCoAMAT[t], C12EnoylCoAMAT[t],  
 C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], NADtMAT, CoAMAT, C12AcylCoAMAT[t],

C16AcylCoAMAT[t], C14AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t],  
 C6AcylCoAMAT[t], NADHMAT[t], AcetylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
 vmtcpC12 → MTP[sftpC12, Vmtp, KmmtpC12EnoylCoAMAT, KmmtpC16EnoylCoAMAT,  
 KmmtpC14EnoylCoAMAT, KmmtpC10EnoylCoAMAT, KmmtpC8EnoylCoAMAT,  
 KmmtpNADMAT, KmmtpCoAMAT, KmmtpC10AcylCoAMAT, KmmtpC16AcylCoAMAT,  
 KmmtpC14AcylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC8AcylCoAMAT,  
 KmmtpC6AcylCoAMAT, KmmtpNADHMAT, KmmtpAcetylCoAMAT, KicrotC4AcetoacylCoA,  
 Keqmtp, C12EnoylCoAMAT[t], C16EnoylCoAMAT[t], C14EnoylCoAMAT[t],  
 C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], NADtMAT, CoAMAT, C10AcylCoAMAT[t],  
 C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t], C8AcylCoAMAT[t],  
 C6AcylCoAMAT[t], NADHMAT[t], AcetylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
 vmtcp10 → MTP[sftpC10, Vmtp, KmmtpC10EnoylCoAMAT, KmmtpC16EnoylCoAMAT,  
 KmmtpC14EnoylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC8EnoylCoAMAT,  
 KmmtpNADMAT, KmmtpCoAMAT, KmmtpC8AcylCoAMAT, KmmtpC16AcylCoAMAT,  
 KmmtpC14AcylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC10AcylCoAMAT,  
 KmmtpC6AcylCoAMAT, KmmtpNADHMAT, KmmtpAcetylCoAMAT, KicrotC4AcetoacylCoA,  
 Keqmtp, C10EnoylCoAMAT[t], C16EnoylCoAMAT[t], C14EnoylCoAMAT[t],  
 C12EnoylCoAMAT[t], C8EnoylCoAMAT[t], NADtMAT, CoAMAT, C8AcylCoAMAT[t],  
 C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t],  
 C6AcylCoAMAT[t], NADHMAT[t], AcetylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
 vmtcp8 → MTP[sftpC8, Vmtp, KmmtpC8EnoylCoAMAT, KmmtpC16EnoylCoAMAT,  
 KmmtpC14EnoylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC10EnoylCoAMAT,  
 KmmtpNADMAT, KmmtpCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC16AcylCoAMAT,  
 KmmtpC14AcylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC10AcylCoAMAT,  
 KmmtpC8AcylCoAMAT, KmmtpNADHMAT, KmmtpAcetylCoAMAT, KicrotC4AcetoacylCoA,  
 Keqmtp, C8EnoylCoAMAT[t], C16EnoylCoAMAT[t], C14EnoylCoAMAT[t],  
 C12EnoylCoAMAT[t], C10EnoylCoAMAT[t], NADtMAT, CoAMAT, C6AcylCoAMAT[t],  
 C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t],  
 C8AcylCoAMAT[t], NADHMAT[t], AcetylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
 vacotC16 → ACOT[sfacotC16, Vmacot, KmacotC16CoA, KmacotC14CoA, KmacotC12CoA,  
 KmacotC10CoA, KmacotC8CoA, KmacotC6CoA, KmacotC4CoA, KmCoA, KmacotC16FFA,  
 KmacotC14FFA, KmacotC12FFA, KmacotC10FFA, KmacotC8FFA, KmacotC6FFA,  
 KmacotC4FFA, KeqacotC16, C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t],  
 C10AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t], C4AcylCoAMAT[t], CoAMAT,  
 C16FFA[t], C14FFA[t], C12FFA[t], C10FFA[t], C8FFA[t], C6FFA[t], C4FFA[t]],  
 vacotC14 → ACOT[sfacotC14, Vmacot, KmacotC14CoA, KmacotC16CoA, KmacotC12CoA,  
 KmacotC10CoA, KmacotC8CoA, KmacotC6CoA, KmacotC4CoA, KmCoA, KmacotC14FFA,  
 KmacotC16FFA, KmacotC12FFA, KmacotC10FFA, KmacotC8FFA, KmacotC6FFA,  
 KmacotC4FFA, KeqacotC14, C14AcylCoAMAT[t], C16AcylCoAMAT[t], C12AcylCoAMAT[t],  
 C10AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t], C4AcylCoAMAT[t], CoAMAT,  
 C14FFA[t], C16FFA[t], C12FFA[t], C10FFA[t], C8FFA[t], C6FFA[t], C4FFA[t]],  
 vacotC12 → ACOT[sfacotC12, Vmacot, KmacotC12CoA, KmacotC16CoA, KmacotC14CoA,  
 KmacotC10CoA, KmacotC8CoA, KmacotC6CoA, KmacotC4CoA, KmCoA, KmacotC12FFA,  
 KmacotC16FFA, KmacotC14FFA, KmacotC10FFA, KmacotC8FFA, KmacotC6FFA,  
 KmacotC4FFA, KeqacotC12, C12AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t],  
 C10AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t], C4AcylCoAMAT[t], CoAMAT,  
 C12FFA[t], C16FFA[t], C14FFA[t], C10FFA[t], C8FFA[t], C6FFA[t], C4FFA[t]],  
 vacotC10 → ACOT[sfacotC10, Vmacot, KmacotC10CoA, KmacotC16CoA, KmacotC14CoA,  
 KmacotC12CoA, KmacotC8CoA, KmacotC6CoA, KmacotC4CoA, KmCoA, KmacotC10FFA,  
 KmacotC16FFA, KmacotC14FFA, KmacotC12FFA, KmacotC8FFA, KmacotC6FFA,  
 KmacotC4FFA, KeqacotC10, C10AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t],  
 C12AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t], C4AcylCoAMAT[t], CoAMAT,  
 C10FFA[t], C16FFA[t], C14FFA[t], C12FFA[t], C8FFA[t], C6FFA[t], C4FFA[t]],  
 vacotC8 → ACOT[sfacotC8, Vmacot, KmacotC8CoA, KmacotC16CoA, KmacotC14CoA,  
 KmacotC12CoA, KmacotC10CoA, KmacotC6CoA, KmacotC4CoA, KmCoA, KmacotC8FFA,

```

KmacotC16FFA, KmacotC14FFA, KmacotC12FFA, KmacotC10FFA, KmacotC6FFA,
KmacotC4FFA, KeqacotC8, C8AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t],
C12AcylCoAMAT[t], C10AcylCoAMAT[t], C6AcylCoAMAT[t], C4AcylCoAMAT[t], CoAMAT,
C8FFA[t], C16FFA[t], C14FFA[t], C12FFA[t], C10FFA[t], C6FFA[t], C4FFA[t]],
vacotC6 → ACOT[sfacotC6, Vmacot, KmacotC6CoA, KmacotC16CoA, KmacotC14CoA,
KmacotC12CoA, KmacotC10CoA, KmacotC8CoA, KmacotC4CoA, KmCoA, KmacotC6FFA,
KmacotC16FFA, KmacotC14FFA, KmacotC12FFA, KmacotC10FFA, KmacotC8FFA,
KmacotC4FFA, KeqacotC6, C6AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t],
C12AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t], C4AcylCoAMAT[t], CoAMAT,
C6FFA[t], C16FFA[t], C14FFA[t], C12FFA[t], C10FFA[t], C8FFA[t], C4FFA[t]],
vacotC4 → ACOT[sfacotC4, Vmacot, KmacotC4CoA, KmacotC16CoA, KmacotC14CoA,
KmacotC12CoA, KmacotC10CoA, KmacotC8CoA, KmacotC6CoA, KmCoA, KmacotC4FFA,
KmacotC16FFA, KmacotC14FFA, KmacotC12FFA, KmacotC10FFA, KmacotC8FFA,
KmacotC6FFA, KeqacotC4, C4AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t],
C12AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t], CoAMAT,
C4FFA[t], C16FFA[t], C14FFA[t], C12FFA[t], C10FFA[t], C8FFA[t], C6FFA[t]],
vffaC16 → ExportRate[keFFA, C16FFA[t]]
vffaC14 → ExportRate[keFFA, C14FFA[t]]
vffaC12 → ExportRate[keFFA, C12FFA[t]]
vffaC10 → ExportRate[keFFA, C10FFA[t]]
vffaC8 → ExportRate[keFFA, C8FFA[t]]
vffaC6 → ExportRate[keFFA, C6FFA[t]],-
vffaC4 → ExportRate[keFFA, C4FFA[t]]
vacesink → RES[Ksacesink, AcetylCoAMAT[t], K1acesink],
vfadhsink → RES[Ksfadhsink, FADHMAT[t], K1fadhsink],
vnadhsink → RES[Ksnadhsink, NADHMAT[t], K1nadhsink}};

CoAMATX =
{CoAMAT → CoAMATT - C16AcylCoAMAT[t] - C16EnoylCoAMAT[t] - C16HydroxyacylCoAMAT[t] -
C16KetoacylCoAMAT[t] - C14AcylCoAMAT[t] - C14EnoylCoAMAT[t] -
C14HydroxyacylCoAMAT[t] - C14KetoacylCoAMAT[t] - C12AcylCoAMAT[t] -
C12EnoylCoAMAT[t] - C12HydroxyacylCoAMAT[t] - C12KetoacylCoAMAT[t] -
C10AcylCoAMAT[t] - C10EnoylCoAMAT[t] - C10HydroxyacylCoAMAT[t] -
C10KetoacylCoAMAT[t] - C8AcylCoAMAT[t] - C8EnoylCoAMAT[t] -
C8HydroxyacylCoAMAT[t] - C8KetoacylCoAMAT[t] - C6AcylCoAMAT[t] - C6EnoylCoAMAT[t] -
C6HydroxyacylCoAMAT[t] - C6KetoacylCoAMAT[t] - C4AcylCoAMAT[t] - C4EnoylCoAMAT[t] -
C4HydroxyacylCoAMAT[t] - C4AcetoacylCoAMAT[t] - AcetylCoAMAT[t]};

```

```

Parm = {
  sfcpt1C16 → 1, Vcpt1 → 0.012, Kmcpt1C16AcylCoACYT → 13.8,
  Kmcpt1CarCYT → 250, 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,
}

```

Kmcp2C10AcylCarMAT → 51, Kmcp2C8AcylCarMAT → 51, Kmcp2C6AcylCarMAT → 51,  
 Kmcp2C4AcylCarMAT → 51, Kmcp2CoAMAT → 30, Kmcp2C16AcylCoAMAT → 38,  
 Kmcp2C14AcylCoAMAT → 38, Kmcp2C12AcylCoAMAT → 38,  
 Kmcp2C10AcylCoAMAT → 38, Kmcp2C8AcylCoAMAT → 38, Kmcp2C6AcylCoAMAT → 1000,  
 Kmcp2C4AcylCoAMAT → 1000 000, Kmcp2CarMAT → 350, Keqcp2 → 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,  
 KmmcadcFAD → 0.12, Kmmcadc12EnoylCoAMAT → 1.08, Kmmcadc10EnoylCoAMAT → 1.08,  
 Kmmcadc8EnoylCoAMAT → 1.08, Kmmcadc6EnoylCoAMAT → 1.08,  
 Kmmcadc4EnoylCoAMAT → 1.08, KmmcadcFADH → 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, Vcrot → 3.6, KmrcrotC16EnoylCoAMAT → 150,  
 KmrcrotC14EnoylCoAMAT → 100, KmrcrotC12EnoylCoAMAT → 25, KmrcrotC10EnoylCoAMAT → 25,  
 KmrcrotC8EnoylCoAMAT → 25, KmrcrotC6EnoylCoAMAT → 25, KmrcrotC4EnoylCoAMAT → 40,  
 KmrcrotC16HydroxyacylCoAMAT → 45, KmrcrotC14HydroxyacylCoAMAT → 45,  
 KmrcrotC12HydroxyacylCoAMAT → 45, KmrcrotC10HydroxyacylCoAMAT → 45,  
 KmrcrotC8HydroxyacylCoAMAT → 45, KmrcrotC6HydroxyacylCoAMAT → 45,  
 KmrcrotC4HydroxyacylCoAMAT → 45, KicrotC4AcetoacylCoA → 1.6, Keqrcrot → 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, Keqmschad →  $2.17 \times 10^{-4}$ ,  
 sfmckatC16 → 0, 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, Keqmckat → 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,

$KmmtpNADMAT \rightarrow 60$ ,  $KmmtpCoAMAT \rightarrow 30$ ,  $KmmtpC14AcylCoAMAT \rightarrow 13.83$ ,  
 $KmmtpC16AcylCoAMAT \rightarrow 13.83$ ,  $KmmtpC12AcylCoAMAT \rightarrow 13.83$ ,  
 $KmmtpC10AcylCoAMAT \rightarrow 13.83$ ,  $KmmtpC8AcylCoAMAT \rightarrow 13.83$ ,  $KmmtpC6AcylCoAMAT \rightarrow 13.83$ ,  
 $KmmtpNADHMAT \rightarrow 50$ ,  $KmmtpAcetylCoAMAT \rightarrow 30$ ,  $Keqmt \rightarrow 0.71$ ,  
 $Vmacot \rightarrow 0.00371$ ,  $sfacotC16 \rightarrow 0.70$ ,  $sfacotC14 \rightarrow 0.86$ ,  $sfacotC12 \rightarrow 0.68$ ,  
 $sfacotC10 \rightarrow 1.0$ ,  $sfacotC8 \rightarrow 0.21$ ,  $sfacotC6 \rightarrow 0.55$ ,  $sfacotC4 \rightarrow 0.70$ ,  
 $KmacotC16CoA \rightarrow 10$ ,  $KmacotC14CoA \rightarrow 15.2$ ,  $KmacotC12CoA \rightarrow 27.5$ ,  $KmacotC10CoA \rightarrow 47.2$ ,  
 $KmacotC8CoA \rightarrow 150.89$ ,  $KmacotC6CoA \rightarrow 138.2$ ,  $KmacotC4CoA \rightarrow 1036.29$ ,  $KmCoA \rightarrow 9$ ,  
 $KmacotC16FFA \rightarrow 27\,000$ ,  $KmacotC14FFA \rightarrow 130\,000$ ,  $KmacotC12FFA \rightarrow 230\,000$ ,  
 $KmacotC10FFA \rightarrow 400\,000$ ,  $KmacotC8FFA \rightarrow 1\,300\,000$ ,  $KmacotC6FFA \rightarrow 350\,000\,000$ ,  
 $KmacotC4FFA \rightarrow 3\,000\,000$ ,  $KeqacotC16 \rightarrow 24\,000$ ,  $KeqacotC14 \rightarrow 76\,000$ ,  $KeqacotC12 \rightarrow 76\,000$ ,  
 $KeqacotC10 \rightarrow 76\,000$ ,  $KeqacotC8 \rightarrow 76\,000$ ,  $KeqacotC6 \rightarrow 76\,000$ ,  $KeqacotC4 \rightarrow 3\,000\,000$ ,  
 $keFFA \rightarrow 2 \times 10^{-6}$ ,  $keC14 \rightarrow 4 \times 10^{-6}$ ,  
 $Ksacesink \rightarrow 6\,000\,000$ ,  $K1acesink \rightarrow 70$ ,  $Ksfadhsink \rightarrow 6\,000\,000$ ,  
 $K1fadhsink \rightarrow 0.46$ ,  $Ksnadhsink \rightarrow 6\,000\,000$ ,  $K1nadhsink \rightarrow 12$ ,  
 $C16AcylCoACYT \rightarrow 25$ ,  $CarCYT \rightarrow 200$ ,  $CoACYT \rightarrow 140$ ,  $MalCoACYT \rightarrow 0$ ,  
 $CarMAT \rightarrow 950$ ,  $FADtMAT \rightarrow 0.77$ ,  $NADtMAT \rightarrow 250$ ,  $CoAMATt \rightarrow 5000$ ,  
 $VCYT \rightarrow 2.2 \times 10^{-6}$ ,  $VMAT \rightarrow 1.8 \times 10^{-6}$ ; }

InitialConditions = {  
 $C16AcylCarCYT[0] = 0$ ,  $C16AcylCarMAT[0] = 0$ ,  $C16AcylCoAMAT[0] = 0$ ,  
 $C16EnoylCoAMAT[0] = 0$ ,  $C16HydroxyacylCoAMAT[0] = 0$ ,  $C16KetoacylCoAMAT[0] = 0$ ,  
 $C14AcylCarCYT[0] = 0$ ,  $C14AcylCarMAT[0] = 0$ ,  $C14AcylCoAMAT[0] = 0$ ,  
 $C14EnoylCoAMAT[0] = 0$ ,  $C14HydroxyacylCoAMAT[0] = 0$ ,  $C14KetoacylCoAMAT[0] = 0$ ,  
 $C12AcylCarCYT[0] = 0$ ,  $C12AcylCarMAT[0] = 0$ ,  $C12AcylCoAMAT[0] = 0$ ,  
 $C12EnoylCoAMAT[0] = 0$ ,  $C12HydroxyacylCoAMAT[0] = 0$ ,  $C12KetoacylCoAMAT[0] = 0$ ,  
 $C10AcylCarCYT[0] = 0$ ,  $C10AcylCarMAT[0] = 0$ ,  $C10AcylCoAMAT[0] = 0$ ,  
 $C10EnoylCoAMAT[0] = 0$ ,  $C10HydroxyacylCoAMAT[0] = 0$ ,  $C10KetoacylCoAMAT[0] = 0$ ,  
 $C8AcylCarCYT[0] = 0$ ,  $C8AcylCarMAT[0] = 0$ ,  $C8AcylCoAMAT[0] = 0$ ,  
 $C8EnoylCoAMAT[0] = 0$ ,  $C8HydroxyacylCoAMAT[0] = 0$ ,  $C8KetoacylCoAMAT[0] = 0$ ,  
 $C6AcylCarCYT[0] = 0$ ,  $C6AcylCarMAT[0] = 0$ ,  $C6AcylCoAMAT[0] = 0$ ,  
 $C6EnoylCoAMAT[0] = 0$ ,  $C6HydroxyacylCoAMAT[0] = 0$ ,  $C6KetoacylCoAMAT[0] = 0$ ,  
 $C4AcylCarCYT[0] = 0$ ,  $C4AcylCarMAT[0] = 0$ ,  $C4AcylCoAMAT[0] = 0$ ,  
 $C4EnoylCoAMAT[0] = 0$ ,  $C4HydroxyacylCoAMAT[0] = 0$ ,  $C4AcetoacylCoAMAT[0] = 0$ ,  
 $AcetylCoAMAT[0] = 70$ ,  $FADHMAT[0] = 0.46$ ,  $NADHMAT[0] = 12$ ,  
 $C16FFA[0] = 0$ ,  $C14FFA[0] = 0$ ,  $C12FFA[0] = 0$ ,  
 $C10FFA[0] = 0$ ,  $C8FFA[0] = 0$ ,  $C6FFA[0] = 0$ ,  $C4FFA[0] = 0$ ; }

Vars = {  
 $C16AcylCarCYT$ ,  $C16AcylCarMAT$ ,  $C16AcylCoAMAT$ ,  
 $C16EnoylCoAMAT$ ,  $C16HydroxyacylCoAMAT$ ,  $C16KetoacylCoAMAT$ ,  
 $C14AcylCarCYT$ ,  $C14AcylCarMAT$ ,  $C14AcylCoAMAT$ ,  $C14EnoylCoAMAT$ ,  
 $C14HydroxyacylCoAMAT$ ,  $C14KetoacylCoAMAT$ ,  
 $C12AcylCarCYT$ ,  $C12AcylCarMAT$ ,  $C12AcylCoAMAT$ ,  $C12EnoylCoAMAT$ ,  
 $C12HydroxyacylCoAMAT$ ,  $C12KetoacylCoAMAT$ ,  
 $C10AcylCarCYT$ ,  $C10AcylCarMAT$ ,  $C10AcylCoAMAT$ ,  $C10EnoylCoAMAT$ ,  
 $C10HydroxyacylCoAMAT$ ,  $C10KetoacylCoAMAT$ ,  
 $C8AcylCarCYT$ ,  $C8AcylCarMAT$ ,  $C8AcylCoAMAT$ ,  $C8EnoylCoAMAT$ ,  
 $C8HydroxyacylCoAMAT$ ,  $C8KetoacylCoAMAT$ ,  
 $C6AcylCarCYT$ ,  $C6AcylCarMAT$ ,  $C6AcylCoAMAT$ ,  $C6EnoylCoAMAT$ ,  
 $C6HydroxyacylCoAMAT$ ,  $C6KetoacylCoAMAT$ ,  
 $C4AcylCarCYT$ ,  $C4AcylCarMAT$ ,  $C4AcylCoAMAT$ ,  $C4EnoylCoAMAT$ ,  
 $C4HydroxyacylCoAMAT$ ,  $C4AcetoacylCoAMAT$ ,  
 $AcetylCoAMAT$ ,  $FADHMAT$ ,  $NADHMAT$ ,  
 $C16FFA$ ,  $C14FFA$ ,  $C12FFA$ ,  $C10FFA$ ,  $C8FFA$ ,  $C6FFA$ ,  $C4FFA$ ; }

```

In[]:= TableForm[Odes];
TableForm[RateEqs];
TableForm[Odes /. RateEqs /. CoAMATX /. Parm];
TableForm[RateEqs /. Parm];
TableForm[InitialConditions];

In[]:= tsol = NDSolve[Join[Odes /. RateEqs /. CoAMATX /. Parm, InitialConditions],
Vars, {t, 0, 1000000000}];

In[]:= Table[{Vars[[i]][t], (Vars[[i]][900000000] /. tsol)[[1]]}, {i, 1, Length[Vars]}]

Out[]= {{C16AcylCarCYT[t], 0.167871}, {C16AcylCarMAT[t], 0.355364},
{C16AcylCoAMAT[t], 0.870444}, {C16EnoylCoAMAT[t], 0.0485765},
{C16HydroxyacylCoAMAT[t], 0.152044}, {C16KetoacylCoAMAT[t], 0.000654373},
{C14AcylCarCYT[t], 0.0372737}, {C14AcylCarMAT[t], 0.17705},
{C14AcylCoAMAT[t], 1.92851}, {C14EnoylCoAMAT[t], 0.0542268},
{C14HydroxyacylCoAMAT[t], 0.154025}, {C14KetoacylCoAMAT[t], 0.000662217},
{C12AcylCarCYT[t], 0.0508391}, {C12AcylCarMAT[t], 0.241486},
{C12AcylCoAMAT[t], 2.63037}, {C12EnoylCoAMAT[t], 0.0618663},
{C12HydroxyacylCoAMAT[t], 0.187162}, {C12KetoacylCoAMAT[t], 0.000802167},
{C10AcylCarCYT[t], 0.0912553}, {C10AcylCarMAT[t], 0.433463},
{C10AcylCoAMAT[t], 4.72147}, {C10EnoylCoAMAT[t], 0.0680884},
{C10HydroxyacylCoAMAT[t], 0.207337}, {C10KetoacylCoAMAT[t], 0.00088605},
{C8AcylCarCYT[t], 0.0936016}, {C8AcylCarMAT[t], 0.444608}, {C8AcylCoAMAT[t], 4.84287},
{C8EnoylCoAMAT[t], 0.147599}, {C8HydroxyacylCoAMAT[t], 0.456175},
{C8KetoacylCoAMAT[t], 0.00194848}, {C6AcylCarCYT[t], 0.248461},
{C6AcylCarMAT[t], 1.18019}, {C6AcylCoAMAT[t], 12.8552}, {C6EnoylCoAMAT[t], 11.0793},
{C6HydroxyacylCoAMAT[t], 34.4789}, {C6KetoacylCoAMAT[t], 0.147256},
{C4AcylCarCYT[t], 0.412546}, {C4AcylCarMAT[t], 1.95959}, {C4AcylCoAMAT[t], 21.3448},
{C4EnoylCoAMAT[t], 41.6664}, {C4HydroxyacylCoAMAT[t], 130.151},
{C4AcetoacylCoAMAT[t], 0.556006}, {AcetylCoAMAT[t], 70.},
{FADHMAT[t], 0.46}, {NADHMAT[t], 12.}, {C16FFA[t], 0.135803},
{C14FFA[t], 0.248805}, {C12FFA[t], 0.148975}, {C10FFA[t], 0.229231},
{C8FFA[t], 0.0154885}, {C6FFA[t], 0.117523}, {C4FFA[t], 0.033139}}

```

## Steady state computation by varying palmitoyl-CoA with ACOT extension

```

In[]:= ParmScan[X_] := {
sfcpt1C16 → 1, Vcpt1 → 0.012, Kmcpt1C16AcylCoACYT → 13.8,
Kmcpt1CarCYT → 250, 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,
}

```

Kmcp2C14AcylCoAMAT → 38, Kmcp2C12AcylCoAMAT → 38,  
 Kmcp2C10Acy1CoAMAT → 38, Kmcp2C8Acyl1CoAMAT → 38, Kmcp2C6AcylCoAMAT → 1000,  
 Kmcp2C4AcylCoAMAT → 1000 000, Kmcp2CarMAT → 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,  
 KmmcadcFAD → 0.12, Kmmcadc12EnoylCoAMAT → 1.08, Kmmcadc10EnoylCoAMAT → 1.08,  
 Kmmcadc8EnoylCoAMAT → 1.08, Kmmcadc6EnoylCoAMAT → 1.08,  
 Kmmcadc4EnoylCoAMAT → 1.08, KmmcadcFADH → 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,  
 sfcrotC16 → 0.13, sfcrotC14 → 0.2, sfcrotC12 → 0.25, sfcrotC10 → 0.33, sfcrotC8 → 0.58,  
 sfcrotC6 → 0.83, sfcrotC4 → 1, Vcrot → 3.6, KmrcrotC16EnoylCoAMAT → 150,  
 KmrcrotC14EnoylCoAMAT → 100, KmrcrotC12EnoylCoAMAT → 25, KmrcrotC10EnoylCoAMAT → 25,  
 KmrcrotC8EnoylCoAMAT → 25, KmrcrotC6EnoylCoAMAT → 25, KmrcrotC4EnoylCoAMAT → 40,  
 KmrcrotC16HydroxyacylCoAMAT → 45, KmrcrotC14HydroxyacylCoAMAT → 45,  
 KmrcrotC12HydroxyacylCoAMAT → 45, KmrcrotC10HydroxyacylCoAMAT → 45,  
 KmrcrotC8HydroxyacylCoAMAT → 45, KmrcrotC6HydroxyacylCoAMAT → 45,  
 KmrcrotC4HydroxyacylCoAMAT → 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, Keqmschad →  $2.17 \times 10^{-4}$ ,  
 sfmckatC16 → 0, 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,  
 KmmckatC8Acyl1CoAMAT → 13.83, KmmckatC6AcylCoAMAT → 13.83,  
 KmmckatC4AcylCoAMAT → 13.83, KmmckatAcetylCoAMAT → 30, Keqmckat → 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, Keqmt → 0.71,
Vmacot → 0.00371, sfacotC16 → 0.70, sfacotC14 → 0.86, sfacotC12 → 0.68,
sfacotC10 → 1.0, sfacotC8 → 0.21, sfacotC6 → 0.55, sfacotC4 → 0.70,
KmacotC16CoA → 10, KmacotC14CoA → 15.2, KmacotC12CoA → 27.5, KmacotC10CoA → 47.2,
KmacotC8CoA → 150.89, KmacotC6CoA → 138.2, KmacotC4CoA → 1036.29, KmCoA → 9,
KmacotC16FFA → 27 000, KmacotC14FFA → 130 000, KmacotC12FFA → 230 000,
KmacotC10FFA → 400 000, KmacotC8FFA → 1 300 000, KmacotC6FFA → 350 000 000,
KmacotC4FFA → 3 000 000, KeqacotC16 → 24 000, KeqacotC14 → 76 000, KeqacotC12 → 76 000,
KeqacotC10 → 76 000, KeqacotC8 → 76 000, KeqacotC6 → 76 000, KeqacotC4 → 3 000 000,
keFFA → 2 * 10-6, keC14 → 4 * 10-6,
Ksacesink → 6 000 000, K1acesink → 70, Ksfadhsink → 6 000 000,
K1fadhsink → 0.46, Ksnadhsink → 6 000 000, K1nadhsink → 12,
C16AcylCoACYT → X, CarCYT → 200, CoACYT → 140, MalCoACYT → 0,
CarMAT → 950, FADtMAT → 0.77, NADtMAT → 250, CoAMATt → 5000,
VCYT → 2.2 * 10-6, VMAT → 1.8 * 10-6};
```

```

tsolScan[X_] :=
NDSolve[Join[Odes /. RateEqs /. CoAMATX /. ParmScan[X], InitialConditions],
Vars, {t, 0, 1000 000 000}];
```

```

SsScan[X_] := Module[{SSGuess},
SSGuess := Table[{Vars[[i]] [t],
(Vars[[i]] [900 000 000] /. tsolScan[X]) [[1]]}, {i, 1, Length[Vars]}];
FindRoot[Table[Odes[[i, 2]] == 0, {i, 1, Length[Odes]}] /. RateEqs /. CoAMATX /.
ParmScan[X], SSGuess]]
```

In[1]:=

```

In[2]:= ScanDownNDS[Xstart_, dX_, Xend_] := Monitor[Module[{SS, SSGuess},
DataDownNDSfluxacot = {};
DataDownNDScconc = {};
DataDownNDSc4coa = {};
DataDownNDSc6coa = {};
DataDownNDSc4c6coa = {};
DataDownNDScintermedcoa = {};
DataDownNDSfreecoa = {};

DataDownNDSvacesink = {};
DataDownNDSvfadhsink = {};
DataDownNDSvnadhsinkACOT = {};
DataDownNDSvacotC4 = {};
DataDownNDSvacotC6 = {};
DataDownNDSvacotC8 = {};
DataDownNDSvacotC10 = {};
DataDownNDSvacotC12 = {};
DataDownNDSvacotC14 = {};
DataDownNDSvacotC16 = {};
tsolStart = tsolScan[Xend];
SSGuess = Table[{Vars[[i]] [t],
(Vars[[i]] [900 000 000] /. tsolStart) [[1]]}, {i, 1, Length[Vars]}];
SSGuess1 = SSGuess[[All, 1]];
SSGuess2 = SSGuess[[All, 2]];
SSGuess1int = SSGuess1 /. t → 0;
```

```

InitialConditionsUD = Thread[SSGuess1int == SSGuess2];

For[X = Xend, X ≥ Xstart,
  tsolScanNDS = NDSolve[Join[Odes /. RateEqs /. CoAMATX /. ParmScan[X],
    InitialConditionsUD], Vars, {t, 0, 1000000000}];
  SSGuess = Table[{Vars[[i]][t], (Vars[[i]][900000000] /. tsolScanNDS)[[1]]},
    {i, 1, Length[Vars]}];
  SSGuess1 = SSGuess[[All, 1]];
  SSGuess2 = SSGuess[[All, 2]];
  SSGuess1int = SSGuess1 /. t → 0;
  InitialConditionsUD = Thread[SSGuess1int == SSGuess2];
  SS = Thread[SSGuess1 → SSGuess2];

c4coa = C4AcylCoAMAT[t] + C4EnoylCoAMAT[t] +
  C4HydroxyacylCoAMAT[t] + C4AcetoacylCoAMAT[t] /. SS;
c6coa = C6AcylCoAMAT[t] + C6EnoylCoAMAT[t] + C6HydroxyacylCoAMAT[t] +
  C6KetoacylCoAMAT[t] /. SS;
c4c6coa = c4coa + c6coa;
intermediatecoa =
  C4AcylCoAMAT[t] + C4EnoylCoAMAT[t] + C4HydroxyacylCoAMAT[t] + C4AcetoacylCoAMAT[t] +
  C6AcylCoAMAT[t] + C6EnoylCoAMAT[t] + C6HydroxyacylCoAMAT[t] +
  C6KetoacylCoAMAT[t] + C8AcylCoAMAT[t] + C8EnoylCoAMAT[t] +
  C8HydroxyacylCoAMAT[t] + C8KetoacylCoAMAT[t] + C10AcylCoAMAT[t] +
  C10EnoylCoAMAT[t] + C10HydroxyacylCoAMAT[t] + C10KetoacylCoAMAT[t] +
  C12AcylCoAMAT[t] + C12EnoylCoAMAT[t] + C12HydroxyacylCoAMAT[t] +
  C12KetoacylCoAMAT[t] + C14AcylCoAMAT[t] + C14EnoylCoAMAT[t] +
  C14HydroxyacylCoAMAT[t] + C14KetoacylCoAMAT[t] + C16AcylCoAMAT[t] +
  C16EnoylCoAMAT[t] + C16HydroxyacylCoAMAT[t] + C16KetoacylCoAMAT[t] /. SS;
freeCoa = CoAMATt - intermediatecoa - 70 /. CoAMATX /. ParmScan[X] /. SS;

C16AcylCarnitineCYT = C16AcylCarCYT[t] /. SS;
C14AcylCarnitineCYT = C14AcylCarCYT[t] /. SS;
C12AcylCarnitineCYT = C12AcylCarCYT[t] /. SS;
C10AcylCarnitineCYT = C10AcylCarCYT[t] /. SS;
C8AcylCarnitineCYT = C8AcylCarCYT[t] /. SS;
C6AcylCarnitineCYT = C6AcylCarCYT[t] /. SS;
C4AcylCarnitineCYT = C4AcylCarCYT[t] /. SS;

AppendTo[DataDownNDSfluxacot,
  {X, 10^3 vcactC16 /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
AppendTo[DataDownNDSc4coa, {X, c4coa}];
AppendTo[DataDownNDSc6coa, {X, c6coa}];
AppendTo[DataDownNDSc4c6coa, {X, c4c6coa}];
AppendTo[DataDownNDScintermedcoa, {X, intermediatecoa}];
AppendTo[DataDownNDSfreecoa, {X, freeCoa}];

AppendTo[DataDownNDSvacesink,
  {X, 10^3 vacesink /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
AppendTo[DataDownNDScfadhsink,
  {X, 10^3 vfadhsink /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
AppendTo[DataDownNDScnadhsinkACOT,
  {X, 10^3 vnadhsink /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];

```

```

AppendTo[DataDownNDSvacotC16,
{X, 103 vacotC16 /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
AppendTo[DataDownNDSvacotC14,
{X, 103 vacotC14 /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
AppendTo[DataDownNDSvacotC12,
{X, 103 vacotC12 /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
AppendTo[DataDownNDSvacotC10,
{X, 103 vacotC10 /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
AppendTo[DataDownNDSvacotC8,
{X, 103 vacotC8 /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
AppendTo[DataDownNDSvacotC6,
{X, 103 vacotC6 /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
AppendTo[DataDownNDSvacotC4,
{X, 103 vacotC4 /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
X = X - dX;
], ProgressIndicator[X, {Xstart, Xend}]]

```

In[6]:= ScanDownNDS[0, 1, 250]

```

In[6]:= ScanUpNDS[Xstart_, dX_, Xend_] := Monitor[Module[{SS, SSGuess},
DataUpNDSfluxacot = {};
DataUpNDSconc = {};
DataUpNDSc4coa = {};
DataUpNDSc6coa = {};
DataUpNDSc4c6coa = {};
DataUpNDScintermedcoa = {};
DataUpNDSfreecoa = {};

DataUpNDSvacesink = {};
DataUpNDSvfadhsink = {};
DataUpNDSvnadhsinkACOT = {};
DataUpNDSvacotC4 = {};
DataUpNDSvacotC6 = {};
DataUpNDSvacotC8 = {};
DataUpNDSvacotC10 = {};
DataUpNDSvacotC12 = {};
DataUpNDSvacotC14 = {};
DataUpNDSvacotC16 = {};
tsolStart = tsolScan[Xstart];
SSGuess = Table[{Vars[[i]][t],
(Vars[[i]][900000000] /. tsolStart)[[1]]}, {i, 1, Length[Vars]}];
SSGuess1 = SSGuess[[All, 1]];
SSGuess2 = SSGuess[[All, 2]];
SSGuess1int = SSGuess1 /. t → 0;
InitialConditionsUD = Thread[SSGuess1int == SSGuess2];

For[X = Xstart, X ≤ Xend,

```

```

tsolScanNDS = NDSolve[Join[Odes /. RateEqs /. CoAMATX /. ParmScan[X],
  InitialConditionsUD], Vars, {t, 0, 1000000000}];
SSGuess = Table[{Vars[[i]][t], (Vars[[i]][900000000] /. tsolScanNDS)[[1]]},
  {i, 1, Length[Vars]}];
SSGuess1 = SSGuess[[All, 1]];
SSGuess2 = SSGuess[[All, 2]];
SSGuess1int = SSGuess1 /. t → 0;
InitialConditionsUD = Thread[SSGuess1int == SSGuess2];
SS = Thread[SSGuess1 → SSGuess2];

c4coa = C4AcylCoAMAT[t] + C4EnoylCoAMAT[t] +
  C4HydroxyacylCoAMAT[t] + C4AcetoacylCoAMAT[t] /. SS;
c6coa = C6AcylCoAMAT[t] + C6EnoylCoAMAT[t] + C6HydroxyacylCoAMAT[t] +
  C6KetoacylCoAMAT[t] /. SS;
c4c6coa = c4coa + c6coa;
intermediatecoa =
  C4AcylCoAMAT[t] + C4EnoylCoAMAT[t] + C4HydroxyacylCoAMAT[t] + C4AcetoacylCoAMAT[t] +
  C6AcylCoAMAT[t] + C6EnoylCoAMAT[t] + C6HydroxyacylCoAMAT[t] +
  C6KetoacylCoAMAT[t] + C8AcylCoAMAT[t] + C8EnoylCoAMAT[t] +
  C8HydroxyacylCoAMAT[t] + C8KetoacylCoAMAT[t] + C10AcylCoAMAT[t] +
  C10EnoylCoAMAT[t] + C10HydroxyacylCoAMAT[t] + C10KetoacylCoAMAT[t] +
  C12AcylCoAMAT[t] + C12EnoylCoAMAT[t] + C12HydroxyacylCoAMAT[t] +
  C12KetoacylCoAMAT[t] + C14AcylCoAMAT[t] + C14EnoylCoAMAT[t] +
  C14HydroxyacylCoAMAT[t] + C14KetoacylCoAMAT[t] + C16AcylCoAMAT[t] +
  C16EnoylCoAMAT[t] + C16HydroxyacylCoAMAT[t] + C16KetoacylCoAMAT[t] /. SS;
freeCoa = CoAMATt - intermediatecoa - 70 /. CoAMATX /. ParmScan[X] /. SS;

C16AcylCarnitineCYT = C16AcylCarCYT[t] /. SS;
C14AcylCarnitineCYT = C14AcylCarCYT[t] /. SS;
C12AcylCarnitineCYT = C12AcylCarCYT[t] /. SS;
C10AcylCarnitineCYT = C10AcylCarCYT[t] /. SS;
C8AcylCarnitineCYT = C8AcylCarCYT[t] /. SS;
C6AcylCarnitineCYT = C6AcylCarCYT[t] /. SS;
C4AcylCarnitineCYT = C4AcylCarCYT[t] /. SS;

AppendTo[DataUpNDSfluxacot,
{X, 10^3 vcactC16 /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
AppendTo[DataUpNDSc4coa, {X, c4coa}];
AppendTo[DataUpNDSc6coa, {X, c6coa}];
AppendTo[DataUpNDSc4c6coa, {X, c4c6coa}];
AppendTo[DataUpNDScintermedcoa, {X, intermediatecoa}];
AppendTo[DataUpNDScfreeCoa, {X, freeCoa}];

AppendTo[DataUpNDSvacesink,
{X, 10^3 vacesink /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
AppendTo[DataUpNDScfadhsink,
{X, 10^3 vfadhsink /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
AppendTo[DataUpNDScvnadhsinkACOT,
{X, 10^3 vnadhsink /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
AppendTo[DataUpNDScvacotC16, {X,
  10^3 vacotC16 /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];

```

```

AppendTo[DataUpNDSvacotC14, {X, 103 vacotC14 /. RateEqs /. CoAMATX /.
  ParmScan[X] /. SS}];
AppendTo[DataUpNDSvacotC12, {X, 103 vacotC12 /. RateEqs /. CoAMATX /.
  ParmScan[X] /. SS}];
AppendTo[DataUpNDSvacotC10, {X, 103 vacotC10 /. RateEqs /. CoAMATX /.
  ParmScan[X] /. SS}];
AppendTo[DataUpNDSvacotC8, {X, 103 vacotC8 /. RateEqs /. CoAMATX /.
  ParmScan[X] /. SS}];
AppendTo[DataUpNDSvacotC6, {X, 103 vacotC6 /. RateEqs /. CoAMATX /.
  ParmScan[X] /. SS}];
AppendTo[DataUpNDSvacotC4, {X, 103 vacotC4 /. RateEqs /. CoAMATX /.
  ParmScan[X] /. SS}];
X = X + dX;
], ProgressIndicator[X, {Xstart, Xend}]]

```

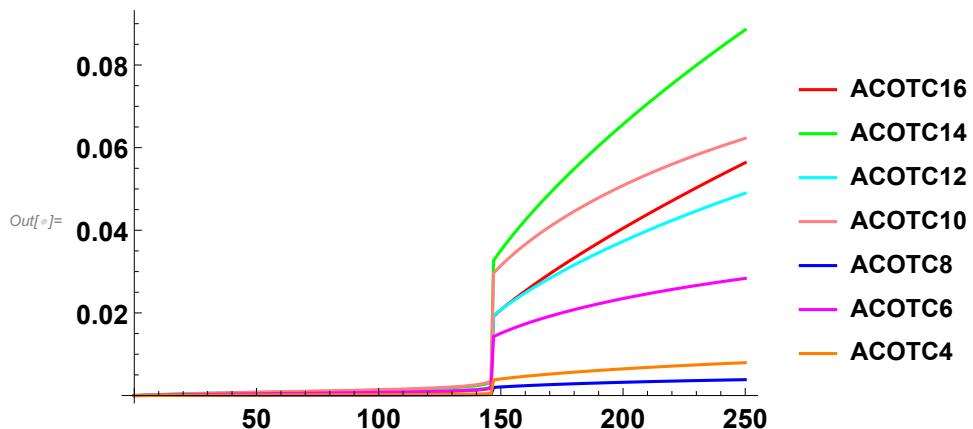
In[1]:= ScanUpNDS[0, 1, 250]

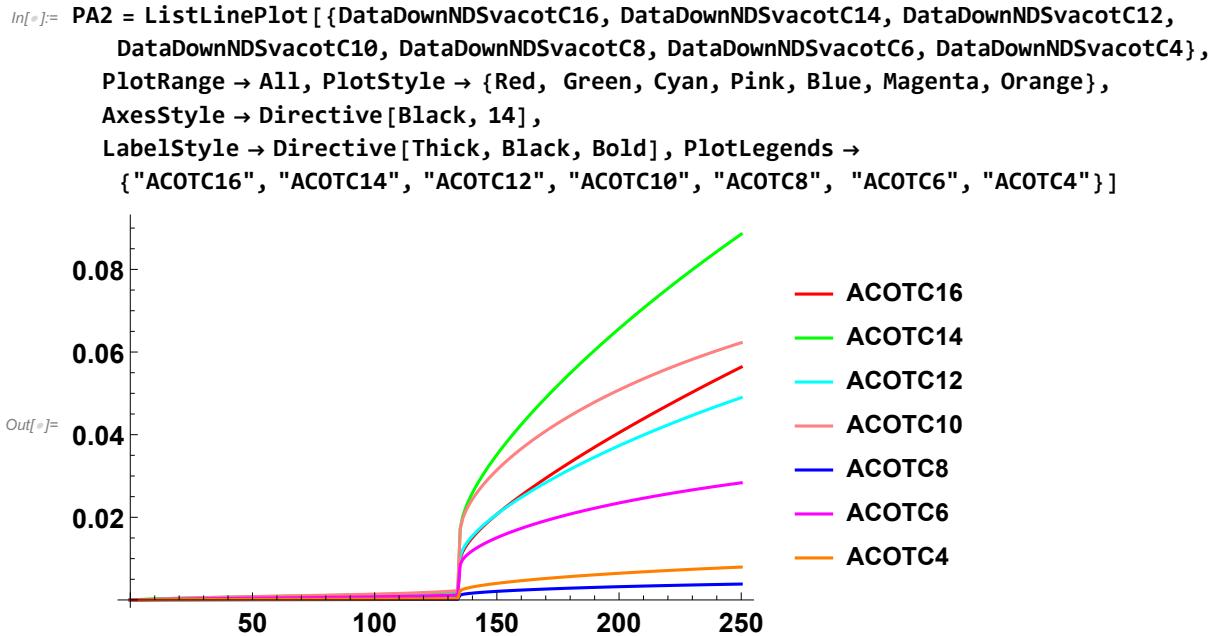
In[2]:=

```

In[3]:= PA1 = ListLinePlot[{DataUpNDSvacotC16, DataUpNDSvacotC14, DataUpNDSvacotC12,
  DataUpNDSvacotC10, DataUpNDSvacotC8, DataUpNDSvacotC6, DataUpNDSvacotC4},
  PlotRange -> All, PlotStyle -> {Red, Green, Cyan, Pink, Blue, Magenta, Orange},
  AxesStyle -> Directive[Black, 14],
  LabelStyle -> Directive[Thick, Black, Bold], PlotLegends ->
  {"ACOTC16", "ACOTC14", "ACOTC12", "ACOTC10", "ACOTC8", "ACOTC6", "ACOTC4"}]

```





# Mitochondrial Fatty Acid Oxidation Kinetic model

## Definitions of the various functions

```
In[1]:= CPT1[sf_, V_, Kms1_, Kms2_, Kmp1_, Kmp2_, Ki1_, Keq_, S1_, S2_, P1_, P2_, I1_, n_] := 
  (sf * V * ((S1 * S2) / (Kms1 * Kms2) - (P1 * P2) / (Kms1 * Kms2 * Keq))) / 
  ((1 + S1 / Kms1 + P1 / Kmp1 + (I1 / Ki1)^n) * (1 + S2 / Kms2 + P2 / Kmp2))

In[2]:= CACT[Vf_, Vr_, Kms1_, Kms2_, Kmp1_, Kmp2_, Kis1_, Kip2_, Keq_, S1_, S2_, P1_, P2_] := 
  (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)))

In[3]:= CPT2[sf_, V_, Kms1_, Kms2_, Kms3_, Kms4_, Kms5_, Kms6_, Kms7_, Kms8_, 
  Kmp1_, Kmp2_, Kmp3_, Kmp4_, Kmp5_, Kmp6_, Kmp7_, Kmp8_, Keq_, S1_, S2_, 
  S3_, S4_, S5_, S6_, S7_, S8_, P1_, P2_, P3_, P4_, P5_, P6_, P7_, P8_] := 
  (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))

In[4]:= VLCAD[sf_, V_, Kms1_, Kms2_, Kms3_, Kms4_, Kmp1_, Kmp2_, 
  Kmp3_, Kmp4_, Keq_, S1_, S2_, S3_, S4_, P1_, P2_, P3_, P4_] := 
  (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))
```

```

In[1]:= LCAD[sf_, V_, Kms1_, Kms2_, Kms3_, Kms4_, Kms5_, Kms6_, Kmp1_, Kmp2_, Kmp3_, Kmp4_,
Kmp5_, Kmp6_, Keq_, S1_, S2_, S3_, S4_, S5_, S6_, P1_, P2_, P3_, P4_, P5_, P6_] :=
(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))

In[2]:= MCAD[sf_, V_, Kms1_, Kms2_, Kms3_, Kms4_, Kms5_, Kms6_, Kmp1_, Kmp2_, Kmp3_, Kmp4_,
Kmp5_, Kmp6_, Keq_, S1_, S2_, S3_, S4_, S5_, S6_, P1_, P2_, P3_, P4_, P5_, P6_] :=
(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))

In[3]:= SCAD[sf_, V_, Kms1_, Kms2_, Kms3_, Kmp1_, Kmp2_, Kmp3_, Keq_, S1_, S2_, S3_, P1_, P2_,
P3_] := (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))

In[4]:= CROT[sf_, V_, Kms1_, Kms2_, Kms3_, Kms4_, Kms5_, Kms6_, Kms7_, Kmp1_, Kmp2_, Kmp3_,
Kmp4_, Kmp5_, Kmp6_, Kmp7_, Ki1_, Keq_, S1_, S2_, S3_, S4_, S5_, S6_, S7_, P1_,
P2_, P3_, P4_, P5_, P6_, P7_, I1_] := (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 / Kmp6 + P6 / Kmp7 + S7 / Kms7 + P7 / Kmp7 + I1 / Ki1)

In[5]:= MSCHAD[sf_, V_, Kms1_, Kms2_, Kms3_, Kms4_, Kms5_, Kms6_, Kms7_, Kms8_,
Kmp1_, Kmp2_, Kmp3_, Kmp4_, Kmp5_, Kmp6_, Kmp7_, Kmp8_, Keq_, S1_, S2_,
S3_, S4_, S5_, S6_, S7_, S8_, P1_, P2_, P3_, P4_, P5_, P6_, P7_, P8_] :=
(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))

In[6]:= MCKATA[sf_, V_, Kms1_, Kms2_, Kms3_, Kms4_, Kms5_, Kms6_, Kms7_, Kms8_,
Kmp1_, Kmp2_, Kmp3_, Kmp4_, Kmp5_, Kmp6_, Kmp7_, Kmp8_, Keq_, S1_, S2_,
S3_, S4_, S5_, S6_, S7_, S8_, P1_, P2_, P3_, P4_, P5_, P6_, P7_, P8_] :=
(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))

In[7]:= MCKATB[sf_, V_, Kms1_, Kms2_, Kms3_, Kms4_, Kms5_, Kms6_, Kms7_, Kms8_,
Kmp1_, Kmp2_, Kmp3_, Kmp4_, Kmp5_, Kmp6_, Kmp7_, Kmp8_, Keq_, S1_, S2_,
S3_, S4_, S5_, S6_, S7_, S8_, P1_, P2_, P3_, P4_, P5_, P6_, P7_, P8_] :=
(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))

In[8]:= MTP[sf_, V_, Kms1_, Kms2_, Kms3_, Kms4_, Kms5_, Kms7_, Kms8_, Kmp1_,
Kmp2_, Kmp3_, Kmp4_, Kmp5_, Kmp6_, Kmp7_, Kmp8_, Ki1_, Keq_, S1_, S2_, S3_,
S4_, S5_, S7_, S8_, P1_, P2_, P3_, P4_, P5_, P6_, P7_, P8_, I1_] := (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 + I1 / Ki1) *
(1 + (S7 - P7) / Kms7 + P7 / Kmp7) * (1 + S8 / Kms8 + P8 / Kmp8))

In[9]:= RES[Ks_, S_, K1_] := Ks * (S - K1)

```

## Define the differential equations

```

In[10]:= Odes = {
C16AcylCarCYT'[t] == (vcpt1C16 - vcactC16) / VCYT,

```

```

C16AcylCarMAT'[t] == (vcactC16 - vcpt2C16) / VMAT,
C16AcylCoAMAT'[t] == (vcpt2C16 - vvlcadC16 - vlcadC16) / VMAT,
C16EnoylCoAMAT'[t] == (vvlcadC16 + vlcadC16 - vcrotC16 - vmtcpC16) / VMAT,
C16HydroxyacylCoAMAT'[t] == (vcrotC16 - vmschadC16) / VMAT,
C16KetoacylCoAMAT'[t] == (vmschadC16 - vmckatC16) / VMAT,
C14AcylCarCYT'[t] == (-vcactC14) / VCYT,
C14AcylCarMAT'[t] == (vcactC14 - vcpt2C14) / VMAT,
C14AcylCoAMAT'[t] == (vcpt2C14 + vmtcpC16 + vmckatC16 - vvlcadC14 - vlcadC14) / VMAT,
C14EnoylCoAMAT'[t] == (vvlcadC14 + vlcadC14 - vcrotC14 - vmtcpC14) / VMAT,
C14HydroxyacylCoAMAT'[t] == (vcrotC14 - vmschadC14) / VMAT,
C14KetoacylCoAMAT'[t] == (vmschadC14 - vmckatC14) / VMAT,
C12AcylCarCYT'[t] == (-vcactC12) / VCYT,
C12AcylCarMAT'[t] == (vcactC12 - vcpt2C12) / VMAT,
C12AcylCoAMAT'[t] ==
  (vcpt2C12 + vmtcpC14 + vmckatC14 - vvlcadC12 - vlcadC12 - vmcadC12) / VMAT,
C12EnoylCoAMAT'[t] == (vvlcadC12 + vlcadC12 + vmcadC12 - vcrotC12 - vmtcpC12) / VMAT,
C12HydroxyacylCoAMAT'[t] == (vcrotC12 - vmschadC12) / VMAT,
C12KetoacylCoAMAT'[t] == (vmschadC12 - vmckatC12) / VMAT,
C10AcylCarCYT'[t] == (-vcactC10) / VCYT,
C10AcylCarMAT'[t] == (vcactC10 - vcpt2C10) / VMAT,
C10AcylCoAMAT'[t] == (vcpt2C10 + vmtcpC12 + vmckatC12 - vlcadC10 - vmcadC10) / VMAT,
C10EnoylCoAMAT'[t] == (vlcadC10 + vmcadC10 - vcrotC10 - vmtcpC10) / VMAT,
C10HydroxyacylCoAMAT'[t] == (vcrotC10 - vmschadC10) / VMAT,
C10KetoacylCoAMAT'[t] == (vmschadC10 - vmckatC10) / VMAT,
C8AcylCarCYT'[t] == (-vcactC8) / VCYT,
C8AcylCarMAT'[t] == (vcactC8 - vcpt2C8) / VMAT,
C8AcylCoAMAT'[t] == (vcpt2C8 + vmtcpC10 + vmckatC10 - vlcadC8 - vmcadC8) / VMAT,
C8EnoylCoAMAT'[t] == (vlcadC8 + vmcadC8 - vcrotC8 - vmtcpC8) / VMAT,
C8HydroxyacylCoAMAT'[t] == (vcrotC8 - vmschadC8) / VMAT,
C8KetoacylCoAMAT'[t] == (vmschadC8 - vmckatC8) / VMAT,
C6AcylCarCYT'[t] == (-vcactC6) / VCYT,
C6AcylCarMAT'[t] == (vcactC6 - vcpt2C6) / VMAT,
C6AcylCoAMAT'[t] == (vcpt2C6 + vmtcpC8 + vmckatC8 - vmcadC6 - vscadC6) / VMAT,
C6EnoylCoAMAT'[t] == (vmcadC6 + vscadC6 - vcrotC6) / VMAT,
C6HydroxyacylCoAMAT'[t] == (vcrotC6 - vmschadC6) / VMAT,
C6KetoacylCoAMAT'[t] == (vmschadC6 - vmckatC6) / VMAT,
C4AcylCarCYT'[t] == (-vcactC4) / VCYT,
C4AcylCarMAT'[t] == (vcactC4 - vcpt2C4) / VMAT,
C4AcylCoAMAT'[t] == (vcpt2C4 + vmckatC6 - vmcadC4 - vscadC4) / VMAT,
C4EnoylCoAMAT'[t] == (vmcadC4 + vscadC4 - vcrotC4) / VMAT,
C4HydroxyacylCoAMAT'[t] == (vcrotC4 - vmschadC4) / VMAT,
C4AcetoacylCoAMAT'[t] == (vmschadC4 - vmckatC4) / VMAT,
AcetylCoAMAT'[t] ==
  (1 / VMAT) (vmtcpC16 + vmckatC16 + vmtcpC14 + vmckatC14 + vmtcpC12 + vmckatC12 +
  vmtcpC10 + vmckatC10 + vmtcpC8 + vmckatC8 + vmckatC6 + 2 * vmckatC4 - vacesink),
FADHMAT'[t] == (1 / VMAT) (vvlcadC16 + vvlcadC14 + vvlcadC12 + vlcadC16 +
  vlcadC14 + vlcadC12 + vlcadC10 + vlcadC8 + vmcadC12 + vmcadC10 +
  vmcadC8 + vmcadC6 + vmcadC4 + vscadC6 + vscadC4 - vfadhsink),
NADHMAT'[t] == (1 / VMAT) (vmtcpC16 + vmtcpC14 + vmtcpC12 + vmtcpC10 +
  vmtcpC8 + vmschadC16 + vmschadC14 + vmschadC12 + vmschadC10 +
  vmschadC8 + vmschadC6 + vmschadC4 - vnadhsink) };
```

```

RateEqs = {vcpt1C16 → CPT1[sfcpt1C16, Vcpt1, Kmcpt1C16AcylCoACYT,
  Kmcpt1CarCYT, Kmcpt1C16AcylCarCYT, Kmcpt1CoACYT, Kicpt1MalCoACYT, Keqcpt1,
  C16AcylCoACYT, CarCYT, C16AcylCarCYT[t], CoACYT, MalCoACYT, ncpt1],

```

$v_{cactC16} \rightarrow CACT[Vfcact, Vrcact, Km_{cactC16}AcylCarCYT, Km_{cactCarMAT}, Km_{cactC16}AcylCarMAT, Km_{cactCarCYT}, Kic_{actC16}AcylCarCYT, Kic_{actCarCYT}, Keq_{cact}, C16AcylCarCYT[t], CarMAT, C16AcylCarMAT[t], CarCYT],$   
 $v_{cactC14} \rightarrow CACT[Vfcact, Vrcact, Km_{cactC14}AcylCarCYT, Km_{cactCarMAT}, Km_{cactC14}AcylCarMAT, Km_{cactCarCYT}, Kic_{actC14}AcylCarCYT, Kic_{actCarCYT}, Keq_{cact}, C14AcylCarCYT[t], CarMAT, C14AcylCarMAT[t], CarCYT],$   
 $v_{cactC12} \rightarrow CACT[Vfcact, Vrcact, Km_{cactC12}AcylCarCYT, Km_{cactCarMAT}, Km_{cactC12}AcylCarMAT, Km_{cactCarCYT}, Kic_{actC12}AcylCarCYT, Kic_{actCarCYT}, Keq_{cact}, C12AcylCarCYT[t], CarMAT, C12AcylCarMAT[t], CarCYT],$   
 $v_{cactC10} \rightarrow CACT[Vfcact, Vrcact, Km_{cactC10}AcylCarCYT, Km_{cactCarMAT}, Km_{cactC10}AcylCarMAT, Km_{cactCarCYT}, Kic_{actC10}AcylCarCYT, Kic_{actCarCYT}, Keq_{cact}, C10AcylCarCYT[t], CarMAT, C10AcylCarMAT[t], CarCYT],$   
 $v_{cactC8} \rightarrow CACT[Vfcact, Vrcact, Km_{cactC8}AcylCarCYT, Km_{cactCarMAT}, Km_{cactC8}AcylCarMAT, Km_{cactCarCYT}, Kic_{actC8}AcylCarCYT, Kic_{actCarCYT}, Keq_{cact}, C8AcylCarCYT[t], CarMAT, C8AcylCarMAT[t], CarCYT],$   
 $v_{cactC6} \rightarrow CACT[Vfcact, Vrcact, Km_{cactC6}AcylCarCYT, Km_{cactCarMAT}, Km_{cactC6}AcylCarMAT, Km_{cactCarCYT}, Kic_{actC6}AcylCarCYT, Kic_{actCarCYT}, Keq_{cact}, C6AcylCarCYT[t], CarMAT, C6AcylCarMAT[t], CarCYT],$   
 $v_{cactC4} \rightarrow CACT[Vfcact, Vrcact, Km_{cactC4}AcylCarCYT, Km_{cactCarMAT}, Km_{cactC4}AcylCarMAT, Km_{cactCarCYT}, Kic_{actC4}AcylCarCYT, Kic_{actCarCYT}, Keq_{cact}, C4AcylCarCYT[t], CarMAT, C4AcylCarMAT[t], CarCYT],$   
 $v_{cpt2C16} \rightarrow CPT2[sfcpt2C16, Vcpt2, Km_{cpt2C16}AcylCarMAT, Km_{cpt2C14}AcylCarMAT, Km_{cpt2C12}AcylCarMAT, Km_{cpt2C10}AcylCarMAT, Km_{cpt2C8}AcylCarMAT, Km_{cpt2C6}AcylCarMAT, Km_{cpt2C4}AcylCarMAT, Km_{cpt2CoAMAT}, Km_{cpt2C16}AcylCoAMAT, Km_{cpt2C14}AcylCoAMAT, Km_{cpt2C12}AcylCoAMAT, Km_{cpt2C10}AcylCoAMAT, Km_{cpt2C8}AcylCoAMAT, Km_{cpt2C6}AcylCoAMAT, Km_{cpt2C4}AcylCoAMAT, Km_{cpt2CarMAT}, Keqcpt2, C16AcylCarMAT[t], C14AcylCarMAT[t], C12AcylCarMAT[t], C10AcylCarMAT[t], C8AcylCarMAT[t], C6AcylCarMAT[t], C4AcylCarMAT[t], CoAMAT, C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t], C4AcylCoAMAT[t], CarMAT],$   
 $v_{cpt2C14} \rightarrow CPT2[sfcpt2C14, Vcpt2, Km_{cpt2C14}AcylCarMAT, Km_{cpt2C16}AcylCarMAT, Km_{cpt2C12}AcylCarMAT, Km_{cpt2C10}AcylCarMAT, Km_{cpt2C8}AcylCarMAT, Km_{cpt2C6}AcylCarMAT, Km_{cpt2C4}AcylCoAMAT, Km_{cpt2CoAMAT}, Km_{cpt2C14}AcylCoAMAT, Km_{cpt2C16}AcylCoAMAT, Km_{cpt2C12}AcylCoAMAT, Km_{cpt2C10}AcylCoAMAT, Km_{cpt2C8}AcylCoAMAT, Km_{cpt2C6}AcylCoAMAT, Km_{cpt2C4}AcylCoAMAT, Km_{cpt2CarMAT}, Keqcpt2, C14AcylCarMAT[t], C16AcylCarMAT[t], C12AcylCarMAT[t], C10AcylCarMAT[t], C8AcylCarMAT[t], C6AcylCarMAT[t], C4AcylCarMAT[t], CoAMAT, C14AcylCoAMAT[t], C16AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t], C4AcylCoAMAT[t], CarMAT],$   
 $v_{cpt2C12} \rightarrow CPT2[sfcpt2C12, Vcpt2, Km_{cpt2C12}AcylCarMAT, Km_{cpt2C16}AcylCarMAT, Km_{cpt2C14}AcylCarMAT, Km_{cpt2C10}AcylCarMAT, Km_{cpt2C8}AcylCarMAT, Km_{cpt2C6}AcylCarMAT, Km_{cpt2C4}AcylCarMAT, Km_{cpt2CoAMAT}, Km_{cpt2C12}AcylCoAMAT, Km_{cpt2C16}AcylCoAMAT, Km_{cpt2C14}AcylCoAMAT, Km_{cpt2C10}AcylCoAMAT, Km_{cpt2C8}AcylCoAMAT, Km_{cpt2C6}AcylCoAMAT, Km_{cpt2C4}AcylCoAMAT, Km_{cpt2CarMAT}, Keqcpt2, C12AcylCarMAT[t], C16AcylCarMAT[t], C14AcylCarMAT[t], C10AcylCarMAT[t], C8AcylCarMAT[t], C6AcylCarMAT[t], C4AcylCarMAT[t], CoAMAT, C12AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t], C4AcylCoAMAT[t], CarMAT],$   
 $v_{cpt2C10} \rightarrow CPT2[sfcpt2C10, Vcpt2, Km_{cpt2C10}AcylCarMAT, Km_{cpt2C16}AcylCarMAT, Km_{cpt2C14}AcylCarMAT, Km_{cpt2C12}AcylCarMAT, Km_{cpt2C8}AcylCarMAT, Km_{cpt2C6}AcylCarMAT, Km_{cpt2C4}AcylCarMAT, Km_{cpt2CoAMAT}, Km_{cpt2C10}AcylCoAMAT, Km_{cpt2C16}AcylCoAMAT, Km_{cpt2C14}AcylCoAMAT, Km_{cpt2C12}AcylCoAMAT, Km_{cpt2C8}AcylCoAMAT, Km_{cpt2C6}AcylCoAMAT, Km_{cpt2C4}AcylCoAMAT, Km_{cpt2CarMAT}, Keqcpt2, C10AcylCarMAT[t], C16AcylCarMAT[t], C14AcylCarMAT[t], C12AcylCarMAT[t], C8AcylCarMAT[t], C6AcylCarMAT[t], C4AcylCarMAT[t], CoAMAT, C10AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t], C4AcylCoAMAT[t], CarMAT],$   
 $v_{cpt2C8} \rightarrow CPT2[sfcpt2C8, Vcpt2, Km_{cpt2C8}AcylCarMAT, Km_{cpt2C16}AcylCarMAT, Km_{cpt2C14}AcylCarMAT, Km_{cpt2C12}AcylCarMAT, Km_{cpt2C10}AcylCarMAT, Km_{cpt2C6}AcylCarMAT,$

$Kmcpt2C4AcylCarMAT, Kmcpt2CoAMAT, Kmcpt2C8AcylCoAMAT, Kmcpt2C16AcylCoAMAT,$   
 $Kmcpt2C14AcylCoAMAT, Kmcpt2C12AcylCoAMAT, Kmcpt2C10AcylCoAMAT, Kmcpt2C6AcylCoAMAT,$   
 $Kmcpt2C4AcylCoAMAT, Kmcpt2CarMAT, Keqcpt2, C8AcylCarMAT[t], C16AcylCarMAT[t],$   
 $C14AcylCarMAT[t], C12AcylCarMAT[t], C10AcylCarMAT[t], C6AcylCarMAT[t],$   
 $C4AcylCarMAT[t], CoAMAT, C8AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t],$   
 $C12AcylCoAMAT[t], C10AcylCoAMAT[t], C6AcylCoAMAT[t], C4AcylCoAMAT[t], CarMAT],$   
 $vcpt2C6 \rightarrow CPT2[sfcpt2C6, Vcpt2, Kmcpt2C6AcylCarMAT, Kmcpt2C16AcylCarMAT,$   
 $Kmcpt2C14AcylCarMAT, Kmcpt2C12AcylCarMAT, Kmcpt2C10AcylCarMAT, Kmcpt2C8AcylCarMAT,$   
 $Kmcpt2C4AcylCarMAT, Kmcpt2CoAMAT, Kmcpt2C6AcylCoAMAT, Kmcpt2C16AcylCoAMAT,$   
 $Kmcpt2C14AcylCoAMAT, Kmcpt2C12AcylCoAMAT, Kmcpt2C10AcylCoAMAT, Kmcpt2C8AcylCoAMAT,$   
 $Kmcpt2C4AcylCoAMAT, Kmcpt2CarMAT, Keqcpt2, C6AcylCarMAT[t], C16AcylCarMAT[t],$   
 $C14AcylCarMAT[t], C12AcylCarMAT[t], C10AcylCarMAT[t], C8AcylCarMAT[t],$   
 $C4AcylCarMAT[t], CoAMAT, C6AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t],$   
 $C12AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t], C4AcylCoAMAT[t], CarMAT],$   
 $vcpt2C4 \rightarrow CPT2[sfcpt2C4, Vcpt2, Kmcpt2C4AcylCarMAT, Kmcpt2C16AcylCarMAT,$   
 $Kmcpt2C14AcylCarMAT, Kmcpt2C12AcylCarMAT, Kmcpt2C10AcylCarMAT, Kmcpt2C8AcylCarMAT,$   
 $Kmcpt2C6AcylCarMAT, Kmcpt2CoAMAT, Kmcpt2C4AcylCoAMAT, Kmcpt2C16AcylCoAMAT,$   
 $Kmcpt2C14AcylCoAMAT, Kmcpt2C12AcylCoAMAT, Kmcpt2C10AcylCoAMAT, Kmcpt2C8AcylCoAMAT,$   
 $Kmcpt2C6AcylCoAMAT, Kmcpt2CarMAT, Keqcpt2, C4AcylCarMAT[t], C16AcylCarMAT[t],$   
 $C14AcylCarMAT[t], C12AcylCarMAT[t], C10AcylCarMAT[t], C8AcylCarMAT[t],$   
 $C6AcylCarMAT[t], CoAMAT, C4AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t],$   
 $C12AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t], CarMAT],$   
 $vvlcadC16 \rightarrow VLCAD[sfvvlcadC16, Vvlcad, KmvlcadC16AcylCoAMAT, KmvlcadC14AcylCoAMAT,$   
 $KmvlcadC12AcylCoAMAT, KmvlcadFAD, KmvlcadC16EnoylCoAMAT,$   
 $KmvlcadC14EnoylCoAMAT, KmvlcadC12EnoylCoAMAT, KmvlcadFADH, Keqvlcad,$   
 $C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t], FADtMAT,$   
 $C16EnoylCoAMAT[t], C14EnoylCoAMAT[t], C12EnoylCoAMAT[t], FADHMAT[t]],$   
 $vvlcadC14 \rightarrow VLCAD[sfvvlcadC14, Vvlcad, KmvlcadC14AcylCoAMAT, KmvlcadC16AcylCoAMAT,$   
 $KmvlcadC12AcylCoAMAT, KmvlcadFAD, KmvlcadC14EnoylCoAMAT,$   
 $KmvlcadC16EnoylCoAMAT, KmvlcadC12EnoylCoAMAT, KmvlcadFADH, Keqvlcad,$   
 $C14AcylCoAMAT[t], C16AcylCoAMAT[t], C12AcylCoAMAT[t], FADtMAT,$   
 $C14EnoylCoAMAT[t], C16EnoylCoAMAT[t], C12EnoylCoAMAT[t], FADHMAT[t]],$   
 $vvlcadC12 \rightarrow VLCAD[sfvvlcadC12, Vvlcad, KmvlcadC12AcylCoAMAT, KmvlcadC16AcylCoAMAT,$   
 $KmvlcadC14AcylCoAMAT, KmvlcadFAD, KmvlcadC12EnoylCoAMAT,$   
 $KmvlcadC16EnoylCoAMAT, KmvlcadC14EnoylCoAMAT, KmvlcadFADH, Keqvlcad,$   
 $C12AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t], FADtMAT,$   
 $C12EnoylCoAMAT[t], C16EnoylCoAMAT[t], C14EnoylCoAMAT[t], FADHMAT[t]],$   
 $vlcadC16 \rightarrow LCAD[sflcadC16, Vlcad, KmlcadC16AcylCoAMAT, KmlcadC14AcylCoAMAT,$   
 $KmlcadC12AcylCoAMAT, KmlcadC10AcylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadFAD,$   
 $KmlcadC16EnoylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC12EnoylCoAMAT,$   
 $KmlcadC10EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, Keqlcad,$   
 $C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t],$   
 $C8AcylCoAMAT[t], FADtMAT, C16EnoylCoAMAT[t], C14EnoylCoAMAT[t],$   
 $C12EnoylCoAMAT[t], C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], FADHMAT[t]],$   
 $vlcadC14 \rightarrow LCAD[sflcadC14, Vlcad, KmlcadC14AcylCoAMAT, KmlcadC16AcylCoAMAT,$   
 $KmlcadC12AcylCoAMAT, KmlcadC10AcylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadFAD,$   
 $KmlcadC14EnoylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC12EnoylCoAMAT,$   
 $KmlcadC10EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, Keqlcad,$   
 $C14AcylCoAMAT[t], C16AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t],$   
 $C8AcylCoAMAT[t], FADtMAT, C14EnoylCoAMAT[t], C16EnoylCoAMAT[t],$   
 $C12EnoylCoAMAT[t], C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], FADHMAT[t]],$   
 $vlcadC12 \rightarrow LCAD[sflcadC12, Vlcad, KmlcadC12AcylCoAMAT, KmlcadC16AcylCoAMAT,$   
 $KmlcadC14AcylCoAMAT, KmlcadC10AcylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadFAD,$   
 $KmlcadC12EnoylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC14EnoylCoAMAT,$   
 $KmlcadC10EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, Keqlcad,$

C12AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t], C10AcylCoAMAT[t],  
 C8AcylCoAMAT[t], FADtMAT, C14EnoylCoAMAT[t], C16EnoylCoAMAT[t],  
 C14EnoylCoAMAT[t], C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], FADHMAT[t]],  
 vlcadC10 → LCAD[sflcadC10, Vlcad, KmlcadC10AcylCoAMAT, KmlcadC16AcylCoAMAT,  
 KmlcadC14AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadFAD,  
 KmlcadC10EnoylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC14EnoylCoAMAT,  
 KmlcadC12EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, Keqlcad,  
 C10AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t],  
 C8AcylCoAMAT[t], FADtMAT, C10EnoylCoAMAT[t], C16EnoylCoAMAT[t],  
 C14EnoylCoAMAT[t], C12EnoylCoAMAT[t], C8EnoylCoAMAT[t], FADHMAT[t]],  
 vlcadC8 → LCAD[sflcadC8, Vlcad, KmlcadC8AcylCoAMAT, KmlcadC16AcylCoAMAT,  
 KmlcadC14AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC10AcylCoAMAT, KmlcadFAD,  
 KmlcadC8EnoylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC14EnoylCoAMAT,  
 KmlcadC12EnoylCoAMAT, KmlcadC10EnoylCoAMAT, KmlcadFADH, Keqlcad,  
 C8AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t],  
 C10AcylCoAMAT[t], FADtMAT, C8EnoylCoAMAT[t], C16EnoylCoAMAT[t],  
 C14EnoylCoAMAT[t], C12EnoylCoAMAT[t], C10EnoylCoAMAT[t], FADHMAT[t]],  
 vmcadC12 → MCAD[sfmcadC12, Vmcad, KmmcadC12AcylCoAMAT, KmmcadC10AcylCoAMAT,  
 KmmcadC8AcylCoAMAT, KmmcadC6AcylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadFAD,  
 KmmcadC12EnoylCoAMAT, KmmcadC10EnoylCoAMAT, KmmcadC8EnoylCoAMAT,  
 KmmcadC6EnoylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadFADH, Keqmcad,  
 C12AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t],  
 C4AcylCoAMAT[t], FADtMAT, C12EnoylCoAMAT[t], C10EnoylCoAMAT[t],  
 C8EnoylCoAMAT[t], C6EnoylCoAMAT[t], C4EnoylCoAMAT[t], FADHMAT[t]],  
 vmcadC10 → MCAD[sfmcadC10, Vmcad, KmmcadC10AcylCoAMAT, KmmcadC12AcylCoAMAT,  
 KmmcadC8AcylCoAMAT, KmmcadC6AcylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadFAD,  
 KmmcadC12EnoylCoAMAT, KmmcadC10EnoylCoAMAT, KmmcadC8EnoylCoAMAT,  
 KmmcadC6EnoylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadFADH, Keqmcad,  
 C10AcylCoAMAT[t], C12AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t],  
 C4AcylCoAMAT[t], FADtMAT, C10EnoylCoAMAT[t], C12EnoylCoAMAT[t],  
 C8EnoylCoAMAT[t], C6EnoylCoAMAT[t], C4EnoylCoAMAT[t], FADHMAT[t]],  
 vmcadC8 → MCAD[sfmcadC8, Vmcad, KmmcadC8AcylCoAMAT, KmmcadC12AcylCoAMAT,  
 KmmcadC10AcylCoAMAT, KmmcadC6AcylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadFAD,  
 KmmcadC8EnoylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC10EnoylCoAMAT,  
 KmmcadC6EnoylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadFADH, Keqmcad,  
 C8AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t], C6AcylCoAMAT[t],  
 C4AcylCoAMAT[t], FADtMAT, C8EnoylCoAMAT[t], C12EnoylCoAMAT[t],  
 C10EnoylCoAMAT[t], C6EnoylCoAMAT[t], C4EnoylCoAMAT[t], FADHMAT[t]],  
 vmcadC6 → MCAD[sfmcadC6, Vmcad, KmmcadC6AcylCoAMAT, KmmcadC12AcylCoAMAT,  
 KmmcadC10AcylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadFAD,  
 KmmcadC6EnoylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC10EnoylCoAMAT,  
 KmmcadC8EnoylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadFADH, Keqmcad,  
 C6AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t],  
 C4AcylCoAMAT[t], FADtMAT, C6EnoylCoAMAT[t], C12EnoylCoAMAT[t],  
 C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], C4EnoylCoAMAT[t], FADHMAT[t]],  
 vmcadC4 → MCAD[sfmcadC4, Vmcad, KmmcadC4AcylCoAMAT, KmmcadC12AcylCoAMAT,  
 KmmcadC10AcylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC6AcylCoAMAT, KmmcadFAD,  
 KmmcadC4EnoylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC10EnoylCoAMAT,  
 KmmcadC8EnoylCoAMAT, KmmcadC6EnoylCoAMAT, KmmcadFADH, Keqmcad,  
 C4AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t],  
 C6AcylCoAMAT[t], FADtMAT, C4EnoylCoAMAT[t], C12EnoylCoAMAT[t],  
 C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], C4EnoylCoAMAT[t], FADHMAT[t]],  
 vscadC6 → SCAD[sfscadC6, Vscad, KmscadC6AcylCoAMAT, KmscadC4AcylCoAMAT, KmscadFAD,  
 KmscadC6EnoylCoAMAT, KmscadC4EnoylCoAMAT, KmscadFADH, Keqscad, C6AcylCoAMAT[t],  
 C4AcylCoAMAT[t], FADtMAT, C6EnoylCoAMAT[t], C4EnoylCoAMAT[t], FADHMAT[t]],

vscadC4 → SCAD[sfscadC4, Vscad, KmscadC4AcylCoAMAT, KmscadC6AcylCoAMAT, KmscadFAD, KmscadC4EnoylCoAMAT, KmscadC6EnoylCoAMAT, KmscadFADH, Keqscad, C4AcylCoAMAT[t], C6AcylCoAMAT[t], FADtMAT, C4EnoylCoAMAT[t], C6EnoylCoAMAT[t], FADHMAT[t]], vcrotC16 → CROT[sfcrotC16, Vcrot, KmcrotC16EnoylCoAMAT, KmcrotC14EnoylCoAMAT, KmcrotC12EnoylCoAMAT, KmcrotC10EnoylCoAMAT, KmcrotC8EnoylCoAMAT, KmcrotC6EnoylCoAMAT, KmcrotC4EnoylCoAMAT, KmcrotC16HydroxyacylCoAMAT, KmcrotC14HydroxyacylCoAMAT, KmcrotC12HydroxyacylCoAMAT, KmcrotC10HydroxyacylCoAMAT, KmcrotC8HydroxyacylCoAMAT, KmcrotC6HydroxyacylCoAMAT, KmcrotC4HydroxyacylCoAMAT, KicrotC4AcetoacylCoA, Keqrot, C16EnoylCoAMAT[t], C14EnoylCoAMAT[t], C12EnoylCoAMAT[t], C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], C6EnoylCoAMAT[t], C4EnoylCoAMAT[t], C16HydroxyacylCoAMAT[t], C14HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t], C8HydroxyacylCoAMAT[t], C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], C4AcetoacylCoAMAT[t]], vcrotC14 → CROT[sfcrotC14, Vcrot, KmcrotC14EnoylCoAMAT, KmcrotC16EnoylCoAMAT, KmcrotC12EnoylCoAMAT, KmcrotC10EnoylCoAMAT, KmcrotC8EnoylCoAMAT, KmcrotC6EnoylCoAMAT, KmcrotC4EnoylCoAMAT, KmcrotC14HydroxyacylCoAMAT, KmcrotC16HydroxyacylCoAMAT, KmcrotC10HydroxyacylCoAMAT, KmcrotC8HydroxyacylCoAMAT, KmcrotC6HydroxyacylCoAMAT, KmcrotC4HydroxyacylCoAMAT, KicrotC4AcetoacylCoA, Keqrot, C14EnoylCoAMAT[t], C16EnoylCoAMAT[t], C12EnoylCoAMAT[t], C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], C6EnoylCoAMAT[t], C4EnoylCoAMAT[t], C14HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t], C8HydroxyacylCoAMAT[t], C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], C4AcetoacylCoAMAT[t]], vcrotC12 → CROT[sfcrotC12, Vcrot, KmcrotC12EnoylCoAMAT, KmcrotC16EnoylCoAMAT, KmcrotC14EnoylCoAMAT, KmcrotC10EnoylCoAMAT, KmcrotC8EnoylCoAMAT, KmcrotC6EnoylCoAMAT, KmcrotC4EnoylCoAMAT, KmcrotC12HydroxyacylCoAMAT, KmcrotC16HydroxyacylCoAMAT, KmcrotC10HydroxyacylCoAMAT, KmcrotC8HydroxyacylCoAMAT, KmcrotC6HydroxyacylCoAMAT, KmcrotC4HydroxyacylCoAMAT, KicrotC4AcetoacylCoA, Keqrot, C12EnoylCoAMAT[t], C16EnoylCoAMAT[t], C14EnoylCoAMAT[t], C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], C6EnoylCoAMAT[t], C4EnoylCoAMAT[t], C12HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t], C14HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t], C8HydroxyacylCoAMAT[t], C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], C4AcetoacylCoAMAT[t]], vcrotC10 → CROT[sfcrotC10, Vcrot, KmcrotC10EnoylCoAMAT, KmcrotC16EnoylCoAMAT, KmcrotC14EnoylCoAMAT, KmcrotC12EnoylCoAMAT, KmcrotC8EnoylCoAMAT, KmcrotC6EnoylCoAMAT, KmcrotC4EnoylCoAMAT, KmcrotC10HydroxyacylCoAMAT, KmcrotC16HydroxyacylCoAMAT, KmcrotC12HydroxyacylCoAMAT, KmcrotC8HydroxyacylCoAMAT, KmcrotC6HydroxyacylCoAMAT, KmcrotC4HydroxyacylCoAMAT, KicrotC4AcetoacylCoA, Keqrot, C10EnoylCoAMAT[t], C16EnoylCoAMAT[t], C14EnoylCoAMAT[t], C12EnoylCoAMAT[t], C8EnoylCoAMAT[t], C6EnoylCoAMAT[t], C4EnoylCoAMAT[t], C10HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t], C14HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C8HydroxyacylCoAMAT[t], C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], C4AcetoacylCoAMAT[t]], vcrotC8 → CROT[sfcrotC8, Vcrot, KmcrotC8EnoylCoAMAT, KmcrotC16EnoylCoAMAT, KmcrotC14EnoylCoAMAT, KmcrotC12EnoylCoAMAT, KmcrotC10EnoylCoAMAT, KmcrotC6EnoylCoAMAT, KmcrotC4EnoylCoAMAT, KmcrotC8HydroxyacylCoAMAT, KmcrotC16HydroxyacylCoAMAT, KmcrotC12HydroxyacylCoAMAT, KmcrotC10HydroxyacylCoAMAT, KmcrotC6HydroxyacylCoAMAT, KmcrotC4HydroxyacylCoAMAT, KicrotC4AcetoacylCoA, Keqrot, C8EnoylCoAMAT[t], C16EnoylCoAMAT[t], C14EnoylCoAMAT[t], C12EnoylCoAMAT[t], C10EnoylCoAMAT[t], C6EnoylCoAMAT[t], C4EnoylCoAMAT[t], C8HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t], C14HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C8HydroxyacylCoAMAT[t], C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], C4AcetoacylCoAMAT[t]]

C4EnoylCoAMAT[t], C8HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t],  
 C14HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t],  
 C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
 vcrotC6 → CROT[sfcrotC6, Vcrot, KmrcrotC6EnoylCoAMAT, KmrcrotC16EnoylCoAMAT,  
 KmrcrotC14EnoylCoAMAT, KmrcrotC12EnoylCoAMAT, KmrcrotC10EnoylCoAMAT,  
 KmrcrotC8EnoylCoAMAT, KmrcrotC4EnoylCoAMAT, KmrcrotC6HydroxyacylCoAMAT,  
 KmrcrotC16HydroxyacylCoAMAT, KmrcrotC14HydroxyacylCoAMAT,  
 KmrcrotC12HydroxyacylCoAMAT, KmrcrotC10HydroxyacylCoAMAT,  
 KmrcrotC8HydroxyacylCoAMAT, KmrcrotC4HydroxyacylCoAMAT, KicrotC4AcetoacylCoA,  
 Keqcrot, C6EnoylCoAMAT[t], C16EnoylCoAMAT[t], C14EnoylCoAMAT[t],  
 C12EnoylCoAMAT[t], C10EnoylCoAMAT[t], C8EnoylCoAMAT[t],  
 C4EnoylCoAMAT[t], C6HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t],  
 C14HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t],  
 C8HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
 vcrotC4 → CROT[sfcrotC4, Vcrot, KmrcrotC4EnoylCoAMAT, KmrcrotC16EnoylCoAMAT,  
 KmrcrotC14EnoylCoAMAT, KmrcrotC12EnoylCoAMAT, KmrcrotC10EnoylCoAMAT,  
 KmrcrotC8EnoylCoAMAT, KmrcrotC6EnoylCoAMAT, KmrcrotC4HydroxyacylCoAMAT,  
 KmrcrotC16HydroxyacylCoAMAT, KmrcrotC14HydroxyacylCoAMAT,  
 KmrcrotC12HydroxyacylCoAMAT, KmrcrotC10HydroxyacylCoAMAT,  
 KmrcrotC8HydroxyacylCoAMAT, KmrcrotC6HydroxyacylCoAMAT, KicrotC4AcetoacylCoA,  
 Keqcrot, C4EnoylCoAMAT[t], C16EnoylCoAMAT[t], C14EnoylCoAMAT[t],  
 C12EnoylCoAMAT[t], C10EnoylCoAMAT[t], C8EnoylCoAMAT[t],  
 C6EnoylCoAMAT[t], C4HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t],  
 C14HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t],  
 C8HydroxyacylCoAMAT[t], C6HydroxyacylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
 vmschadC16 → MSCHAD[sfmschadC16, Vmschad, KmmschadC16HydroxyacylCoAMAT,  
 KmmschadC14HydroxyacylCoAMAT, KmmschadC12HydroxyacylCoAMAT,  
 KmmschadC10HydroxyacylCoAMAT, KmmschadC8HydroxyacylCoAMAT,  
 KmmschadC6HydroxyacylCoAMAT, KmmschadC4HydroxyacylCoAMAT,  
 KmmschadNADMAT, KmmschadC16KetoacylCoAMAT, KmmschadC14KetoacylCoAMAT,  
 KmmschadC12KetoacylCoAMAT, KmmschadC10KetoacylCoAMAT, KmmschadC8KetoacylCoAMAT,  
 KmmschadC6KetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT, KmmschadNADHMAT,  
 Keqmschad, C16HydroxyacylCoAMAT[t], C14HydroxyacylCoAMAT[t],  
 C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t], C8HydroxyacylCoAMAT[t],  
 C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], NADtMAT, C16KetoacylCoAMAT[t],  
 C14KetoacylCoAMAT[t], C12KetoacylCoAMAT[t], C10KetoacylCoAMAT[t],  
 C8KetoacylCoAMAT[t], C6KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], NADHMAT[t]],  
 vmschadC14 → MSCHAD[sfmschadC14, Vmschad, KmmschadC14HydroxyacylCoAMAT,  
 KmmschadC16HydroxyacylCoAMAT, KmmschadC12HydroxyacylCoAMAT,  
 KmmschadC10HydroxyacylCoAMAT, KmmschadC8HydroxyacylCoAMAT,  
 KmmschadC6HydroxyacylCoAMAT, KmmschadC4HydroxyacylCoAMAT,  
 KmmschadNADMAT, KmmschadC14KetoacylCoAMAT, KmmschadC16KetoacylCoAMAT,  
 KmmschadC12KetoacylCoAMAT, KmmschadC10KetoacylCoAMAT, KmmschadC8KetoacylCoAMAT,  
 KmmschadC6KetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT, KmmschadNADHMAT,  
 Keqmschad, C14HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t],  
 C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t], C8HydroxyacylCoAMAT[t],  
 C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], NADtMAT, C14KetoacylCoAMAT[t],  
 C16KetoacylCoAMAT[t], C12KetoacylCoAMAT[t], C10KetoacylCoAMAT[t],  
 C8KetoacylCoAMAT[t], C6KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], NADHMAT[t]],  
 vmschadC12 → MSCHAD[sfmschadC12, Vmschad, KmmschadC12HydroxyacylCoAMAT,  
 KmmschadC16HydroxyacylCoAMAT, KmmschadC14HydroxyacylCoAMAT,  
 KmmschadC10HydroxyacylCoAMAT, KmmschadC8HydroxyacylCoAMAT,  
 KmmschadC6HydroxyacylCoAMAT, KmmschadC4HydroxyacylCoAMAT,  
 KmmschadNADMAT, KmmschadC12KetoacylCoAMAT, KmmschadC16KetoacylCoAMAT,  
 KmmschadC14KetoacylCoAMAT, KmmschadC10KetoacylCoAMAT, KmmschadC8KetoacylCoAMAT,

KmmschadC6KetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT, KmmschadNADHMAT,  
 Keqmschad, C12HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t],  
 C14HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t], C8HydroxyacylCoAMAT[t],  
 C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], NADtMAT, C12KetoacylCoAMAT[t],  
 C16KetoacylCoAMAT[t], C14KetoacylCoAMAT[t], C10KetoacylCoAMAT[t],  
 C8KetoacylCoAMAT[t], C6KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], NADHMAT[t]],  
 vmschadC10 → MSCHAD [sfmschadC10, Vmschad, KmmschadC10HydroxyacylCoAMAT,  
 KmmschadC16HydroxyacylCoAMAT, KmmschadC14HydroxyacylCoAMAT,  
 KmmschadC12HydroxyacylCoAMAT, KmmschadC8HydroxyacylCoAMAT,  
 KmmschadC6HydroxyacylCoAMAT, KmmschadC4HydroxyacylCoAMAT,  
 KmmschadNADMAT, KmmschadC10KetoacylCoAMAT, KmmschadC16KetoacylCoAMAT,  
 KmmschadC14KetoacylCoAMAT, KmmschadC12KetoacylCoAMAT, KmmschadC8KetoacylCoAMAT,  
 KmmschadC6KetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT, KmmschadNADHMAT,  
 Keqmschad, C10HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t],  
 C14HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C8HydroxyacylCoAMAT[t],  
 C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], NADtMAT, C10KetoacylCoAMAT[t],  
 C16KetoacylCoAMAT[t], C14KetoacylCoAMAT[t], C12KetoacylCoAMAT[t],  
 C8KetoacylCoAMAT[t], C6KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], NADHMAT[t]],  
 vmschadC8 → MSCHAD [sfmschadC8, Vmschad, KmmschadC8HydroxyacylCoAMAT,  
 KmmschadC16HydroxyacylCoAMAT, KmmschadC14HydroxyacylCoAMAT,  
 KmmschadC12HydroxyacylCoAMAT, KmmschadC10HydroxyacylCoAMAT,  
 KmmschadC6HydroxyacylCoAMAT, KmmschadC4HydroxyacylCoAMAT,  
 KmmschadNADMAT, KmmschadC8KetoacylCoAMAT, KmmschadC16KetoacylCoAMAT,  
 KmmschadC14KetoacylCoAMAT, KmmschadC12KetoacylCoAMAT, KmmschadC10KetoacylCoAMAT,  
 KmmschadC6KetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT, KmmschadNADHMAT,  
 Keqmschad, C8HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t],  
 C14HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t],  
 C6HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], NADtMAT, C8KetoacylCoAMAT[t],  
 C16KetoacylCoAMAT[t], C14KetoacylCoAMAT[t], C12KetoacylCoAMAT[t],  
 C10KetoacylCoAMAT[t], C6KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], NADHMAT[t]],  
 vmschadC6 → MSCHAD [sfmschadC6, Vmschad, KmmschadC6HydroxyacylCoAMAT,  
 KmmschadC16HydroxyacylCoAMAT, KmmschadC14HydroxyacylCoAMAT,  
 KmmschadC12HydroxyacylCoAMAT, KmmschadC10HydroxyacylCoAMAT,  
 KmmschadC8HydroxyacylCoAMAT, KmmschadC4HydroxyacylCoAMAT,  
 KmmschadNADMAT, KmmschadC6KetoacylCoAMAT, KmmschadC16KetoacylCoAMAT,  
 KmmschadC14KetoacylCoAMAT, KmmschadC12KetoacylCoAMAT, KmmschadC10KetoacylCoAMAT,  
 KmmschadC8KetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT, KmmschadNADHMAT,  
 Keqmschad, C6HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t],  
 C14HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t],  
 C8HydroxyacylCoAMAT[t], C4HydroxyacylCoAMAT[t], NADtMAT, C6KetoacylCoAMAT[t],  
 C16KetoacylCoAMAT[t], C14KetoacylCoAMAT[t], C12KetoacylCoAMAT[t],  
 C10KetoacylCoAMAT[t], C8KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], NADHMAT[t]],  
 vmschadC4 → MSCHAD [sfmschadC4, Vmschad, KmmschadC4HydroxyacylCoAMAT,  
 KmmschadC16HydroxyacylCoAMAT, KmmschadC14HydroxyacylCoAMAT,  
 KmmschadC12HydroxyacylCoAMAT, KmmschadC10HydroxyacylCoAMAT,  
 KmmschadC8HydroxyacylCoAMAT, KmmschadC6HydroxyacylCoAMAT,  
 KmmschadNADMAT, KmmschadC4AcetoacylCoAMAT, KmmschadC16KetoacylCoAMAT,  
 KmmschadC14KetoacylCoAMAT, KmmschadC12KetoacylCoAMAT, KmmschadC10KetoacylCoAMAT,  
 KmmschadC8KetoacylCoAMAT, KmmschadC6KetoacylCoAMAT, KmmschadNADHMAT,  
 Keqmschad, C4HydroxyacylCoAMAT[t], C16HydroxyacylCoAMAT[t],  
 C14HydroxyacylCoAMAT[t], C12HydroxyacylCoAMAT[t], C10HydroxyacylCoAMAT[t],  
 C8HydroxyacylCoAMAT[t], C6HydroxyacylCoAMAT[t], NADtMAT, C4AcetoacylCoAMAT[t],  
 C16KetoacylCoAMAT[t], C14KetoacylCoAMAT[t], C12KetoacylCoAMAT[t],  
 C10KetoacylCoAMAT[t], C8KetoacylCoAMAT[t], C6KetoacylCoAMAT[t], NADHMAT[t]],  
 vmckatC16 → MCKATA [sfmckatC16, Vmckat, KmmckatC16KetoacylCoAMAT,



C16KetoacylCoAMAT[t], C14KetoacylCoAMAT[t], C12KetoacylCoAMAT[t],  
 C10KetoacylCoAMAT[t], C8KetoacylCoAMAT[t], C4AcetoacylCoAMAT[t], CoAMAT,  
 C4AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t],  
 C10AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t], AcetylCoAMAT[t]],  
 vmtckatC4 → MCKATB[sfmckatC4, Vmckat, KmmckatC4AcetoacylCoAMAT,  
 KmmckatC16KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT, KmmckatC12KetoacylCoAMAT,  
 KmmckatC10KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC6KetoacylCoAMAT,  
 KmmckatCoAMAT, KmmckatC4AcylCoAMAT, KmmckatC16AcylCoAMAT, KmmckatC14AcylCoAMAT,  
 KmmckatC12AcylCoAMAT, KmmckatC10AcylCoAMAT, KmmckatC8AcylCoAMAT,  
 KmmckatC6AcylCoAMAT, KmmckatAcetylCoAMAT, Keqmtckat, C4AcetoacylCoAMAT[t],  
 C16KetoacylCoAMAT[t], C14KetoacylCoAMAT[t], C12KetoacylCoAMAT[t],  
 C10KetoacylCoAMAT[t], C8KetoacylCoAMAT[t], C6KetoacylCoAMAT[t], CoAMAT,  
 C4AcylCoAMAT[t], C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t],  
 C10AcylCoAMAT[t], C8AcylCoAMAT[t], C6AcylCoAMAT[t], AcetylCoAMAT[t]],  
 vmtcp16 → MTP[sfntpC16, Vmtp, KmmtpC16EnoylCoAMAT, KmmtpC14EnoylCoAMAT,  
 KmmtpC12EnoylCoAMAT, KmmtpC10EnoylCoAMAT, KmmtpC8EnoylCoAMAT,  
 KmmtpNADMAT, KmmtpCoAMAT, KmmtpC14AcylCoAMAT, KmmtpC16AcylCoAMAT,  
 KmmtpC12AcylCoAMAT, KmmtpC10AcylCoAMAT, KmmtpC8AcylCoAMAT,  
 KmmtpC6AcylCoAMAT, KmmtpNADHMAT, KmmtpAcetylCoAMAT, KicrotC4AcetoacylCoA,  
 Keqmtcp, C16EnoylCoAMAT[t], C14EnoylCoAMAT[t], C12EnoylCoAMAT[t],  
 C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], NADtMAT, CoAMAT, C12AcylCoAMAT[t],  
 C16AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t],  
 C6AcylCoAMAT[t], NADHMAT[t], AcetylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
 vmtcp14 → MTP[sfntpC14, Vmtp, KmmtpC14EnoylCoAMAT, KmmtpC16EnoylCoAMAT,  
 KmmtpC12EnoylCoAMAT, KmmtpC10EnoylCoAMAT, KmmtpC8EnoylCoAMAT,  
 KmmtpNADMAT, KmmtpCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC16AcylCoAMAT,  
 KmmtpC14AcylCoAMAT, KmmtpC10AcylCoAMAT, KmmtpC8AcylCoAMAT,  
 KmmtpC6AcylCoAMAT, KmmtpNADHMAT, KmmtpAcetylCoAMAT, KicrotC4AcetoacylCoA,  
 Keqmtcp, C14EnoylCoAMAT[t], C16EnoylCoAMAT[t], C12EnoylCoAMAT[t],  
 C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], NADtMAT, CoAMAT, C12AcylCoAMAT[t],  
 C16AcylCoAMAT[t], C14AcylCoAMAT[t], C10AcylCoAMAT[t], C8AcylCoAMAT[t],  
 C6AcylCoAMAT[t], NADHMAT[t], AcetylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
 vmtcp12 → MTP[sfntpC12, Vmtp, KmmtpC12EnoylCoAMAT, KmmtpC16EnoylCoAMAT,  
 KmmtpC14EnoylCoAMAT, KmmtpC10EnoylCoAMAT, KmmtpC8EnoylCoAMAT,  
 KmmtpNADMAT, KmmtpCoAMAT, KmmtpC10AcylCoAMAT, KmmtpC16AcylCoAMAT,  
 KmmtpC14AcylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC8AcylCoAMAT,  
 KmmtpC6AcylCoAMAT, KmmtpNADHMAT, KmmtpAcetylCoAMAT, KicrotC4AcetoacylCoA,  
 Keqmtcp, C12EnoylCoAMAT[t], C16EnoylCoAMAT[t], C14EnoylCoAMAT[t],  
 C10EnoylCoAMAT[t], C8EnoylCoAMAT[t], NADtMAT, CoAMAT, C10AcylCoAMAT[t],  
 C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t], C8AcylCoAMAT[t],  
 C6AcylCoAMAT[t], NADHMAT[t], AcetylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
 vmtcp10 → MTP[sfntpC10, Vmtp, KmmtpC10EnoylCoAMAT, KmmtpC16EnoylCoAMAT,  
 KmmtpC14EnoylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC8EnoylCoAMAT,  
 KmmtpNADMAT, KmmtpCoAMAT, KmmtpC8AcylCoAMAT, KmmtpC16AcylCoAMAT,  
 KmmtpC14AcylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC10AcylCoAMAT,  
 KmmtpC6AcylCoAMAT, KmmtpNADHMAT, KmmtpAcetylCoAMAT, KicrotC4AcetoacylCoA,  
 Keqmtcp, C10EnoylCoAMAT[t], C16EnoylCoAMAT[t], C14EnoylCoAMAT[t],  
 C12EnoylCoAMAT[t], C8EnoylCoAMAT[t], NADtMAT, CoAMAT, C8AcylCoAMAT[t],  
 C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t],  
 C6AcylCoAMAT[t], NADHMAT[t], AcetylCoAMAT[t], C4AcetoacylCoAMAT[t]],  
 vmtcp8 → MTP[sfntpC8, Vmtp, KmmtpC8EnoylCoAMAT, KmmtpC16EnoylCoAMAT,  
 KmmtpC14EnoylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC10EnoylCoAMAT,  
 KmmtpNADMAT, KmmtpCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC16AcylCoAMAT,  
 KmmtpC14AcylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC10AcylCoAMAT,  
 KmmtpC8AcylCoAMAT, KmmtpNADHMAT, KmmtpAcetylCoAMAT, KicrotC4AcetoacylCoA,

```

Keqmtip, C8EnoylCoAMAT[t], C16EnoylCoAMAT[t], C14EnoylCoAMAT[t],
C12EnoylCoAMAT[t], C10EnoylCoAMAT[t], NADtMAT, CoAMAT, C6AcylCoAMAT[t],
C16AcylCoAMAT[t], C14AcylCoAMAT[t], C12AcylCoAMAT[t], C10AcylCoAMAT[t],
C8AcylCoAMAT[t], NADHMAT[t], AcetylCoAMAT[t], C4AcetoacylCoAMAT[t]],

vacesink → RES[Ksacesink, AcetylCoAMAT[t], K1acesink],
vfadhsink → RES[Ksfadhsink, FADHMAT[t], K1fadhsink],
vnadhsink → RES[Ksnadhsink, NADHMAT[t], K1nadhsink}];

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

Parm = {
sfcpt1C16 → 1, Vcpt1 → 0.012, Kmcp1C16AcylCoACYT → 13.8,
Kmcp1CarCYT → 250, Kmcp1C16AcylCarCYT → 136, Kmcp1CoACYT → 40.7,
Kicp1MalCoACYT → 9.1, Keqcpt1 → 0.45, ncpt1 → 2.4799,
Vfcact → 0.42, Vrcact → 0.42, KmactC16AcylCarCYT → 15,
KmactC14AcylCarCYT → 15, KmactC12AcylCarCYT → 15, KmactC10AcylCarCYT → 15,
KmactC8AcylCarCYT → 15, KmactC6AcylCarCYT → 15, KmactC4AcylCarCYT → 15,
KmactCarMAT → 130, KmactC16AcylCarMAT → 15, KmactC14AcylCarMAT → 15,
KmactC12AcylCarMAT → 15, KmactC10AcylCarMAT → 15, KmactC8AcylCarMAT → 15,
KmactC6AcylCarMAT → 15, KmactC4AcylCarMAT → 15, KmactCarCYT → 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,
Kmcp2C16AcylCarMAT → 51, Kmcp2C14AcylCarMAT → 51, Kmcp2C12AcylCarMAT → 51,
Kmcp2C10AcylCarMAT → 51, Kmcp2C8AcylCarMAT → 51, Kmcp2C6AcylCarMAT → 51,
Kmcp2C4AcylCarMAT → 51, Kmcp2CoAMAT → 30, Kmcp2C16AcylCoAMAT → 38,
Kmcp2C14AcylCoAMAT → 38, Kmcp2C12AcylCoAMAT → 38,
Kmcp2C10AcylCoAMAT → 38, Kmcp2C8AcylCoAMAT → 38, Kmcp2C6AcylCoAMAT → 1000,
Kmcp2C4AcylCoAMAT → 1000 000, Kmcp2CarMAT → 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, Keqlcad → 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,
}
```

$KmmcadC8EnoylCoAMAT \rightarrow 1.08$ ,  $KmmcadC6EnoylCoAMAT \rightarrow 1.08$ ,  
 $KmmcadC4EnoylCoAMAT \rightarrow 1.08$ ,  $KmmcadFADH \rightarrow 24.2$ ,  $Keqmcad \rightarrow 6$ ,  
 $sfscadC6 \rightarrow 0.3$ ,  $sfscadC4 \rightarrow 1$ ,  $Vscad \rightarrow 0.081$ ,  $KmscadC6AcylCoAMAT \rightarrow 285$ ,  
 $KmscadC4AcylCoAMAT \rightarrow 10.7$ ,  $KmscadFAD \rightarrow 0.12$ ,  $KmscadC6EnoylCoAMAT \rightarrow 1.08$ ,  
 $KmscadC4EnoylCoAMAT \rightarrow 1.08$ ,  $KmscadFADH \rightarrow 24.2$ ,  $Keqscad \rightarrow 6$ ,  
 $sfcrotC16 \rightarrow 0.13$ ,  $sfcrotC14 \rightarrow 0.2$ ,  $sfcrotC12 \rightarrow 0.25$ ,  $sfcrotC10 \rightarrow 0.33$ ,  $sfcrotC8 \rightarrow 0.58$ ,  
 $sfcrotC6 \rightarrow 0.83$ ,  $sfcrotC4 \rightarrow 1$ ,  $Vcrot \rightarrow 3.6$ ,  $KmcrotC16EnoylCoAMAT \rightarrow 150$ ,  
 $KmcrotC14EnoylCoAMAT \rightarrow 100$ ,  $KmcrotC12EnoylCoAMAT \rightarrow 25$ ,  $KmcrotC10EnoylCoAMAT \rightarrow 25$ ,  
 $KmcrotC8EnoylCoAMAT \rightarrow 25$ ,  $KmcrotC6EnoylCoAMAT \rightarrow 25$ ,  $KmcrotC4EnoylCoAMAT \rightarrow 40$ ,  
 $KmcrotC16HydroxyacylCoAMAT \rightarrow 45$ ,  $KmcrotC14HydroxyacylCoAMAT \rightarrow 45$ ,  
 $KmcrotC12HydroxyacylCoAMAT \rightarrow 45$ ,  $KmcrotC10HydroxyacylCoAMAT \rightarrow 45$ ,  
 $KmcrotC8HydroxyacylCoAMAT \rightarrow 45$ ,  $KmcrotC6HydroxyacylCoAMAT \rightarrow 45$ ,  
 $KmcrotC4HydroxyacylCoAMAT \rightarrow 45$ ,  $KicrotC4AcetoacylCoA \rightarrow 1.6$ ,  $Keqcrot \rightarrow 3.13$ ,  
 $sfmschadC16 \rightarrow 0.6$ ,  $sfmschadC14 \rightarrow 0.5$ ,  $sfmschadC12 \rightarrow 0.43$ ,  $sfmschadC10 \rightarrow 0.64$ ,  
 $sfmschadC8 \rightarrow 0.89$ ,  $sfmschadC6 \rightarrow 1$ ,  $sfmschadC4 \rightarrow 0.67$ ,  $Vmschad \rightarrow 1$ ,  
 $KmmschadC16HydroxyacylCoAMAT \rightarrow 1.5$ ,  $KmmschadC14HydroxyacylCoAMAT \rightarrow 1.8$ ,  
 $KmmschadC12HydroxyacylCoAMAT \rightarrow 3.7$ ,  $KmmschadC10HydroxyacylCoAMAT \rightarrow 8.8$ ,  
 $KmmschadC8HydroxyacylCoAMAT \rightarrow 16.3$ ,  $KmmschadC6HydroxyacylCoAMAT \rightarrow 28.6$ ,  
 $KmmschadC4HydroxyacylCoAMAT \rightarrow 69.9$ ,  $KmmschadNADMAT \rightarrow 58.5$ ,  
 $KmmschadC16KetoacylCoAMAT \rightarrow 1.4$ ,  $KmmschadC14KetoacylCoAMAT \rightarrow 1.4$ ,  
 $KmmschadC12KetoacylCoAMAT \rightarrow 1.6$ ,  $KmmschadC10KetoacylCoAMAT \rightarrow 2.3$ ,  
 $KmmschadC8KetoacylCoAMAT \rightarrow 4.1$ ,  $KmmschadC6KetoacylCoAMAT \rightarrow 5.8$ ,  
 $KmmschadC4AcetoacylCoAMAT \rightarrow 16.9$ ,  $KmmschadNADHMAT \rightarrow 5.4$ ,  $Keqmschad \rightarrow 2.17 * 10^{-4}$ ,  
 $sfmckatC16 \rightarrow 0$ ,  $sfmckatC14 \rightarrow 0.2$ ,  $sfmckatC12 \rightarrow 0.38$ ,  $sfmckatC10 \rightarrow 0.65$ ,  
 $sfmckatC8 \rightarrow 0.81$ ,  $sfmckatC6 \rightarrow 1$ ,  $sfmckatC4 \rightarrow 0.49$ ,  $Vmckat \rightarrow 0.377$ ,  
 $KmmckatC16KetoacylCoAMAT \rightarrow 1.1$ ,  $KmmckatC14KetoacylCoAMAT \rightarrow 1.2$ ,  
 $KmmckatC12KetoacylCoAMAT \rightarrow 1.3$ ,  $KmmckatC10KetoacylCoAMAT \rightarrow 2.1$ ,  
 $KmmckatC8KetoacylCoAMAT \rightarrow 3.2$ ,  $KmmckatC6KetoacylCoAMAT \rightarrow 6.7$ ,  
 $KmmckatC4AcetoacylCoAMAT \rightarrow 12.4$ ,  $KmmckatCoAMAT \rightarrow 26.6$ ,  
 $KmmckatC14AcylCoAMAT \rightarrow 13.83$ ,  $KmmckatC16AcylCoAMAT \rightarrow 13.83$ ,  
 $KmmckatC12AcylCoAMAT \rightarrow 13.83$ ,  $KmmckatC10AcylCoAMAT \rightarrow 13.83$ ,  
 $KmmckatC8AcylCoAMAT \rightarrow 13.83$ ,  $KmmckatC6AcylCoAMAT \rightarrow 13.83$ ,  
 $KmmckatC4AcylCoAMAT \rightarrow 13.83$ ,  $KmmckatAcetylCoAMAT \rightarrow 30$ ,  $Keqmckat \rightarrow 1051$ ,  
 $sfmtpC16 \rightarrow 1$ ,  $sfmtpC14 \rightarrow 0.9$ ,  $sfmtpC12 \rightarrow 0.81$ ,  $sfmtpC10 \rightarrow 0.73$ ,  $sfmtpC8 \rightarrow 0.34$ ,  
 $Vmtp \rightarrow 2.84$ ,  $KmmtpC16EnoylCoAMAT \rightarrow 25$ ,  $KmmtpC14EnoylCoAMAT \rightarrow 25$ ,  
 $KmmtpC12EnoylCoAMAT \rightarrow 25$ ,  $KmmtpC10EnoylCoAMAT \rightarrow 25$ ,  $KmmtpC8EnoylCoAMAT \rightarrow 25$ ,  
 $KmmtpNADMAT \rightarrow 60$ ,  $KmmtpCoAMAT \rightarrow 30$ ,  $KmmtpC14AcylCoAMAT \rightarrow 13.83$ ,  
 $KmmtpC16AcylCoAMAT \rightarrow 13.83$ ,  $KmmtpC12AcylCoAMAT \rightarrow 13.83$ ,  
 $KmmtpC10AcylCoAMAT \rightarrow 13.83$ ,  $KmmtpC8AcylCoAMAT \rightarrow 13.83$ ,  $KmmtpC6AcylCoAMAT \rightarrow 13.83$ ,  
 $KmmtpNADHMAT \rightarrow 50$ ,  $KmmtpAcetylCoAMAT \rightarrow 30$ ,  $Keqmt \rightarrow 0.71$ ,  
 $Ksacesink \rightarrow 6000000$ ,  $K1acesink \rightarrow 70$ ,  $Ksfadhsink \rightarrow 6000000$ ,  
 $K1fadhsink \rightarrow 0.46$ ,  $Ksnadhsink \rightarrow 6000000$ ,  $K1nadhsink \rightarrow 12$ ,  
 $C16AcylCoACYT \rightarrow 25$ ,  $CarCYT \rightarrow 200$ ,  $CoACYT \rightarrow 140$ ,  $MalCoACYT \rightarrow 0$ ,  
 $CarMAT \rightarrow 950$ ,  $FADtMAT \rightarrow 0.77$ ,  $NADtMAT \rightarrow 250$ ,  $CoAMATT \rightarrow 5000$ ,  
 $VCYT \rightarrow 2.2 * 10^{-6}$ ,  $VMAT \rightarrow 1.8 * 10^{-6}$ ; }

```

InitialConditions = {
  C16AcylCarCYT[0] = 0, C16AcylCarMAT[0] = 0, C16AcylCoAMAT[0] = 0,
  C16EnoylCoAMAT[0] = 0, C16HydroxyacylCoAMAT[0] = 0, C16KetoacylCoAMAT[0] = 0,
  C14AcylCarCYT[0] = 0, C14AcylCarMAT[0] = 0, C14AcylCoAMAT[0] = 0,
  C14EnoylCoAMAT[0] = 0, C14HydroxyacylCoAMAT[0] = 0, C14KetoacylCoAMAT[0] = 0,
  C12AcylCarCYT[0] = 0, C12AcylCarMAT[0] = 0, C12AcylCoAMAT[0] = 0,
  C12EnoylCoAMAT[0] = 0, C12HydroxyacylCoAMAT[0] = 0, C12KetoacylCoAMAT[0] = 0,
  C10AcylCarCYT[0] = 0, C10AcylCarMAT[0] = 0, C10AcylCoAMAT[0] = 0,
  C10EnoylCoAMAT[0] = 0, C10HydroxyacylCoAMAT[0] = 0, C10KetoacylCoAMAT[0] = 0,
}

```

```

C8AcylCarCYT[0] == 0, C8AcylCarMAT[0] == 0, C8AcylCoAMAT[0] == 0,
C8EnoylCoAMAT[0] == 0, C8HydroxyacylCoAMAT[0] == 0, C8KetoacylCoAMAT[0] == 0,
C6AcylCarCYT[0] == 0, C6AcylCarMAT[0] == 0, C6AcylCoAMAT[0] == 0,
C6EnoylCoAMAT[0] == 0, C6HydroxyacylCoAMAT[0] == 0, C6KetoacylCoAMAT[0] == 0,
C4AcylCarCYT[0] == 0, C4AcylCarMAT[0] == 0, C4AcylCoAMAT[0] == 0,
C4EnoylCoAMAT[0] == 0, C4HydroxyacylCoAMAT[0] == 0, C4AcetoacylCoAMAT[0] == 0,
AcetylCoAMAT[0] == 70, FADHMAT[0] == 0.46, NADHMAT[0] == 12};

Vars = {
  C16AcylCarCYT, C16AcylCarMAT, C16AcylCoAMAT,
  C16EnoylCoAMAT, C16HydroxyacylCoAMAT, C16KetoacylCoAMAT,
  C14AcylCarCYT, C14AcylCarMAT, C14AcylCoAMAT, C14EnoylCoAMAT,
  C14HydroxyacylCoAMAT, C14KetoacylCoAMAT,
  C12AcylCarCYT, C12AcylCarMAT, C12AcylCoAMAT, C12EnoylCoAMAT,
  C12HydroxyacylCoAMAT, C12KetoacylCoAMAT,
  C10AcylCarCYT, C10AcylCarMAT, C10AcylCoAMAT, C10EnoylCoAMAT,
  C10HydroxyacylCoAMAT, C10KetoacylCoAMAT,
  C8AcylCarCYT, C8AcylCarMAT, C8AcylCoAMAT, C8EnoylCoAMAT,
  C8HydroxyacylCoAMAT, C8KetoacylCoAMAT,
  C6AcylCarCYT, C6AcylCarMAT, C6AcylCoAMAT, C6EnoylCoAMAT,
  C6HydroxyacylCoAMAT, C6KetoacylCoAMAT,
  C4AcylCarCYT, C4AcylCarMAT, C4AcylCoAMAT, C4EnoylCoAMAT,
  C4HydroxyacylCoAMAT, C4AcetoacylCoAMAT,
  AcetylCoAMAT, FADHMAT, NADHMAT};

In[=]:= TableForm[Odes];
TableForm[RateEqs];
TableForm[Odes /. RateEqs /. CoAMATX /. Parm];
TableForm[RateEqs /. Parm];
TableForm[InitialConditions];

In[=]:= tsol = NDSolve[Join[Odes /. RateEqs /. CoAMATX /. Parm, InitialConditions],
  Vars, {t, 0, 1000000000}];
```

```
In[1]:= Table[{Vars[[i]][t], (Vars[[i]][900000000] /. tsol)[[1]]}, {i, 1, Length[Vars]}]

Out[1]= {{C16AcylCarCYT[t], 0.167997}, {C16AcylCarMAT[t], 0.355963}, {C16AcylCoAMAT[t], 0.872403}, {C16EnoylCoAMAT[t], 0.0487436}, {C16HydroxyacylCoAMAT[t], 0.152568}, {C16KetoacylCoAMAT[t], 0.000656626}, {C14AcylCarCYT[t], 0.0373818}, {C14AcylCarMAT[t], 0.177564}, {C14AcylCoAMAT[t], 1.93364}, {C14EnoylCoAMAT[t], 0.0544366}, {C14HydroxyacylCoAMAT[t], 0.154607}, {C14KetoacylCoAMAT[t], 0.000664719}, {C12AcylCarCYT[t], 0.0510162}, {C12AcylCarMAT[t], 0.242327}, {C12AcylCoAMAT[t], 2.63889}, {C12EnoylCoAMAT[t], 0.0621263}, {C12HydroxyacylCoAMAT[t], 0.187943}, {C12KetoacylCoAMAT[t], 0.000805513}, {C10AcylCarCYT[t], 0.0916998}, {C10AcylCarMAT[t], 0.435574}, {C10AcylCoAMAT[t], 4.74332}, {C10EnoylCoAMAT[t], 0.0684024}, {C10HydroxyacylCoAMAT[t], 0.208289}, {C10KetoacylCoAMAT[t], 0.000890113}, {C8AcylCarCYT[t], 0.0941203}, {C8AcylCarMAT[t], 0.447072}, {C8AcylCoAMAT[t], 4.86853}, {C8EnoylCoAMAT[t], 0.148284}, {C8HydroxyacylCoAMAT[t], 0.458288}, {C8KetoacylCoAMAT[t], 0.0019575}, {C6AcylCarCYT[t], 0.249827}, {C6AcylCarMAT[t], 1.18668}, {C6AcylCoAMAT[t], 12.9227}, {C6EnoylCoAMAT[t], 11.1239}, {C6HydroxyacylCoAMAT[t], 34.6175}, {C6KetoacylCoAMAT[t], 0.147847}, {C4AcylCarCYT[t], 0.414653}, {C4AcylCarMAT[t], 1.9696}, {C4AcylCoAMAT[t], 21.4486}, {C4EnoylCoAMAT[t], 41.836}, {C4HydroxyacylCoAMAT[t], 130.681}, {C4AcetoacylCoAMAT[t], 0.558265}, {AcetylCoAMAT[t], 70.}, {FADHMAT[t], 0.46}, {NADHMAT[t], 12.}}
```

## Steady state computation by varying palmitoyl-CoA

```
In[2]:= ParmScan[X_] := {
  sfcpt1C16 → 1, Vcpt1 → 0.012, Kmcpt1C16AcylCoACYT → 13.8,
  Kmcpt1CarCYT → 250, Kmcpt1C16AcylCarCYT → 136, Kmcpt1CoACYT → 40.7,
  Kicpt1MalCoACYT → 9.1, Keqcppt1 → 0.45, ncpt1 → 2.4799,
  Vfcact → 0.42, Vrcact → 0.42, KmcaactC16AcylCarCYT → 15,
  KmcaactC14AcylCarCYT → 15, KmcaactC12AcylCarCYT → 15, KmcaactC10AcylCarCYT → 15,
  KmcaactC8AcylCarCYT → 15, KmcaactC6AcylCarCYT → 15, KmcaactC4AcylCarCYT → 15,
  KmcaactCarMAT → 130, KmcaactC16AcylCarMAT → 15, KmcaactC14AcylCarMAT → 15,
  KmcaactC12AcylCarMAT → 15, KmcaactC10AcylCarMAT → 15, KmcaactC8AcylCarMAT → 15,
  KmcaactC6AcylCarMAT → 15, KmcaactC4AcylCarMAT → 15, KmcaactCarCYT → 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, Keqcppt2 → 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, Keqvvlcad → 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,
```

$KmlcadFAD \rightarrow 0.12$ ,  $KmlcadC16EnoylCoAMAT \rightarrow 1.08$ ,  $KmlcadC14EnoylCoAMAT \rightarrow 1.08$ ,  
 $KmlcadC12EnoylCoAMAT \rightarrow 1.08$ ,  $KmlcadC10EnoylCoAMAT \rightarrow 1.08$ ,  
 $KmlcadC8EnoylCoAMAT \rightarrow 1.08$ ,  $KmlcadFADH \rightarrow 24.2$ ,  $Keqlcad \rightarrow 6$ ,  
 $sfmcadC12 \rightarrow 0.38$ ,  $sfmcadC10 \rightarrow 0.8$ ,  $sfmcadC8 \rightarrow 0.87$ ,  $sfmcadC6 \rightarrow 1$ ,  $sfmcadC4 \rightarrow 0.12$ ,  
 $Vmcad \rightarrow 0.081$ ,  $Kmmcadc12AcylCoAMAT \rightarrow 5.7$ ,  $Kmmcadc10AcylCoAMAT \rightarrow 5.4$ ,  
 $Kmmcadc8AcylCoAMAT \rightarrow 4$ ,  $Kmmcadc6AcylCoAMAT \rightarrow 9.4$ ,  $Kmmcadc4AcylCoAMAT \rightarrow 135$ ,  
 $KmmcadcFAD \rightarrow 0.12$ ,  $Kmmcadc12EnoylCoAMAT \rightarrow 1.08$ ,  $Kmmcadc10EnoylCoAMAT \rightarrow 1.08$ ,  
 $Kmmcadc8EnoylCoAMAT \rightarrow 1.08$ ,  $Kmmcadc6EnoylCoAMAT \rightarrow 1.08$ ,  
 $Kmmcadc4EnoylCoAMAT \rightarrow 1.08$ ,  $KmmcadcFADH \rightarrow 24.2$ ,  $Keqmcad \rightarrow 6$ ,  
 $sfscadC6 \rightarrow 0.3$ ,  $sfscadC4 \rightarrow 1$ ,  $Vscad \rightarrow 0.081$ ,  $KmscadC6AcylCoAMAT \rightarrow 285$ ,  
 $KmscadC4AcylCoAMAT \rightarrow 10.7$ ,  $KmscadFAD \rightarrow 0.12$ ,  $KmscadC6EnoylCoAMAT \rightarrow 1.08$ ,  
 $KmscadC4EnoylCoAMAT \rightarrow 1.08$ ,  $KmscadFADH \rightarrow 24.2$ ,  $Keqscad \rightarrow 6$ ,  
 $sfcrotC16 \rightarrow 0.13$ ,  $sfcrotC14 \rightarrow 0.2$ ,  $sfcrotC12 \rightarrow 0.25$ ,  $sfcrotC10 \rightarrow 0.33$ ,  $sfcrotC8 \rightarrow 0.58$ ,  
 $sfcrotC6 \rightarrow 0.83$ ,  $sfcrotC4 \rightarrow 1$ ,  $Vcrot \rightarrow 3.6$ ,  $KmcrotC16EnoylCoAMAT \rightarrow 150$ ,  
 $KmcrotC14EnoylCoAMAT \rightarrow 100$ ,  $KmcrotC12EnoylCoAMAT \rightarrow 25$ ,  $KmcrotC10EnoylCoAMAT \rightarrow 25$ ,  
 $KmcrotC8EnoylCoAMAT \rightarrow 25$ ,  $KmcrotC6EnoylCoAMAT \rightarrow 25$ ,  $KmcrotC4EnoylCoAMAT \rightarrow 40$ ,  
 $KmcrotC16HydroxyacylCoAMAT \rightarrow 45$ ,  $KmcrotC14HydroxyacylCoAMAT \rightarrow 45$ ,  
 $KmcrotC12HydroxyacylCoAMAT \rightarrow 45$ ,  $KmcrotC10HydroxyacylCoAMAT \rightarrow 45$ ,  
 $KmcrotC8HydroxyacylCoAMAT \rightarrow 45$ ,  $KmcrotC6HydroxyacylCoAMAT \rightarrow 45$ ,  
 $KmcrotC4HydroxyacylCoAMAT \rightarrow 45$ ,  $KicrotC4AcetoacylCoA \rightarrow 1.6$ ,  $Keqrot \rightarrow 3.13$ ,  
 $sfmschadC16 \rightarrow 0.6$ ,  $sfmschadC14 \rightarrow 0.5$ ,  $sfmschadC12 \rightarrow 0.43$ ,  $sfmschadC10 \rightarrow 0.64$ ,  
 $sfmschadC8 \rightarrow 0.89$ ,  $sfmschadC6 \rightarrow 1$ ,  $sfmschadC4 \rightarrow 0.67$ ,  $Vmschad \rightarrow 1$ ,  
 $KmmschadC16HydroxyacylCoAMAT \rightarrow 1.5$ ,  $KmmschadC14HydroxyacylCoAMAT \rightarrow 1.8$ ,  
 $KmmschadC12HydroxyacylCoAMAT \rightarrow 3.7$ ,  $KmmschadC10HydroxyacylCoAMAT \rightarrow 8.8$ ,  
 $KmmschadC8HydroxyacylCoAMAT \rightarrow 16.3$ ,  $KmmschadC6HydroxyacylCoAMAT \rightarrow 28.6$ ,  
 $KmmschadC4HydroxyacylCoAMAT \rightarrow 69.9$ ,  $KmmschadNADMAT \rightarrow 58.5$ ,  
 $KmmschadC16KetoacylCoAMAT \rightarrow 1.4$ ,  $KmmschadC14KetoacylCoAMAT \rightarrow 1.4$ ,  
 $KmmschadC12KetoacylCoAMAT \rightarrow 1.6$ ,  $KmmschadC10KetoacylCoAMAT \rightarrow 2.3$ ,  
 $KmmschadC8KetoacylCoAMAT \rightarrow 4.1$ ,  $KmmschadC6KetoacylCoAMAT \rightarrow 5.8$ ,  
 $KmmschadC4AcetoacylCoAMAT \rightarrow 16.9$ ,  $KmmschadNADMAT \rightarrow 5.4$ ,  $Keqmschad \rightarrow 2.17 * 10^{-4}$ ,  
 $sfmckatC16 \rightarrow 0$ ,  $sfmckatC14 \rightarrow 0.2$ ,  $sfmckatC12 \rightarrow 0.38$ ,  $sfmckatC10 \rightarrow 0.65$ ,  
 $sfmckatC8 \rightarrow 0.81$ ,  $sfmckatC6 \rightarrow 1$ ,  $sfmckatC4 \rightarrow 0.49$ ,  $Vmckat \rightarrow 0.377$ ,  
 $KmmckatC16KetoacylCoAMAT \rightarrow 1.1$ ,  $KmmckatC14KetoacylCoAMAT \rightarrow 1.2$ ,  
 $KmmckatC12KetoacylCoAMAT \rightarrow 1.3$ ,  $KmmckatC10KetoacylCoAMAT \rightarrow 2.1$ ,  
 $KmmckatC8KetoacylCoAMAT \rightarrow 3.2$ ,  $KmmckatC6KetoacylCoAMAT \rightarrow 6.7$ ,  
 $KmmckatC4AcetoacylCoAMAT \rightarrow 12.4$ ,  $KmmckatCoAMAT \rightarrow 26.6$ ,  
 $KmmckatC14AcylCoAMAT \rightarrow 13.83$ ,  $KmmckatC16AcylCoAMAT \rightarrow 13.83$ ,  
 $KmmckatC12AcylCoAMAT \rightarrow 13.83$ ,  $KmmckatC10AcylCoAMAT \rightarrow 13.83$ ,  
 $KmmckatC8AcylCoAMAT \rightarrow 13.83$ ,  $KmmckatC6AcylCoAMAT \rightarrow 13.83$ ,  
 $KmmckatC4AcylCoAMAT \rightarrow 13.83$ ,  $KmmckatAcetylCoAMAT \rightarrow 30$ ,  $Keqmckat \rightarrow 1051$ ,  
 $SfntpC16 \rightarrow 1$ ,  $SfntpC14 \rightarrow 0.9$ ,  $SfntpC12 \rightarrow 0.81$ ,  $SfntpC10 \rightarrow 0.73$ ,  $SfntpC8 \rightarrow 0.34$ ,  
 $Vntp \rightarrow 2.84$ ,  $KmmtpC16EnoylCoAMAT \rightarrow 25$ ,  $KmmtpC14EnoylCoAMAT \rightarrow 25$ ,  
 $KmmtpC12EnoylCoAMAT \rightarrow 25$ ,  $KmmtpC10EnoylCoAMAT \rightarrow 25$ ,  $KmmtpC8EnoylCoAMAT \rightarrow 25$ ,  
 $KmmtpNADMAT \rightarrow 60$ ,  $KmmtpCoAMAT \rightarrow 30$ ,  $KmmtpC14AcylCoAMAT \rightarrow 13.83$ ,  
 $KmmtpC16AcylCoAMAT \rightarrow 13.83$ ,  $KmmtpC12AcylCoAMAT \rightarrow 13.83$ ,  
 $KmmtpC10AcylCoAMAT \rightarrow 13.83$ ,  $KmmtpC8AcylCoAMAT \rightarrow 13.83$ ,  $KmmtpC6AcylCoAMAT \rightarrow 13.83$ ,  
 $KmmtpNADMAT \rightarrow 50$ ,  $KmmtpAcetylCoAMAT \rightarrow 30$ ,  $Keqmt \rightarrow 0.71$ ,  
 $Ksacesink \rightarrow 6\ 000\ 000$ ,  $K1acesink \rightarrow 70$ ,  $Ksfadhsink \rightarrow 6\ 000\ 000$ ,  
 $K1fadhsink \rightarrow 0.46$ ,  $Ksnadhsink \rightarrow 6\ 000\ 000$ ,  $K1nadhsink \rightarrow 12$ ,  
 $C16AcylCoACYT \rightarrow X$ ,  $CarCYT \rightarrow 200$ ,  $CoACYT \rightarrow 140$ ,  $MalCoACYT \rightarrow 0$ ,  
 $CarMAT \rightarrow 950$ ,  $FADtMAT \rightarrow 0.77$ ,  $NADtMAT \rightarrow 250$ ,  $CoAMATT \rightarrow 5000$ ,  
 $VCYT \rightarrow 2.2 * 10^{-6}$ ,  $VMAT \rightarrow 1.8 * 10^{-6}$ ; };

```

tsolScanW0[X_] :=
NDSolve[Join[ODEs /. RateEqs /. CoAMATX /. ParmScan[X], InitialConditions],
```

```

Vars, {t, 0, 1000000000}];

SsScan[X_] := Module[{SSGuess},
  SSGuess := Table[{Vars[[i]][t],
    (Vars[[i]][900000000] /. tsolScanWO[X])[[1]]}, {i, 1, Length[Vars]}];
  FindRoot[Table[Odes[[i, 2]] == 0, {i, 1, Length[Odes]}] /. RateEqs /. CoAMATX /.
    ParmScan[X], SSGuess]];

In[]:= ScanDownNDSWO[Xstart_, dX_, Xend_] := Monitor[Module[{SS, SSGuess},
  DataDownNDSflux = {};
  DataDownC16AcylCoAMAT = {};
  DataDownNDSconc = {};
  DataDownNDSc4coa = {};
  DataDownNDSc6coa = {};
  DataDownNDSc4c6coa = {};
  DataDownNDScintermedcoa = {};
  DataDownNDSfreecoawa = {};

  DataDownNDSvacesink = {};
  DataDownNDSvfadhsink = {};
  DataDownNDSvnadhsink = {};
  tsolStart = tsolScanWO[Xend];
  SSGuess = Table[{Vars[[i]][t],
    (Vars[[i]][900000000] /. tsolStart)[[1]]}, {i, 1, Length[Vars]}];
  SSGuess1 = SSGuess[[All, 1]];
  SSGuess2 = SSGuess[[All, 2]];
  SSGuess1int = SSGuess1 /. t → 0;
  InitialConditionsUD = Thread[SSGuess1int == SSGuess2];

  For[X = Xend, X ≥ Xstart,
    tsolScanNDS = NDSolve[Join[Odes /. RateEqs /. CoAMATX /. ParmScan[X],
      InitialConditionsUD], Vars, {t, 0, 1000000000}];
    SSGuess = Table[{Vars[[i]][t], (Vars[[i]][900000000] /. tsolScanNDS)[[1]]},
      {i, 1, Length[Vars]}];
    SSGuess1 = SSGuess[[All, 1]];
    SSGuess2 = SSGuess[[All, 2]];
    SSGuess1int = SSGuess1 /. t → 0;
    InitialConditionsUD = Thread[SSGuess1int == SSGuess2];
    SS = Thread[SSGuess1 → SSGuess2];

    c4coa = C4AcylCoAMAT[t] + C4EnoylCoAMAT[t] +
      C4HydroxyacylCoAMAT[t] + C4AcetoacylCoAMAT[t] /. SS;
    c6coa = C6AcylCoAMAT[t] + C6EnoylCoAMAT[t] + C6HydroxyacylCoAMAT[t] +
      C6KetoacylCoAMAT[t] /. SS;
    c4c6coa = c4coa + c6coa;
    intermediatecoa =
      C4AcylCoAMAT[t] + C4EnoylCoAMAT[t] + C4HydroxyacylCoAMAT[t] + C4AcetoacylCoAMAT[t] +
      C6AcylCoAMAT[t] + C6EnoylCoAMAT[t] + C6HydroxyacylCoAMAT[t] +
      C6KetoacylCoAMAT[t] + C8AcylCoAMAT[t] + C8EnoylCoAMAT[t] +
      C8HydroxyacylCoAMAT[t] + C8KetoacylCoAMAT[t] + C10AcylCoAMAT[t] +
      C10EnoylCoAMAT[t] + C10HydroxyacylCoAMAT[t] + C10KetoacylCoAMAT[t] +
      C12AcylCoAMAT[t] + C12EnoylCoAMAT[t] + C12HydroxyacylCoAMAT[t] +
      C12KetoacylCoAMAT[t] + C14AcylCoAMAT[t] + C14EnoylCoAMAT[t] +
      C14HydroxyacylCoAMAT[t] + C14KetoacylCoAMAT[t]
  ];

```

```

C14HydroxyacylCoAMAT[t] + C14KetoacylCoAMAT[t] + C16AcylCoAMAT[t] +
C16EnoylCoAMAT[t] + C16HydroxyacylCoAMAT[t] + C16KetoacylCoAMAT[t] /. SS;
freeCoa = CoAMATt - intermediatecoa - 70 /. CoAMATX /. ParmScan[X] /. SS;

DC16AcylCoAMAT = C16AcylCoAMAT[t] /. SS;
C16AcylCarnitineCYT = C16AcylCarCYT[t] /. SS;
C14AcylCarnitineCYT = C14AcylCarCYT[t] /. SS;
C12AcylCarnitineCYT = C12AcylCarCYT[t] /. SS;
C10AcylCarnitineCYT = C10AcylCarCYT[t] /. SS;
C8AcylCarnitineCYT = C8AcylCarCYT[t] /. SS;
C6AcylCarnitineCYT = C6AcylCarCYT[t] /. SS;
C4AcylCarnitineCYT = C4AcylCarCYT[t] /. SS;
AppendTo[DataDownC16AcylCoAMAT, {X, DC16AcylCoAMAT}];
AppendTo[DataDownNDSflux,
{X, 10^3 vcactC16 /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}]];
AppendTo[DataDownNDSc4coa, {X, c4coa}];
AppendTo[DataDownNDSc6coa, {X, c6coa}];
AppendTo[DataDownNDSc4c6coa, {X, c4c6coa}];
AppendTo[DataDownNDScintermedcoa, {X, intermediatecoa}];
AppendTo[DataDownNDSfreecoawa, {X, freeCoa}];

AppendTo[DataDownNDSvacesink,
{X, 10^3 vacesink /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
AppendTo[DataDownNDSvfadhsink,
{X, 10^3 vfadhsink /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
AppendTo[DataDownNDSvnadhsink,
{X, 10^3 vnadhsink /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
X = X - dX;
], ProgressIndicator[X, {Xstart, Xend}]]

```

In[]:= ScanDownNDSWO[0, 1, 250]

```

In[]:= ScanUpNDSWO[Xstart_, dx_, Xend_] := Monitor[Module[{SS, SSGuess},
DataUpNDSflux = {};
DataUpC16AcylCoAMAT == {};
DataUpNDSconc = {};
DataUpNDSc4coa = {};
DataUpNDSc6coa = {};
DataUpNDSc4c6coa = {};
DataUpNDScintermedcoa = {};
DataUpNDSfreecoawa = {};

DataUpNDSvacesink = {};
DataUpNDSvfadhsink = {};
DataUpNDSvnadhsink = {};

tsolStart = tsolScanWO[Xstart];
SSGuess = Table[{Vars[[i]][t],
(Vars[[i]][900000000] /. tsolStart)[[1]]}, {i, 1, Length[Vars]}];
SSGuess1 = SSGuess[[All, 1]];

```

```

SSGuess2 = SSGuess[[All, 2]];
SSGuess1int = SSGuess1 /. t → 0;
InitialConditionsUD = Thread[SSGuess1int == SSGuess2];

For[X = Xstart, X ≤ Xend,

  tsolScanNDS = NDSolve[Join[Odes /. RateEqs /. CoAMATX /. ParmScan[X],
    InitialConditionsUD], Vars, {t, 0, 1000000000}];
  SSGuess = Table[{Vars[[i]][t], (Vars[[i]][900000000] /. tsolScanNDS)[[1]]},
    {i, 1, Length[Vars]}];
  SSGuess1 = SSGuess[[All, 1]];
  SSGuess2 = SSGuess[[All, 2]];
  SSGuess1int = SSGuess1 /. t → 0;
  InitialConditionsUD = Thread[SSGuess1int == SSGuess2];
  SS = Thread[SSGuess1 → SSGuess2];

  c4coa = C4AcylCoAMAT[t] + C4EnoylCoAMAT[t] +
    C4HydroxyacylCoAMAT[t] + C4AcetoacylCoAMAT[t] /. SS;
  c6coa = C6AcylCoAMAT[t] + C6EnoylCoAMAT[t] + C6HydroxyacylCoAMAT[t] +
    C6KetoacylCoAMAT[t] /. SS;
  c4c6coa = c4coa + c6coa;
  intermediatecoa =
    C4AcylCoAMAT[t] + C4EnoylCoAMAT[t] + C4HydroxyacylCoAMAT[t] + C4AcetoacylCoAMAT[t] +
    C6AcylCoAMAT[t] + C6EnoylCoAMAT[t] + C6HydroxyacylCoAMAT[t] +
    C6KetoacylCoAMAT[t] + C8AcylCoAMAT[t] + C8EnoylCoAMAT[t] +
    C8HydroxyacylCoAMAT[t] + C8KetoacylCoAMAT[t] + C10AcylCoAMAT[t] +
    C10EnoylCoAMAT[t] + C10HydroxyacylCoAMAT[t] + C10KetoacylCoAMAT[t] +
    C12AcylCoAMAT[t] + C12EnoylCoAMAT[t] + C12HydroxyacylCoAMAT[t] +
    C12KetoacylCoAMAT[t] + C14AcylCoAMAT[t] + C14EnoylCoAMAT[t] +
    C14HydroxyacylCoAMAT[t] + C14KetoacylCoAMAT[t] + C16AcylCoAMAT[t] +
    C16EnoylCoAMAT[t] + C16HydroxyacylCoAMAT[t] + C16KetoacylCoAMAT[t] /. SS;
  freeCoa = CoAMATt - intermediatecoa - 70 /. CoAMATX /. ParmScan[X] /. SS;

  DC16AcylCoAMAT = C16AcylCoAMAT[t] /. SS;
  C16AcylCarnitineCYT = C16AcylCarCYT[t] /. SS;
  C14AcylCarnitineCYT = C14AcylCarCYT[t] /. SS;
  C12AcylCarnitineCYT = C12AcylCarCYT[t] /. SS;
  C10AcylCarnitineCYT = C10AcylCarCYT[t] /. SS;
  C8AcylCarnitineCYT = C8AcylCarCYT[t] /. SS;
  C6AcylCarnitineCYT = C6AcylCarCYT[t] /. SS;
  C4AcylCarnitineCYT = C4AcylCarCYT[t] /. SS;
  AppendTo[DataUpC16AcylCoAMAT, {X, DC16AcylCoAMAT}];

  AppendTo[DataUpNDSflux,
    {X, 10^3 vcactC16 /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
  AppendTo[DataUpNDSc4coa, {X, c4coa}];
  AppendTo[DataUpNDSc6coa, {X, c6coa}];
  AppendTo[DataUpNDSc4c6coa, {X, c4c6coa}];
  AppendTo[DataUpNDScintermedcoa, {X, intermediatecoa}];
  AppendTo[DataUpNDSfreecoawa, {X, freeCoa}];

  AppendTo[DataUpNDSvacesink,
    {X, 10^3 vacesink /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];

```

```

AppendTo[DataUpNDSvfadhsink,
{X, 103 vfadhsink /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
AppendTo[DataUpNDSvnadhsink,
{X, 103 vnadhsink /. RateEqs /. CoAMATX /. ParmScan[X] /. SS}];
X = X + dX;
], ProgressIndicator[X, {Xstart, Xend}]]

```

In[<sup>10</sup>]:= ScanUpNDSW0[0, 1, 250]

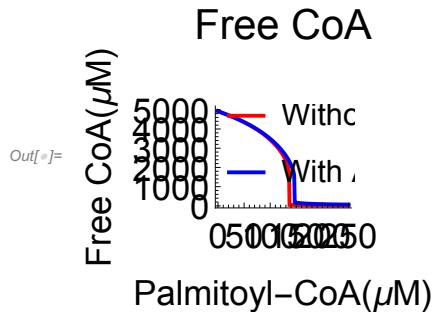
... AppendTo: DataUpC16AcylCoAMAT is not a variable with a value, so its value cannot be changed.  
... AppendTo: DataUpC16AcylCoAMAT is not a variable with a value, so its value cannot be changed.  
... AppendTo: DataUpC16AcylCoAMAT is not a variable with a value, so its value cannot be changed.  
... General: Further output of AppendTo::value will be suppressed during this calculation.

## Steady state plots for varying palmitoyl-CoA with and without ACOT

```

In[11]:= ListLinePlot[{DataUpNDSfreecoawa, DataUpNDSfreecoa},
PlotRange -> All, PlotStyle -> {Red, Blue}, AxesStyle -> Directive[Black, 16],
LabelStyle -> Directive[Black], Frame -> {{True, False}, {True, False}},
FrameLabel -> {"Free CoA(μM)", "None", {"Palmitoyl-CoA(μM)", "Palmitoyl-CoA(μM)"}, None},
PlotLegends -> Placed[LineLegend[{"Without ACOT", "With ACOT"}, {FontSize -> 16}], {Left, Bottom}],
PlotLabel -> "Free CoA",
BaseStyle -> {FontSize -> 18, FontWeight -> "3", AbsoluteThickness[2]},
FrameStyle -> Thickness[0.00005], ImageSize -> Scaled[0.3], AspectRatio -> 0.75]

```



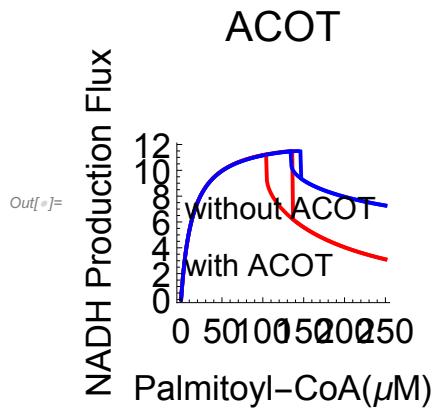
In[<sup>12</sup>]:=

```

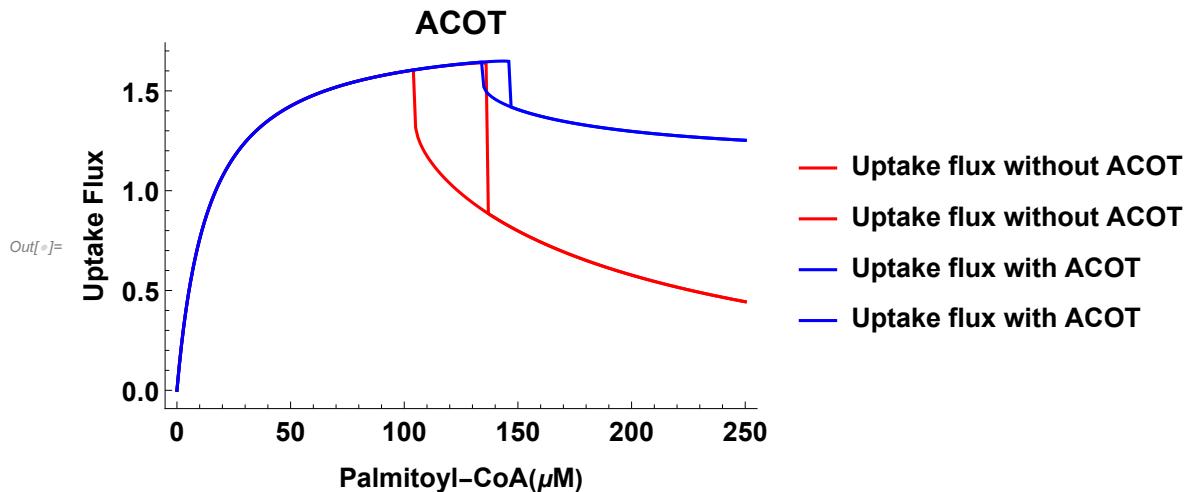
PlotLegends -> Placed[LineLegend[{"WT", "ShcKO"}, {LegendMarkerSize -> {{30, 10}}, LabelStyle -> {FontSize -> 18}}], {Right, Bottom}]

```

```
In[]:= ListLinePlot[{DataUpNDSvnadhsink, DataUpNDSvnadhsinkACOT, DataDownNDSvnadhsink,
  DataDownNDSvnadhsinkACOT}, PlotRange -> All, PlotStyle -> {Red, Blue, Red, Blue},
  AxesStyle -> Directive[Black, 16], LabelStyle -> Directive[Black],
  Frame -> {{True, False}, {True, False}}, FrameLabel -> {"NADH Production Flux", None},
  {"Palmitoyl-CoA(μM)", "Palmitoyl-CoA(μM)"}, PlotLegends ->
  Placed[LineLegend[{"NADH production without ACOT", "NADH production with ACOT"}, 
    LabelStyle -> {FontSize -> 16}], {Right, Bottom}], PlotLabel -> "ACOT",
  BaseStyle -> {FontSize -> 18, FontWeight -> "3", AbsoluteThickness[2]},
  FrameStyle -> Thickness[0.00005], ImageSize -> Scaled[0.3], AspectRatio -> 0.75]
```



```
In[]:= ListLinePlot[{DataUpNDSflux, DataDownNDSflux, DataUpNDSfluxacot, DataDownNDSfluxacot},
  PlotRange -> All, PlotStyle -> {Red, Red, Blue, Blue}, AxesStyle -> Directive[Black, 14],
  LabelStyle -> Directive[14, Black, Bold], Frame -> {{True, False}, {True, False}},
  FrameLabel -> {"Uptake Flux", None}, {"Palmitoyl-CoA(μM)", "Palmitoyl-CoA(μM)"}, 
  PlotLegends -> {"Uptake flux without ACOT", "Uptake flux without ACOT",
    "Uptake flux with ACOT", "Uptake flux with ACOT"}, PlotLabel -> "ACOT"]
```



### Ratio of NADH production flux to CPT1 or Uptake flux without and with ACOT

```
In[]:= NADHtoCPT1upwithoutACOT = DataUpNDSvnadhsink[[All, 2]] / DataUpNDSflux[[All, 2]];
In[]:= NADHtoCPT1downwithoutACOT = DataDownNDSvnadhsink[[All, 2]] / DataDownNDSflux[[All, 2]];
```

```

In[]:= NADHtoCPT1upwithACOT = DataUpNDSvnadhsinkACOT[[All, 2]] / DataUpNDSfluxacot[[All, 2]];

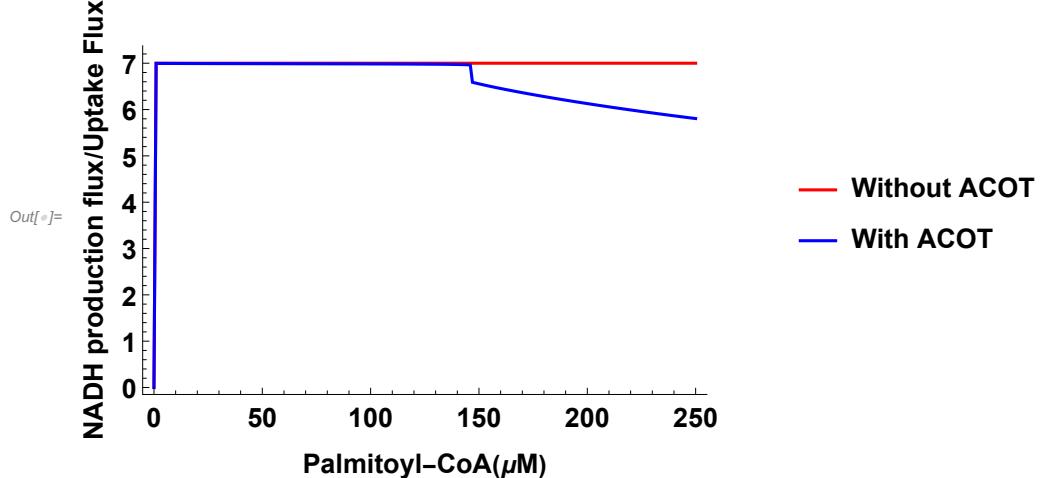
NADHtoCPT1DownwithACOT =
  DataDownNDSvnadhsinkACOT[[All, 2]] / DataDownNDSfluxacot[[All, 2]];

In[]:= (*ListLinePlot[{Thread[{DataUpNDSflux[[All,1]],NADHtoCPT1upwithoutACOT}],
 Thread[{DataDownNDSflux[[All,1]],NADHtoCPT1downwithoutACOT}],
 Thread[{DataUpNDSflux[[All,1]],NADHtoCPT1upwithACOT}],
 Thread[{DataDownNDSflux[[All,1]],NADHtoCPT1DownwithACOT}]],PlotRange->All,
 PlotStyle->{Red,Red,Blue,Blue}, AxesStyle->Directive[Black,14],
 LabelStyle->Directive[14,Black,Bold], Frame->{{True,False},{True,False}},
 FrameLabel->{{"NADH production flux/Uptake Flux",None},
 {"Palmitoyl-CoA(μM)", "Palmitoyl-CoA(μM)"}},
 PlotLegends->{"NADH production flux/Uptake Flux without ACOT",
 "NADH production flux/Uptake Flux without ACOT",
 "NADH production flux/Uptake Flux with ACOT",
 "NADH production flux/Uptake Flux with ACOT"},PlotLabel->"ACOT"]*)

In[]:= ListLinePlot[{Thread[{DataUpNDSflux[[All, 1]], NADHtoCPT1upwithoutACOT}],
 Thread[{DataUpNDSflux[[All, 1]], NADHtoCPT1upwithACOT}]},
 PlotRange -> All, PlotStyle -> {Red, Blue}, AxesStyle -> Directive[Black, 14],
 LabelStyle -> Directive[14, Black, Bold], Frame -> {{True, False}, {True, False}},
 FrameLabel -> {{"NADH production flux/Uptake Flux", None},
 {"Palmitoyl-CoA(μM)", "Palmitoyl-CoA(μM)"}},
 PlotLegends -> {"Without ACOT", "With ACOT"},
 PlotLabel -> "Ratio of NADH production flux to uptake flux"]

```

### Ratio of NADH production flux to uptake flux



```
In[]:= ListLinePlot[{Thread[{DataDownNDSflux[[All, 1]], NADHtoCPT1downwithoutACOT}],  
 Thread[{DataDownNDSflux[[All, 1]], NADHtoCPT1DownwithACOT}]],  
 PlotRange → All, PlotStyle → {Red, Blue}, AxesStyle → Directive[Black, 14],  
 LabelStyle → Directive[14, Black, Bold], Frame → {{True, False}, {True, False}},  
 FrameLabel → {"NADH production flux/Uptake Flux", None},  
 {"Palmitoyl-CoA(μM)", "Palmitoyl-CoA(μM)"},  
 PlotLegends → {"Without ACOT", "With ACOT"},  
 PlotLabel → "Ratio of NADH production flux to uptake flux"]
```

