SBML Model Report

Model name: "Rao2014 - Fatty acid beta-oxidation (reduced model)"



May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: RaoShodhan¹ and JutyNick² at February 28th 2014 at 12:50 a. m. Table 1 gives an overview of the quantities of all components of this model.

Table 1: Number of components in this model, which are described in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	2
species types	0	species	55
events	0	constraints	0
reactions	37	function definitions	48
global parameters	140	unit definitions	2
rules	2	initial assignments	0

Model Notes

This represents the reduced version of the {\textquotestraightdblbase}time course model{

¹University Medical Center, Groningen, shodhanr@gmail.com

²EMBL-EBI, juty@ebi.ac.uk

2 Unit Definitions

This is an overview of five unit definitions of which three are predefined by SBML and not mentioned in the model.

2.1 Unit time

Definition 60 s

2.2 Unit substance

Definition µmol

2.3 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition 1

2.4 Unit area

Notes Square metre is the predefined SBML unit for area since SBML Level 2 Version 1.

Definition m²

2.5 Unit length

Notes Metre is the predefined SBML unit for length since SBML Level 2 Version 1.

Definition m

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
VCYT	VCYT		3	0.01	1		
VMAT	VMAT		3	$1.8\cdot10^{-6}$	1	$\overline{\mathbb{Z}}$	

3.1 Compartment VCYT

This is a three dimensional compartment with a constant size of 0.01 litre.

Name VCYT

3.2 Compartment VMAT

This is a three dimensional compartment with a constant size of $1.8 \cdot 10^{-6}$ litre.

Name VMAT

4 Species

This model contains 55 species. The boundary condition of 24 of these species is set to true so that these species' amount cannot be changed by any reaction. Section 9 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
C16AcylCarCYT	C16AcylCarCYT	VCYT	$\mu \text{mol} \cdot l^{-1}$ $\mu \text{mol} \cdot l^{-1}$	 B	
C14AcylCarCYT C12AcylCarCYT	C14AcylCarCYT C12AcylCarCYT	VCYT VCYT	$\mu \text{mol} \cdot l^{-1}$		
C10AcylCarCYT C8AcylCarCYT	C10AcylCarCYT C8AcylCarCYT	VCYT VCYT	μ mol \cdot l $^{-1}$ μ mol \cdot l $^{-1}$		
C6AcylCarCYT	C6AcylCarCYT	VCYT	$\mu \text{mol} \cdot l^{-1}$		\Box
C4AcylCarCYT C16AcylCoACYT	C4AcylCarCYT C16AcylCoACYT	VCYT VCYT	$μ$ mol · l $^{-1}$ $μ$ mol · l $^{-1}$		⊟ ☑
CarCYT	CarCYT	VCYT	$\begin{array}{c} \mu mol \cdot l^{-1} \\ \mu mol \cdot l^{-1} \end{array}$	$\mathbf{Z}_{\underline{\cdot}}$	\square
CoACYT MalCoACYT	CoACYT MalCoACYT	VCYT VCYT	$\mu mol \cdot l^{-1}$	✓	1
C16AcylCarMAT C16AcylCoAMAT	C16AcylCarMAT C16AcylCoAMAT	VMAT VMAT	μ mol \cdot l $^{-1}$ μ mol \cdot l $^{-1}$		
C16EnoylCoAMAT	C16EnoylCoAMAT	VMAT	$\mu \text{mol} \cdot l^{-1}$		
C16HydroxyacylCoAM C16KetoacylCoAMAT	ATC16HydroxyacylCoAMAT C16KetoacylCoAMAT	VMAT VMAT	μ mol · l $^{-1}$ μ mol · l $^{-1}$	Z	Z
C14AcylCarMAT	C14AcylCarMAT	VMAT	$\mu \text{mol} \cdot l^{-1}$		\Box
C14AcylCoAMAT C14EnoylCoAMAT	C14AcylCoAMAT C14EnoylCoAMAT	VMAT VMAT	μ mol · l ⁻¹ μ mol · l ⁻¹		
C14HydroxyacylCoAM	ATC14HydroxyacylCoAMAT	VMAT	$\mu \text{mol} \cdot l^{-1}$		
C14KetoacylCoAMAT	C14KetoacylCoAMAT	VMAT	μ mol·l ⁻¹		

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
C12AcylCarMAT	C12AcylCarMAT	VMAT	μ mol·l ⁻¹		
C12AcylCoAMAT	C12AcylCoAMAT	VMAT	$\mu \text{mol} \cdot l^{-1}$		
C12EnoylCoAMAT	C12EnoylCoAMAT	VMAT	$\mu mol \cdot l^{-1}$		
C12HydroxyacylCoAM	ATC12HydroxyacylCoAMAT	VMAT	μ mol·l ⁻¹	\square	
C12KetoacylCoAMAT	C12KetoacylCoAMAT	VMAT	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$	$\overline{\mathbf{Z}}$
C10AcylCarMAT	C10AcylCarMAT	VMAT	$\mu \text{mol} \cdot l^{-1}$		
C10AcylCoAMAT	C10AcylCoAMAT	VMAT	μ mol·l ⁻¹		
C10EnoylCoAMAT	C10EnoylCoAMAT	VMAT	μ mol·l ⁻¹		
C10HydroxyacylCoAM	ATC10HydroxyacylCoAMAT	VMAT	$\mu \text{mol} \cdot l^{-1}$	\square	
C10KetoacylCoAMAT	C10KetoacylCoAMAT	VMAT	$\mu \text{mol} \cdot l^{-1}$	$\overline{\mathbf{Z}}$	$\overline{\mathbf{Z}}$
C8AcylCarMAT	C8AcylCarMAT	VMAT	$\mu mol \cdot l^{-1}$		
C8AcylCoAMAT	C8AcylCoAMAT	VMAT	$\mu mol \cdot l^{-1}$		
C8EnoylCoAMAT	C8EnoylCoAMAT	VMAT	μ mol·l ⁻¹		
C8HydroxyacylCoAMA'	T C8HydroxyacylCoAMAT	VMAT	$\mu \text{mol} \cdot l^{-1}$	\square	
C8KetoacylCoAMAT	C8KetoacylCoAMAT	VMAT	$\mu mol \cdot l^{-1}$		$\overline{\mathbf{Z}}$
C6AcylCarMAT	C6AcylCarMAT	VMAT	$\mu mol \cdot l^{-1}$		
C6AcylCoAMAT	C6AcylCoAMAT	VMAT	μ mol·l ⁻¹		
C6EnoylCoAMAT	C6EnoylCoAMAT	VMAT	$\mu \text{mol} \cdot l^{-1}$		
C6HydroxyacylCoAMA	T C6HydroxyacylCoAMAT	VMAT	$\mu mol \cdot l^{-1}$	\square	
C6KetoacylCoAMAT	C6KetoacylCoAMAT	VMAT	μ mol·l ⁻¹		
C4AcylCarMAT	C4AcylCarMAT	VMAT	μ mol·l ⁻¹		
C4AcylCoAMAT	C4AcylCoAMAT	VMAT	μ mol·l ⁻¹		
C4EnoylCoAMAT	C4EnoylCoAMAT	VMAT	μ mol·l ⁻¹		
C4HydroxyacylCoAMA	T C4HydroxyacylCoAMAT	VMAT	$\mu mol \cdot l^{-1}$	\square	
C4AcetoacylCoAMAT	C4AcetoacylCoAMAT	VMAT	$\mu mol \cdot l^{-1}$		
AcetylCoAMAT	AcetylCoAMAT	VMAT	$\mu mol \cdot l^{-1}$		
FADHMAT	FADHMAT	VMAT	$\mu \text{mol} \cdot l^{-1}$	\square	

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi-
					tion
NADHMAT	NADHMAT	VMAT	μ mol·l ⁻¹		$ \overline{Z} $
CoAMAT	CoAMAT	VMAT	μ mol·l ⁻¹		$\overline{\mathbf{Z}}$
CarMAT	CarMAT	VMAT	μ mol·l $^{-1}$		$\overline{\mathbf{Z}}$
FADtMAT	FADtMAT	VMAT	μ mol·l $^{-1}$	$ \overline{\mathbf{Z}} $	$\overline{\mathbf{Z}}$
NADtMAT	NADtMAT	VMAT	$\mu mol \cdot l^{-1}$	$ \overline{\mathbf{Z}} $	$\overline{\mathbf{Z}}$
CoAMATt	CoAMATt	VMAT	$\mu mol \cdot l^{-1}$		
${ t species}_{ extsf{-}} 1$	NAD	VMAT	$\mu mol \cdot l^{-1}$	\square	

5 Parameters

This model contains 140 global parameters.

Table 4: Properties of each parameter.

Id	Name SBO	Value Value	Unit	Constant
Vfcact	Vfcact	0.420		✓
Vrcact	Vrcact	0.420		$\overline{\mathbb{Z}}$
${\tt KmcactCarMAT}$	KmcactCarMAT	130.000		$\overline{\mathbb{Z}}$
${\tt KmcactCarCYT}$	KmcactCarCYT	130.000		$\overline{\mathbb{Z}}$
KicactCarCYT	KicactCarCYT	200.000		$\overline{\checkmark}$
Keqcact	Keqcact	1.000		$\overline{\mathbf{Z}}$
Vcpt2	Vcpt2	0.391		$\overline{\mathbf{Z}}$
Kmcpt2C16Acyl	Cakemacpt2C16AcylCarMAT	51.000		$\overline{\mathbf{Z}}$
Kmcpt2C14Acyl	Cakemacpt2C14AcylCarMAT	51.000		$\overline{\mathbf{Z}}$
Kmcpt2C12Acyl	Cakemacpt2C12AcylCarMAT	51.000		$\overline{\mathbf{Z}}$
Kmcpt2C10Acyl	Caccomaca de la Caccomaca de l	51.000		
Kmcpt2C8AcylC	arknatept2C8AcylCarMAT	51.000		
Kmcpt2C6AcylC	arknatept2C6AcylCarMAT	51.000		\square
Kmcpt2C4AcylC	addatept2C4AcylCarMAT	51.000		
Kmcpt2CoAMAT	Kmcpt2CoAMAT	30.000		$ \overline{\mathscr{A}} $
Kmcpt2C16Acyl	Cdamattt2C16AcylCoAMAT	38.000		
Kmcpt2C14Acyl	С <mark>фатаст</mark> рт2С14AcylCoAMAT	38.000		
Kmcpt2C12Acyl	С <mark>фамаф</mark> t2С12AcylCoAMAT	38.000		\square
Kmcpt2C10Acyl	С ф\mar pt2С10AcylCoAMAT	38.000		\square
Kmcpt2C8AcylC	oAMATept2C8AcylCoAMAT	38.000		\square
Kmcpt2C6AcylC	oAMATept2C6AcylCoAMAT	1000.000		
Kmcpt2C4AcylC	o ARMATE pt 2C4A cylCoAMAT	1000000.000		\square
${\tt Kmcpt2CarMAT}$	Kmcpt2CarMAT	350.000		\square
Keqcpt2	Keqcpt2	2.220		\square
Vvlcad	Vvlcad	0.008		\square
KmvlcadC16Acy	1 06an√a dadC16AcylCoAMA′	Γ 6.500		
KmvlcadC14Acy	1 КыАМА ФаdC14AcylCoAMA	Γ 4.000		\square
KmvlcadC12Acy	1 -166/AWA cTadC12AcylCoAMA	Γ 2.700		\square
KmvlcadFAD	KmvlcadFAD	0.120		\square
KmvlcadC16Eno	y lKonAili&atil C16EnoylCoAM <i>I</i>	AT 1.080		\square
KmvlcadC14Eno	y lKonAili&atil C14EnoylCoAM	AT 1.080		\square
KmvlcadC12Eno	y lKonAili&atil C12EnoylCoAM <i>I</i>	AT 1.080		
KmvlcadFADH	KmvlcadFADH	24.200		
Keqvlcad	Keqvlcad	6.000		$ \overline{\checkmark} $
Vlcad	Vlcad	0.010		$\overline{\mathbf{Z}}$
KmlcadC16Acyl	CdAmadadC16AcylCoAMAT	2.500		$\overline{\mathbf{Z}}$
KmlcadC14Acyl	CdamadadC14AcylCoAMAT	7.400		\mathbf{Z}

Id	Name SBO	Value	Unit	Constant
KmlcadC12Ac	y1Cd AmA tadC12AcylCoAMAT	9.000	<u></u>	✓
KmlcadC10Ac	y1CdamadadC10AcylCoAMAT	24.300		
KmlcadC8Acy	LCo AXIATI cadC8AcylCoAMAT	123.000		
KmlcadFAD	KmlcadFAD	0.120		$ \mathbf{Z} $
KmlcadC16End	oyl (KankatiC16EnoylCoAMAT	1.080		$ \mathbf{Z} $
KmlcadC14End	oyl (KankatiC14EnoylCoAMAT	1.080		$ \mathbf{Z} $
KmlcadC12End	oyl (KankardC12EnoylCoAMAT	1.080		
KmlcadC10End	oyl (KankatiC10EnoylCoAMAT	1.080		
KmlcadC8Eno	y1Cd AMA dadC8EnoylCoAMAT	1.080		
${\tt KmlcadFADH}$	KmlcadFADH	24.200		
Keqlcad	Keqlcad	6.000		
Vmcad	Vmcad	0.081		
KmmcadC12Ac	y1CdAmancadC12AcylCoAMAT	5.700		\square
KmmcadC10Ac	y1CdAmancadC10AcylCoAMAT	5.400		\square
KmmcadC8Acy	LCo ÆĭAtī ncadC8AcylCoAMAT	4.000		\square
KmmcadC6Acy	LCo AXIA TncadC6AcylCoAMAT	9.400		
KmmcadC4Acy	LCo ÆMAT ncadC4AcylCoAMAT	135.000		
KmmcadFAD	KmmcadFAD	0.120		
KmmcadC12End	oy1 66AMA TadC12EnoylCoAMAT	1.080		
KmmcadC10Enc	oy1 06AMA @adC10EnoylCoAMAT	1.080		\square
KmmcadC8Eno	y1Cd4MantcadC8EnoylCoAMAT	1.080		\square
KmmcadC6Eno	y1CdAmancadC6EnoylCoAMAT	1.080		\square
KmmcadC4Eno	y1Cd4MantcadC4EnoylCoAMAT	1.080		\square
${\tt KmmcadFADH}$	KmmcadFADH	24.200		\square
Keqmcad	Keqmcad	6.000		\square
Vscad	Vscad	0.081		
KmscadC6Acy	LCoAMATEcadC6AcylCoAMAT	285.000		\square
KmscadC4Acy	LCoAMATEcadC4AcylCoAMAT	10.700		\square
${\tt KmscadFAD}$	KmscadFAD	0.120		
KmscadC6Eno	y1Cd Ama tadC6EnoylCoAMAT	1.080		\square
KmscadC4Eno	y1Cd Ama tadC4EnoylCoAMAT	1.080		\square
${\tt KmscadFADH}$	KmscadFADH	24.200		\square
Keqscad	Keqscad	6.000		\square
Vcrot	Vcrot	3.600		
KmcrotC16En	oyl (KantacitC16EnoylCoAMAT	150.000		
	oyl (KantactC14EnoylCoAMAT	100.000		
	oyl (Kantant C12 Enoyl CoAMAT	25.000		\square
	oyl (Kantant C10 Enoyl CoAMAT	25.000		\square
•	y1Cd4MacFotC8EnoylCoAMAT	25.000		
	y1Cd4MacFotC6EnoylCoAMAT	25.000		
•	y1Cd4MacFotC4EnoylCoAMAT	40.000		
KmcrotC16Hy	dro xkymcydi@dAMA JfdroxyacylCoA	MAT 45.000		\square

Id	Name	SBO	Value	Unit	Constant
KmcrotC14H	ydrox KymcydiColAMA yd	roxyacylCoAM	AT 45.000		Ø
KmcrotC12H	ydrox KymcydtColAMA yId	roxyacylCoAM	AT 45.000		\square
KmcrotC10H	ydrox KymcydtColAYHJ Jd	roxyacylCoAM	AT 45.000		\square
KmcrotC8Hy	droxy KanychotoAMA yTdro	oxyacylCoAMA	T 45.000		\square
KmcrotC6Hy	droxy KanychotoA9Hay dro	oxyacylCoAMA	T 45.000		$ \overline{\mathbf{Z}} $
KmcrotC4Hy	droxy KanychotoAMA yTdro	oxyacylCoAMA	T 45.000		$ \overline{\mathscr{A}} $
KicrotC4Ac	etoad yibCot/ C4Acetoa	cylCoA	1.600		$ \mathbf{Z} $
Keqcrot	Keqcrot		3.130		
Vmschad	Vmschad		1.000		
KmmschadC1	6HydrKonnynascyhla d6AM6A	H ydroxyacylCo.	AMAT.500		$\overline{\mathbf{Z}}$
KmmschadC1	4Hydr Komynascyhlad GAIMM	f ydroxyacylCo.	AMAT.800		
KmmschadC1	2Hydr Komynascyliad6AMA	f ydroxyacylCo.	AMA T .700		
KmmschadC1	OHydr Kornynascyhlad GANOA	f ydroxyacylCo.	AMA % .800		
KmmschadC8	Hydrd xiyrancs;ch@d@N84T	ydroxyacylCoA	MAT6.300		$\overline{\mathbf{Z}}$
KmmschadC6	Hydrd xiyrancs;ch@d@MAT	ydroxyacylCoA	MAT8.600		$ \overline{\mathscr{A}} $
KmmschadC4	Hydrd xiynancs;ch@d@441 T	ydroxyacylCoA	MA T 69.900		
KmmschadNA	DMAT KmmschadNAD	OMAT	58.500		$\overline{\mathbf{Z}}$
KmmschadC1	6KetdKannyn1.CohAnMC1161	KetoacylCoAM	AT 1.400		$\overline{\mathbf{Z}}$
KmmschadC1	4KetdKannynikCohAnMCI141	KetoacylCoAM	AT 1.400		$\overline{\mathbf{Z}}$
KmmschadC1	2KetdKannynikCohAnMCII2I	KetoacylCoAM	AT 1.600		$\overline{\mathbf{Z}}$
KmmschadC1	OKetdKannynikCohAnMCIIOI	KetoacylCoAM	AT 2.300		$\overline{\mathbf{Z}}$
KmmschadC8	Ketoa kcynin0xxx4MAdC 8K	etoacylCoAMA	T 4.100		$\overline{\mathbf{Z}}$
KmmschadC6	Ketoa kiyihûxxAMAIC 6K	etoacylCoAMA	T 5.800		$\overline{\mathbf{Z}}$
KmmschadC4	Acetdamynl.Cohand.CAA	cetoacylCoAM	AT 16.900		$\overline{\mathbb{Z}}$
KmmschadNA	DHMA T KmmschadNAD	HMAT	5.400		$\overline{\mathbf{Z}}$
Keqmschad	Keqmschad		$2.17 \cdot 10^{-4}$		$\overline{\mathbf{Z}}$
Vmckat	Vmckat		0.377		$\overline{\mathbf{Z}}$
KmmckatC16	Ketoa kininodamo 16K	etoacylCoAMA'	Γ 1.100		$\overline{\mathbf{Z}}$
KmmckatC14	Ketoa kin in Kelan (CT 4Ke	etoacylCoAMA	Γ 1.200		$ \overline{\mathbf{Z}} $
KmmckatC12	Ketoa kiyih0kd4MQT 2K6	etoacylCoAMA	Γ 1.300		$\overline{\mathbf{Z}}$
KmmckatC10	Ketoa KryninGckAMCT OK	etoacylCoAMA	Γ 2.100		$\overline{\mathbf{Z}}$
KmmckatC8K	etoad yihthodMAtC 8Ket	oacylCoAMAT	3.200		$\overline{\mathbf{Z}}$
KmmckatC6K	etoad yihthodMAtC 6Ket	oacylCoAMAT	6.700		<u></u>
KmmckatC4A	cetoa kininodamo aAc	etoacylCoAMA	Γ 12.400		<u></u>
KmmckatCoA	MAT KmmckatCoAM	IAT	26.600		<u></u>
KmmckatC14	Acyl Kolamad katC14A	cylCoAMAT	13.830		$\overline{\mathbf{Z}}$
KmmckatC16	Acylo Kannad katC16A	cylCoAMAT	13.830		$\overline{\mathbf{Z}}$
KmmckatC12	Acylo Kannad katC12A	cylCoAMAT	13.830		$\overline{\mathbf{Z}}$
	Acylo Kannad katC10A	•	13.830		$\overline{\mathbf{Z}}$
	cy1Cd AMA nTckatC8Acy	•	13.830		$\overline{\mathbf{Z}}$
KmmckatC6A	cy1Cd AMA nTckatC6Acy	ylCoAMAT	13.830		$\overline{\mathbf{Z}}$
	cylCd AMA nTckatC4Acy		13.830		$\overline{\mathbf{Z}}$

Id	Name SBC) Value	Unit	Constant
KmmckatAcet	y1Cd Ama ntckatAcetylCoAMAT	30.000		
Keqmckat	Keqmckat	1051.000		$\overline{\mathbf{Z}}$
Vmtp	Vmtp	2.840		$ \overline{\checkmark} $
KmmtpC16Eno	y1CdAMantpC16EnoylCoAMA	T 25.000		$\overline{\mathbf{Z}}$
KmmtpC14Eno	y1CdAMantpC14EnoylCoAMA	T 25.000		$\overline{\mathbf{Z}}$
KmmtpC12Eno	y1CdAMantpC12EnoylCoAMA	T 25.000		$\overline{\mathbf{Z}}$
KmmtpC10Eno	y1CdAMantpC10EnoylCoAMA	T 25.000		$\overline{\mathbf{Z}}$
KmmtpC8Enoy	LCo AiXia timtpC8EnoylCoAMAT	25.000		$\overline{\mathbf{Z}}$
KmmtpNADMAT	KmmtpNADMAT	60.000		7
KmmtpCoAMAT	KmmtpCoAMAT	30.000		<u></u>
KmmtpC14Acy	LCo AiMaii mtpC14AcylCoAMAT	13.830		$\overline{\mathbf{Z}}$
KmmtpC16Acy	LCo AiMaii mtpC16AcylCoAMAT	13.830		7
KmmtpC12Acy	LCoAMAThtpC12AcylCoAMAT	13.830		$\overline{\mathbf{Z}}$
KmmtpC10Acy	LCo AiMaii mtpC10AcylCoAMAT	13.830		$\overline{\mathbf{Z}}$
KmmtpC8Acyl	CoAMMITmtpC8AcylCoAMAT	13.830		$\overline{\mathbf{Z}}$
KmmtpC6Acyl	CoAMAThmtpC6AcylCoAMAT	13.830		
KmmtpNADHMA	Г KmmtpNADHMAT	50.000		$\overline{\mathbf{Z}}$
KmmtpAcety10	CoAMAThmtpAcetylCoAMAT	30.000		$\overline{\mathbf{Z}}$
Keqmtp	Keqmtp	0.710		$\overline{\mathbf{Z}}$

6 Function definitions

This is an overview of 48 function definitions.

6.1 Function definition MTP

Name MTP₋₂

Arguments 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

Mathematical Expression

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

6.2 Function definition MCKATB

Name MCKATB_2

Arguments 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

Mathematical Expression

$$\frac{sf \cdot V \cdot \left(\frac{S1 \cdot S8}{Kms1 \cdot Kms8} - \frac{P8 \cdot P8}{Kms1 \cdot Kms8} - \frac{(2)}{Kms1 \cdot Kms8 \cdot Keq}\right)}{\left(1 + \frac{S1}{Kms1} + \frac{P1}{Kmp1} + \frac{S2}{Kms2} + \frac{P2}{Kmp2} + \frac{S3}{Kms3} + \frac{P3}{Kmp3} + \frac{S4}{Kms4} + \frac{P4}{Kmp4} + \frac{S5}{Kms5} + \frac{P5}{Kmp5} + \frac{S6}{Kms6} + \frac{P6}{Kmp6} + \frac{S7}{Kms7} + \frac{P7}{Kmp8} + \frac{P7}{Kmp8}$$

6.3 Function definition MCKATA

Name MCKATA_2

Arguments 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

Mathematical Expression

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

6.4 Function definition RES

Name RES_2

Arguments Ks, S, K1

Mathematical Expression

$$Ks \cdot (S - K1) \tag{4}$$

6.5 Function definition SCAD

Name SCAD_2

Arguments sf, V, Kms1, Kms2, Kms3, Kmp1, Kmp2, Kmp3, Keq, S1, S2, S3, P1, P2, P3

Mathematical Expression

$$\frac{sf \cdot V \cdot \left(\frac{S1 \cdot (S3-P3)}{Kms1 \cdot Kms3} - \frac{P1 \cdot P3}{Kms1 \cdot Kms3 \cdot Keq}\right)}{\left(1 + \frac{S1}{Kms1} + \frac{P1}{Kmp1} + \frac{S2}{Kms2} + \frac{P2}{Kmp2}\right) \cdot \left(1 + \frac{S3-P3}{Kms3} + \frac{P3}{Kmp3}\right)}$$
 (5)

6.6 Function definition LCAD

Name LCAD_2

Arguments 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

Mathematical Expression

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

6.7 Function definition CPT1

Name CPT1_2

Arguments sf, V, Kms1, Kms2, Kmp1, Kmp2, Ki1, Keq, S1, S2, P1, P2, I1, n

Mathematical Expression

$$\frac{sf \cdot V \cdot \left(\frac{S1 \cdot S2}{Kms1 \cdot Kms2} - \frac{P1 \cdot P2}{Kms1 \cdot Kms2 \cdot Keq}\right)}{\left(1 + \frac{S1}{Kms1} + \frac{P1}{Kmp1} + \left(\frac{I1}{Ki1}\right)^n\right) \cdot \left(1 + \frac{S2}{Kms2} + \frac{P2}{Kmp2}\right)}$$
(7)

6.8 Function definition VLCAD

Name VLCAD_2

Arguments sf, V, Kms1, Kms2, Kms3, Kms4, Kmp1, Kmp2, Kmp3, Kmp4, Keq, S1, S2, S3, S4, P1, P2, P3, P4

Mathematical Expression

$$\frac{sf \cdot V \cdot \left(\frac{S1 \cdot (S4 - P4)}{Kms1 \cdot Kms4} - \frac{P1 \cdot P4}{Kms1 \cdot Kms4 \cdot Keq}\right)}{\left(1 + \frac{S1}{Kms1} + \frac{P1}{Kmp1} + \frac{S2}{Kms2} + \frac{P2}{Kmp2} + \frac{S3}{Kms3} + \frac{P3}{Kmp3}\right) \cdot \left(1 + \frac{S4 - P4}{Kms4} + \frac{P4}{Kmp4}\right)}$$
(8)

6.9 Function definition CPT2

Name CPT2_2

Arguments 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

Mathematical Expression

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

6.10 Function definition MCAD

Name MCAD_2

Arguments 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

Mathematical Expression

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

6.11 Function definition function_4_vcpt1C16_1

Name function_4_vcpt1C16_1

Arguments [C16AcylCarCYT], [C16AcylCoACYT], [CarCYT], [CoACYT], Keqcpt1, Kicpt1MalCoACYT, Kmcpt1C16AcylCarCYT, Kmcpt1C16AcylCoACYT, Kmcpt1CarCYT, Kmcpt1CoACYT, [MalCoACYT], vol (VCYT), Vcpt1, ncpt1, sfcpt1C16

Mathematical Expression

CPT1 (sfcpt1C16, Vcpt1, Kmcpt1C16AcylCoACYT, Kmcpt1CarCYT, Kmcpt1C16AcylCarCYT, Kmcpt1CoACYT, (11) vol (V

6.12 Function definition function_4_vcactC16_1

Name function_4_vcactC16_1

Arguments [C16AcylCarCYT], [C16AcylCarMAT], [CarCYT], [CarMAT], Keqcact, KicactC16AcylCarCYT, KicactCarCYT, KmcactC16AcylCarCYT, KmcactC16AcylCarMAT, KmcactCarCYT, KmcactCarMAT, Vfcact, Vrcact

Mathematical Expression

 $\frac{\text{Vfcact} \cdot }{[\text{C16AcylCarCYT}] \cdot [\text{CarMAT}] + \text{KmcactCarMAT} \cdot [\text{C16AcylCarCYT}] + \text{KmcactC16AcylCarCYT} \cdot [\text{CarMAT}] \cdot \left(\frac{(12)}{(12)} + \frac{(12)}{$

6.13 Function definition function_4_vcactC14_1

Name function_4_vcactC14_1

Arguments [C14AcylCarCYT], [C14AcylCarMAT], [CarCYT], [CarMAT], Keqcact, KicactC14AcylCarCYT, KicactCarCYT, KmcactC14AcylCarCYT, KmcactC14AcylCarMAT, KmcactCarCYT, KmcactCarMAT, Vfcact, Vrcact

Mathematical Expression

 $\frac{\text{Vfcact} \cdot }{\left[\text{C14AcylCarCYT}\right] \cdot \left[\text{CarMAT}\right] + \text{KmcactCarMAT} \cdot \left[\text{C14AcylCarCYT}\right] + \text{KmcactC14AcylCarCYT} \cdot \left[\text{CarMAT}\right] \cdot \left(\text{CarMAT}\right] \cdot \left(\text{CarMAT}\right) \cdot \left(\text$

6.14 Function definition function 4 vcactC12 1

Name function_4_vcactC12_1

Arguments [C12AcylCarCYT], [C12AcylCarMAT], [CarCYT], [CarMAT], Keqcact, KicactC12AcylCarCYT, KicactCarCYT, KmcactC12AcylCarCYT, KmcactC12AcylCarMAT, KmcactCarCYT, KmcactCarMAT, Vfcact, Vrcact

Mathematical Expression

 $\frac{\text{Vfcact} \cdot }{[\text{C12AcylCarCYT}] \cdot [\text{CarMAT}] + \text{KmcactCarMAT} \cdot [\text{C12AcylCarCYT}] + \text{KmcactC12AcylCarCYT} \cdot [\text{CarMAT}] \cdot \left(\frac{(14)}{(14)} + \frac{(14)}{$

6.15 Function definition function_4_vcactC10_1

Name function_4_vcactC10_1

Arguments [C10AcylCarCYT], [C10AcylCarMAT], [CarCYT], [CarMAT], Keqcact, KicactC10AcylCarCYT, KicactCarCYT, KmcactC10AcylCarCYT, KmcactC10AcylCarMAT, KmcactCarCYT, KmcactCarMAT, Vfcact, Vrcact

Mathematical Expression

 $\frac{\text{Vfcact} \cdot \\ (15)}{[\text{C10AcylCarCYT}] \cdot [\text{CarMAT}] + \text{KmcactCarMAT} \cdot [\text{C10AcylCarCYT}] + \text{KmcactC10AcylCarCYT} \cdot [\text{CarMAT}] \cdot \left(\frac{(15)}{(15)} \right)}$

6.16 Function definition function_4_vcactC8_1

Name function_4_vcactC8_1

Arguments [C8AcylCarCYT], [C8AcylCarMAT], [CarCYT], [CarMAT], Keqcact, KicactC8AcylCarCYT, KicactCarCYT, KmcactC8AcylCarCYT, KmcactC8AcylCarMAT, KmcactCarCYT, KmcactCarMAT, Vfcact, Vrcact

Mathematical Expression

$$\frac{\text{Vfcact} \cdot \left([\text{CSAcylCarCYT}] \cdot [\text{CarMAT}] + \text{KmcactCarMAT} \cdot [\text{C8AcylCarCYT}] + \text{KmcactC8AcylCarCYT} \cdot [\text{CarMAT}] \cdot \left(1 + \text{CACYLCarCYT} \right) + \text{CACYLCarCYT} \cdot [\text{CarMAT}] \cdot \left(1 + \text{CACYLCarCYT} \right) + \text{CACYLCarCYT} \cdot [\text{CarMAT}] \cdot \left(1 + \text{CACYLCarCYT} \right) + \text{CACYLCarCYT} \cdot [\text{CarMAT}] \cdot \left(1 + \text{CACYLCarCYT} \right) + \text{CACYLCarCYT} \cdot [\text{CarMAT}] \cdot \left(1 + \text{CACYLCarCYT} \right) + \text{CACYLCarCYT} \cdot [\text{CarMAT}] \cdot \left(1 + \text{CACYLCarCYT} \right) + \text{CACYLCarCYT} \cdot [\text{CarMAT}] \cdot \left(1 + \text{CACYLCarCYT} \right) + \text{CACYLCarCYT} \cdot [\text{CarMAT}] \cdot \left(1 + \text{CACYLCarCYT} \right) + \text{CACYLCarCYT} \cdot [\text{CarMAT}] \cdot \left(1 + \text{CACYLCarCYT} \right) + \text{CACYLCarCYT} \cdot [\text{CarMAT}] \cdot \left(1 + \text{CACYLCarCYT} \right) + \text{CACYLCarCYT} \cdot [\text{CarMAT}] \cdot \left(1 + \text{CACYLCarCYT} \right) + \text{CACYLCarCYT} \cdot [\text{CarMAT}] \cdot \left(1 + \text{CACYLCarCYT} \right) + \text{CACYLCarCYT} \cdot [\text{CarMAT}] \cdot \left(1 + \text{CACYLCarCYT} \right) + \text{CACYLCarCYT} \cdot [\text{CarMAT}] \cdot (1 + \text{CACYLCarCYT}) + \text{CACYLCarCYT} \cdot$$

6.17 Function definition function 4 vcactC6 1

Name function_4_vcactC6_1

Arguments [C6AcylCarCYT], [C6AcylCarMAT], [CarCYT], [CarMAT], Keqcact, KicactC6AcylCarCYT, KicactCarCYT, KmcactC6AcylCarCYT, KmcactC6AcylCarMAT, KmcactCarCYT, KmcactCarMAT, Vfcact, Vrcact

Mathematical Expression

$$\frac{\text{Vfcact} \cdot \left([Colored Colored Co$$

6.18 Function definition function_4_vcactC4_1

Name function_4_vcactC4_1

Arguments [C4AcylCarCYT], [C4AcylCarMAT], [CarCYT], [CarMAT], Keqcact, KicactC4AcylCarCYT, KicactCarCYT, KmcactC4AcylCarCYT, KmcactC4AcylCarMAT, KmcactCarCYT, KmcactCarMAT, Vfcact, Vrcact

Mathematical Expression

$$\frac{\text{Vfcact} \cdot \left([\text{C4AcylCarCYT}] \cdot [\text{CarMAT}] + \text{KmcactCarMAT} \cdot [\text{C4AcylCarCYT}] + \text{KmcactC4AcylCarCYT} \cdot [\text{CarMAT}] \cdot \left(1 + \text{C4AcylCarCYT} \right) \right)}{\text{C4AcylCarCYT} \cdot [\text{CarMAT}] \cdot \left(1 + \text{C4AcylCarCYT} \right) \cdot [\text{CarMAT}] \cdot \left(1 + \text{C4AcylCarCYT} \right)}$$

6.19 Function definition function_4_vcpt2C16_1

Name function_4_vcpt2C16_1

Arguments [C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], [C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCarMAT], [C16AcylCarMAT], [C16AcylCarMAT], [C4AcylCarMAT], [C4AcylCarMAT], [C4AcylCarMAT], [C6AcylCoAMAT], [C6AcylCoAMAT], [C8AcylCarMAT], [C8AcylCarMA

Mathematical Expression

CPT2 (sfcpt2C16, Vcpt2, Kmcpt2C16AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C12AcylCarMAT, Kmcp

6.20 Function definition function_4_vcpt2C14_1

Name function_4_vcpt2C14_1

Arguments [C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], [C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCarMAT], [C14AcylCarMAT], [C16AcylCarMAT], [C16AcylCarMAT], [C4AcylCarMAT], [C4AcylCarMAT], [C6AcylCarMAT], [C6AcylCarMAT], [C8AcylCarMAT], [C8AcylC

Mathematical Expression

CPT2 (sfcpt2C14, Vcpt2, Kmcpt2C14AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C12AcylCarMAT, Kmcpt2

6.21 Function definition function_4_vcpt2C12_1

Name function_4_vcpt2C12_1

Arguments [C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], [C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCarMAT], [C14AcylCarMAT], [C16AcylCarMAT], [C16AcylCarMAT], [C4AcylCarMAT], [C4AcylCarMAT], [C6AcylCoAMAT], [C6AcylCoAMAT], [C8AcylCarMAT], [C8AcylC

Mathematical Expression

CPT2 (sfcpt2C12, Vcpt2, Kmcpt2C12AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2

6.22 Function definition function_4_vcpt2C10_1

Name function_4_vcpt2C10_1

Arguments [C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], [C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCarMAT], [C16AcylCarMAT], [C16AcylCarMAT], [C4AcylCarMAT], [C4AcylCarMAT], [C4AcylCarMAT], [C6AcylCarMAT], [C6AcylCarMAT], [C8AcylCarMAT], [C8AcylCarMA

Mathematical Expression

CPT2 (sfcpt2C10, Vcpt2, Kmcpt2C10AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C

6.23 Function definition function_4_vcpt2C8_1

Name function_4_vcpt2C8_1

Arguments [C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], [C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCarMAT], [C16AcylCarMAT], [C16AcylCarMAT], [C4AcylCarMAT], [C4AcylCarMAT], [C4AcylCarMAT], [C6AcylCarMAT], [C6AcylCarMAT], [C8AcylCarMAT], [C8AcylCarMAT], [C8AcylCarMAT], [CarMAT], [CarMAT], [CoAMAT], Keqcpt2, Kmcpt2C10AcylCarMAT, Kmcpt2C10AcylCarMAT, Kmcpt2C12AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C4AcylCarMAT, Kmcpt2C4AcylCarMAT, Kmcpt2C6AcylCarMAT, Kmcpt2C6AcylCarMAT, Kmcpt2C6AcylCarMAT, Kmcpt2C6AcylCarMAT, Kmcpt2C6AcylCarMAT, Kmcpt2C8AcylCarMAT, Kmcpt2C8AcylCarMAT, Kmcpt2CarMAT, Kmcpt2CarMAT, Kmcpt2CarMAT, Kmcpt2CarMAT, Vol (VMAT), Vcpt2, sfcpt2C8

Mathematical Expression

CPT2 (sfcpt2C8, Vcpt2, Kmcpt2C8AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C12AcylCarMAT, Kmcpt2C1

6.24 Function definition function_4_vcpt2C6_1

Name function_4_vcpt2C6_1

Arguments [C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], [C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCarMAT], [C16AcylCarMAT], [C16AcylCarMAT], [C16AcylCoAMAT], [C4AcylCarMAT], [C4AcylCarMAT], [C6AcylCarMAT], [C8AcylCarMAT], [C8AcylC

Mathematical Expression

CPT2 (sfcpt2C6, Vcpt2, Kmcpt2C6AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C12AcylCarMAT, Kmcpt2C1

6.25 Function definition function_4_vcpt2C4_1

Name function_4_vcpt2C4_1

Arguments [C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], [C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCarMAT], [C16AcylCarMAT], [C16AcylCarMAT], [C4AcylCarMAT], [C4AcylCarMAT], [C4AcylCarMAT], [C6AcylCoAMAT], [C6AcylCoAMAT], [C8AcylCarMAT], [C8AcylCarMAT], [C8AcylCarMAT], [CarMAT], [CarMAT], Keqcpt2, Kmcpt2C10AcylCarMAT, Kmcpt2C10AcylCoAMAT, Kmcpt2C12AcylCarMAT, Kmcpt2C12AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C4AcylCarMAT, Kmcpt2C4AcylCarMAT, Kmcpt2C6AcylCarMAT, Vol (VMAT), Vcpt2, sfcpt2C4

Mathematical Expression

CPT2 (sfcpt2C4, Vcpt2, Kmcpt2C4AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C12AcylCarMAT, Kmcpt2C1

6.26 Function definition function_4_vvlcadC16_1

Name function_4_vvlcadC16_1

Arguments [C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [FADHMAT], [FADHMAT], Keqvlcad, KmvlcadC12AcylCoAMAT KmvlcadC12EnoylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC14EnoylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC16EnoylCoAMAT, KmvlcadFAD, KmvlcadFADH, vol (VMAT), Vvlcad, sfvlcadC16

Mathematical Expression

 $\underline{VLCAD\,(sfvlcadC16,Vvlcad,KmvlcadC16AcylCoAMAT,KmvlcadC14AcylCoAMAT,KmvlcadC12AcylCoAMAT,KmvlcadC12AcylCoAMAT,KmvlcadC12AcylCoAMAT,KmvlcadC12AcylCoAMAT,KmvlcadC14AcylCoAMAT,KmvlcadC12AcylCoAMAT,KmvlcadC14AcylCoAMAT,KmvlcadC12AcylCoAMAT,KmvlcadC12AcylCoAMAT,KmvlcadC14AcylCoAMAT,KmvlcadC12AcylCoAMAT,KmvlcadC12AcylCoAMAT,KmvlcadC14AcylCoAMAT,KmvlcadC12AcylCoAMAT,K$

6.27 Function definition function_4_vvlcadC14_1

Name function_4_vvlcadC14_1

Arguments [C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqvlcad, KmvlcadC12AcylCoAMAT KmvlcadC12EnoylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC14EnoylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC16EnoylCoAMAT, KmvlcadFAD, KmvlcadFADH, vol (VMAT), Vvlcad, sfvlcadC14

Mathematical Expression

VLCAD (sfvlcadC14, Vvlcad, KmvlcadC14AcylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC16AcylCoA

6.28 Function definition function_4_vvlcadC12_1

Name function_4_vvlcadC12_1

Arguments [C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [FADHMAT], [FADHMAT], Keqvlcad, KmvlcadC12AcylCoAMAT KmvlcadC12EnoylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC14EnoylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC16EnoylCoAMAT, KmvlcadFADH, vol (VMAT), Vvlcad, sfvlcadC12

Mathematical Expression

 $\underline{VLCAD}(sfvlcadC12, Vvlcad, KmvlcadC12AcylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC14Acy$

6.29 Function definition function_4_vlcadC16_1

Name function_4_vlcadC16_1

Arguments [C10AcylCoAMAT], [C10EnoylCoAMAT], [C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [C16EnoylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [FADHMAT], [FADHMAT], Keqlcad, KmlcadC10AcylCoAMAT, KmlcadC10EnoylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12EnoylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, vol (VMAT), Vlcad, sflcadC16

Mathematical Expression

LCAD (sflcadC16, Vlcad, KmlcadC16AcylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC16AcylCoAMAT, Kmlcad

6.30 Function definition function_4_vlcadC14_1

Name function_4_vlcadC14_1

Arguments [C10AcylCoAMAT], [C10EnoylCoAMAT], [C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [C16EnoylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [FADHMAT], [FADHMAT], Keqlcad, KmlcadC10AcylCoAMAT, KmlcadC10EnoylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12EnoylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadC8AcylCoAMAT, Vlcad, sflcadC14

Mathematical Expression

LCAD (sflcadC14, Vlcad, KmlcadC14AcylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC16AcylCoAMAT, Kmlcad

6.31 Function definition function_4_vlcadC12_1

Name function_4_vlcadC12_1

Arguments [C10AcylCoAMAT], [C10EnoylCoAMAT], [C12AcylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [FADHMAT], [FADHMAT], Keqlcad, KmlcadC10AcylCoAMAT, KmlcadC10EnoylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12EnoylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, vol (VMAT), Vlcad, sflcadC12

Mathematical Expression

LCAD (sfleadC12, Vlcad, KmlcadC12AcylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC16AcylCoAMAT, Kmlcad

6.32 Function definition function_4_vlcadC10_1

Name function_4_vlcadC10_1

Arguments [C10AcylCoAMAT], [C10EnoylCoAMAT], [C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [C16EnoylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [FADHMAT], [FADHMAT], Keqlcad, KmlcadC10AcylCoAMAT, KmlcadC10EnoylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12EnoylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, vol (VMAT), Vlcad, sflcadC10

Mathematical Expression

LCAD (sflcad C10, Vlcad, Kmlcad C10 Acyl CoAMAT, Kmlcad C16 Acyl C0AMAT, Kml

6.33 Function definition function_4_vmcadC12_1

Name function_4_vmcadC12_1

Arguments [C10AcylCoAMAT], [C10EnoylCoAMAT], [C12AcylCoAMAT], [C12EnoylCoAMAT], [C4AcylCoAMAT], [C4EnoylCoAMAT], [C6EnoylCoAMAT], [C6EnoylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqmcad, KmmcadC10AcylCoAMAT, KmmcadC10EnoylCoAMAT, KmmcadC12AcylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadC6AcylCoAMAT, KmmcadC6EnoylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC8EnoylCoAMAT, KmmcadFAD, KmmcadFADH, vol (VMAT), Vmcad, sfmcadC12

Mathematical Expression

 $\underline{MCAD}(sfmcadC12, Vmcad, KmmcadC12AcylCoAMAT, KmmcadC10AcylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC10AcylCoAMAT, Kmmc$

6.34 Function definition function_4_vmcadC10_1

Name function_4_vmcadC10_1

Arguments [C10AcylCoAMAT], [C10EnoylCoAMAT], [C12AcylCoAMAT], [C12EnoylCoAMAT], [C4AcylCoAMAT], [C4EnoylCoAMAT], [C6EnoylCoAMAT], [C8AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [FADHMAT], [FADHMAT], Keqmcad, KmmcadC10AcylCoAMAT, KmmcadC10EnoylCoAMAT, KmmcadC12AcylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadC6AcylCoAMAT, KmmcadC6EnoylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC8EnoylCoAMAT, KmmcadFADH, vol (VMAT), Vmcad, sfmcadC10

Mathematical Expression

MCAD (sfmcadC10, Vmcad, KmmcadC10AcylCoAMAT, KmmcadC12AcylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC8AcylCoAMAT

6.35 Function definition function_4_vmcadC8_1

Name function_4_vmcadC8_1

Arguments [C10AcylCoAMAT], [C10EnoylCoAMAT], [C12AcylCoAMAT], [C12EnoylCoAMAT], [C4AcylCoAMAT], [C4EnoylCoAMAT], [C6EnoylCoAMAT], [C6EnoylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqmcad, KmmcadC10AcylCoAMAT, KmmcadC10EnoylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadC6AcylCoAMAT, KmmcadC6EnoylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC8EnoylCoAMAT, KmmcadFADH, vol (VMAT), Vmcad, sfmcadC8

Mathematical Expression

MCAD (sfmcadC8, Vmcad, KmmcadC8AcylCoAMAT, KmmcadC12AcylCoAMAT, KmmcadC10AcylCoAMAT, KmmcadC1

6.36 Function definition function_4_vmcadC6_1

Name function_4_vmcadC6_1

Arguments [C10AcylCoAMAT], [C10EnoylCoAMAT], [C12AcylCoAMAT], [C12EnoylCoAMAT], [C4AcylCoAMAT], [C4EnoylCoAMAT], [C6EnoylCoAMAT], [C6EnoylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqmcad, KmmcadC10AcylCoAMAT, KmmcadC10EnoylCoAMAT, KmmcadC12AcylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadC6AcylCoAMAT, KmmcadC6EnoylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC8EnoylCoAMAT, KmmcadFAD, KmmcadFADH, vol (VMAT), Vmcad, sfmcadC6

Mathematical Expression

 $\underline{MCAD}(sfmcadC6, Vmcad, KmmcadC6AcylCoAMAT, KmmcadC12AcylCoAMAT, KmmcadC10AcylCoAMAT, Kmmc$

6.37 Function definition function_4_vscadC4_1

Name function_4_vscadC4_1

Arguments [C4AcylCoAMAT], [C4EnoylCoAMAT], [C6AcylCoAMAT], [C6EnoylCoAMAT], [FADHMAT], [FADHMAT], Keqscad, KmscadC4AcylCoAMAT, KmscadC4EnoylCoAMAT, KmscadC6AcylCoAMAT, KmscadC6EnoylCoAMAT, KmscadFADH, vol (VMAT), Vscad, sfscadC4

Mathematical Expression

SCAD (sfscadC4, Vscad, KmscadC4AcylCoAMAT, KmscadC6AcylCoAMAT, KmscadC4EnoylCoAMAT, KmscadC

6.38 Function definition function_4_vmckatC6_1

Name function_4_vmckatC6_1

Arguments [AcetylCoAMAT], [C10AcylCoAMAT], [C10KetoacylCoAMAT], [C12AcylCoAMAT], [C12KetoacylCoAMAT], [C14AcylCoAMAT], [C14KetoacylCoAMAT], [C16AcylCoAMAT], [C16KetoacylCoAMAT], [C4AcetoacylCoAMAT], [C4AcylCoAMAT], [C6AcylCoAMAT], [C6KetoacylCoAMAT], [C8AcylCoAMAT], [C8KetoacylCoAMAT], [C0AMAT], Keqmckat, KmmckatAcetylCoAMAT, KmmckatC10AcylCoAMAT, KmmckatC10KetoacylCoAMAT, KmmckatC12AcylCoAMAT, KmmckatC12KetoacylCoAMAT, KmmckatC14AcylCoAMAT,

KmmckatC14KetoacylCoAMAT, KmmckatC16AcylCoAMAT, KmmckatC16KetoacylCoAMAT, KmmckatC4AcetoacylCoAMAT, KmmckatC4AcylCoAMAT, KmmckatC6AcylCoAMAT, KmmckatC6KetoacylCoAMAT, KmmckatC8AcylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC0AMAT, vol (VMAT), Vmckat, sfmckatC6

Mathematical Expression

 $\underline{MCKATA} (sfmckatC6, Vmckat, KmmckatC6KetoacylCoAMAT, KmmckatC16KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT, KmmckatC14Ket$

6.39 Function definition function_4_vmckatC4_1

Name function_4_vmckatC4_1

Arguments [AcetylCoAMAT], [C10AcylCoAMAT], [C10KetoacylCoAMAT], [C12AcylCoAMAT], [C12KetoacylCoAMAT], [C14AcylCoAMAT], [C14KetoacylCoAMAT], [C16AcylCoAMAT], [C16KetoacylCoAMAT], [C4AcetoacylCoAMAT], [C4AcylCoAMAT], [C6AcylCoAMAT], [C6KetoacylCoAMAT], [C8KetoacylCoAMAT], [C6KetoacylCoAMAT], [C8KetoacylCoAMAT], [C0AMAT], Keqmckat, KmmckatAcetylCoAMAT, KmmckatC10AcylCoAMAT, KmmckatC10KetoacylCoAMAT, KmmckatC12AcylCoAMAT, KmmckatC12KetoacylCoAMAT, KmmckatC14AcylCoAMAT, KmmckatC14KetoacylCoAMAT, KmmckatC16AcylCoAMAT, KmmckatC16KetoacylCoAMAT, KmmckatC4AcylCoAMAT, KmmckatC4AcylCoAMAT, KmmckatC6KetoacylCoAMAT, KmmckatC4AcylCoAMAT, KmmckatC6KetoacylCoAMAT, KmmckatC8AcylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC6KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC6KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC6KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC0AMAT, Vol (VMAT), Vmckat, sfmckatC4

Mathematical Expression

 $\underline{MCKATB} (sfmckatC4, Vmckat, KmmckatC4AcetoacylCoAMAT, KmmckatC16KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT, KmmckatC14Ke$

6.40 Function definition function_4_vmtpC16_1

Name function_4_vmtpC16_1

Arguments [AcetylCoAMAT], [C10AcylCoAMAT], [C10EnoylCoAMAT], [C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [C4AcetoacylCoAMAT], [C6AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [C0AMAT], Keqmtp, KicrotC4AcetoacylCoA, KmmtpAcetylCoAMAT, KmmtpC10AcylCoAMAT, KmmtpC10EnoylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC14AcylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16AcylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT, KmmtpC8EnoylCoAMAT, KmmtpC0AMAT, KmmtpC0AMAT, KmmtpNADHMAT, KmmtpNADHMAT, [NADHMAT], [NADtMAT], vol (VMAT), Vmtp, sfmtpC16

Mathematical Expression

 $\underline{MTP}(sfmtpC16, Vmtp, KmmtpC16EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC14EnoylCoAMAT, Kmmtp$

6.41 Function definition function_4_vmtpC14_1

Name function_4_vmtpC14_1

Arguments [AcetylCoAMAT], [C10AcylCoAMAT], [C10EnoylCoAMAT], [C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [C4AcetoacylCoAMAT], [C6AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [C0AMAT], Keqmtp, KicrotC4AcetoacylCoA, KmmtpAcetylCoAMAT, KmmtpC10AcylCoAMAT, KmmtpC10EnoylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC14AcylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16AcylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT, KmmtpC8EnoylCoAMAT, KmmtpC0AMAT, KmmtpNADHMAT, KmmtpNADHMAT, [NADHMAT], [NADHMAT], vol (VMAT), Vmtp, sfmtpC14

Mathematical Expression

 $\underline{MTP(sfmtpC14,Vmtp,KmmtpC14EnoylCoAMAT,KmmtpC16EnoylCoAMAT,KmmtpC12EnoylCoAMAT,KmmtpC12EnoylCoAMAT,KmmtpC14EnoylCoAMAT,KmmtpC16EnoylCoAMAT,Kmmt$

6.42 Function definition function_4_vmtpC12_1

Name function_4_vmtpC12_1

Arguments [AcetylCoAMAT], [C10AcylCoAMAT], [C10EnoylCoAMAT], [C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [C4AcetoacylCoAMAT], [C6AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [CoAMAT], Keqmtp, KicrotC4AcetoacylCoA, KmmtpAcetylCoAMAT, KmmtpC10AcylCoAMAT, KmmtpC10EnoylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC14AcylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16AcylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT, KmmtpC8EnoylCoAMAT, KmmtpCoAMAT, KmmtpNADHMAT, KmmtpNADHMAT, [NADHMAT], [NADtMAT], vol (VMAT), Vmtp, sfmtpC12

Mathematical Expression

 $\underline{MTP(sfmtpC12,Vmtp,KmmtpC12EnoylCoAMAT,KmmtpC16EnoylCoAMAT,KmmtpC14EnoylCoAMAT,KmmtpC14EnoylCoAMAT,KmmtpC16EnoylCoAMAT,Kmmt$

6.43 Function definition function_4_vmtpC10_1

Name function_4_vmtpC10_1

Arguments [AcetylCoAMAT], [C10AcylCoAMAT], [C10EnoylCoAMAT], [C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [C4AcetoacylCoAMAT], [C6AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [CoAMAT], Keqmtp, KicrotC4AcetoacylCoA, KmmtpAcetylCoAMAT, KmmtpC10AcylCoAMAT, KmmtpC10EnoylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC12EnoylCoAMAT

KmmtpC14AcylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16AcylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT, KmmtpC8EnoylCoAMAT, KmmtpCoAMAT, KmmtpNADHMAT, KmmtpNADHMAT, [NADHMAT], [NADtMAT], vol (VMAT), Vmtp, sfmtpC10

Mathematical Expression

MTP (sfmtpC10, Vmtp, KmmtpC10EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC16E

6.44 Function definition function_4_vmtpC8_1

Name function_4_vmtpC8_1

Arguments [AcetylCoAMAT], [C10AcylCoAMAT], [C10EnoylCoAMAT], [C12AcylCoAMAT], [C12EnoylCoAMAT], [C14EnoylCoAMAT], [C16EnoylCoAMAT], [C16EnoylCoAMAT], [C4AcetoacylCoAMAT], [C6AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [C0AMAT], Keqmtp, KicrotC4AcetoacylCoA, KmmtpAcetylCoAMAT,

KmmtpC10AcylCoAMAT, KmmtpC10EnoylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC14AcylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16AcylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT, KmmtpC8EnoylCoAMAT, KmmtpC0AMAT, KmmtpNADHMAT, KmmtpNADHMAT, [NADHMAT], [NADHMAT], vol (VMAT), Vmtp,

sfmtpC8

Mathematical Expression

 $\underline{MTP}(sfmtpC8, Vmtp, KmmtpC8EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC1$

6.45 Function definition function_4_vacesink_1

Name function_4_vacesink_1

Arguments [AcetylCoAMAT], K1acesink, Ksacesink, vol (VMAT)

Mathematical Expression

$$\frac{\text{RES}\left(\text{Ksacesink}, [\text{AcetylCoAMAT}], \text{K1acesink}\right)}{\text{vol}\left(\text{VMAT}\right)}$$

$$(45)$$

6.46 Function definition CRMS

Name CRMS

Arguments sfc, Vc, sfm, Vm, S1, P0, Kms1, Kmms1, Kmp0, P1, P3, Keqc, Keqm, Kmp1, P2, Kmp2, Kmp3, S2, Kms2, I1, Ki

Mathematical Expression

$$\frac{sfc \cdot Vc \cdot sfm \cdot Vm \cdot \left(\frac{S1 \cdot P0}{Kms1 \cdot Kmms1 \cdot Kmp0} - \frac{P1 \cdot P3}{Kms1 \cdot Kmms1 \cdot Kmp0 \cdot Keqc \cdot Keqm}\right)}{\frac{sfc \cdot Vc \cdot \left(1 + \frac{P1}{Kmp1} + \frac{P2}{Kmp2}\right) \cdot \left(1 + \frac{P0}{Kmp0} + \frac{P3}{Kmp3}\right)}{Kms1 \cdot Keqc}} + \frac{sfm \cdot Vm \cdot P0 \cdot \left(1 + \frac{S1}{Kms1} + \frac{S2}{Kms2} + \frac{I1}{Ki}\right)}{Kmms1 \cdot Kmp0}}$$

$$(46)$$

6.47 Function definition CRMS_C6

Name CRMS_C6

Arguments sfcrotC6, Vcrot, sfmschadC6, Vmschad, [C6EnoylCoAMAT], NAD, KmcrotC6EnoylCoAMAT, KmmschadC6HydroxyacylCoAMAT, KmmschadNADMAT, [C6KetoacylCoAMAT], [NADHMAT], Keqcrot, Keqmschad, KmmschadC6KetoacylCoAMAT, [C4AcetoacylCoAMAT], KmmschadC4AcetoacylCoAMAT, KmmschadNADHMAT, [C4EnoylCoAMAT], KmcrotC4EnoylCoAMAT, KicrotC4AcetoacylCoA, vol (VMAT)

Mathematical Expression

 $\underline{CRMS}\,(sfcrotC6,Vcrot,sfmschadC6,Vmschad,[C6EnoylCoAMAT],NAD,KmcrotC6EnoylCoAMAT,KmmschadC6,Vcrot,sfmschadC6,Vmschad,[C6EnoylCoAMAT],NAD,KmcrotC6EnoylCoAMAT,KmmschadC6,Vcrot,sfmschadC6,Vmschad,[C6EnoylCoAMAT],NAD,KmcrotC6EnoylCoAMAT,KmmschadC6,Vmschad$

6.48 Function definition CRMS_C4

Name CRMS_C4

Arguments sfcrotC4, Vcrot, sfmschadC4, Vmschad, [C4EnoylCoAMAT], NAD, KmcrotC4EnoylCoAMAT, KmmschadC4HydroxyacylCoAMAT, KmmschadNADMAT, [C4AcetoacylCoAMAT], [NADHMAT], Keqcrot, Keqmschad, KmmschadC4AcetoacylCoAMAT, [C6KetoacylCoAMAT], KmmschadC6KetoacylCoAKmmschadNADHMAT, [C6EnoylCoAMAT], KmcrotC6EnoylCoAMAT, KicrotC4AcetoacylCoA, vol (VMAT)

Mathematical Expression

 $\underline{CRMS}\,(sfcrotC4,Vcrot,sfmschadC4,Vmschad,[C4EnoylCoAMAT],NAD,KmcrotC4EnoylCoAMAT,KmmschadC4,Vcrot,SfmschadC4,Vmschad,[C4EnoylCoAMAT],NAD,KmcrotC4EnoylCoAMAT,KmmschadC4,Vmschad,SfmschadC4,SfmschadC4,S$

7 Rules

This is an overview of two rules.

7.1 Rule C16AcylCoACYT

Rule C16AcylCoACYT is an assignment rule for species C16AcylCoACYT:

C16AcylCoACYT =
$$26.8 \cdot 2.71828^{0.18 \cdot \text{time}}$$
 (49)

7.2 Rule Coamat

Rule CoAMAT is an assignment rule for species CoAMAT:

```
\begin{aligned} \text{CoAMAT} &= \left[ \text{CoAMAT} \right] - \left( \left[ \text{C16AcylCoAMAT} \right] + \left[ \text{C16EnoylCoAMAT} \right] \\ &+ \left[ \text{C16HydroxyacylCoAMAT} \right] + \left[ \text{C16KetoacylCoAMAT} \right] + \left[ \text{C14AcylCoAMAT} \right] \\ &+ \left[ \text{C14EnoylCoAMAT} \right] + \left[ \text{C14HydroxyacylCoAMAT} \right] + \left[ \text{C12HydroxyacylCoAMAT} \right] \\ &+ \left[ \text{C12AcylCoAMAT} \right] + \left[ \text{C12EnoylCoAMAT} \right] + \left[ \text{C10EnoylCoAMAT} \right] \\ &+ \left[ \text{C10EnoylCoAMAT} \right] + \left[ \text{C10AcylCoAMAT} \right] + \left[ \text{C10EnoylCoAMAT} \right] \\ &+ \left[ \text{C8EnoylCoAMAT} \right] + \left[ \text{C10KetoacylCoAMAT} \right] + \left[ \text{C8KetoacylCoAMAT} \right] \\ &+ \left[ \text{C6EnoylCoAMAT} \right] + \left[ \text{C6EnoylCoAMAT} \right] + \left[ \text{C6HydroxyacylCoAMAT} \right] \\ &+ \left[ \text{C6KetoacylCoAMAT} \right] + \left[ \text{C4AcylCoAMAT} \right] + \left[ \text{C4EnoylCoAMAT} \right] \\ &+ \left[ \text{C4HydroxyacylCoAMAT} \right] + \left[ \text{C4AcetoacylCoAMAT} \right] + \left[ \text{AcetylCoAMAT} \right] \end{aligned}
```

Derived unit $\mu mol \cdot l^{-1}$

8 Reactions

This model contains 37 reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 5: Overview of all reactions

		Tuble 51 Overview of	an reactions	
No	Id	Name	Reaction Equation SBO	
1	vcpt1C16	vcpt1C16	C16AcylCoACYT, CarCYT, CoACYT, MalCoACYT, C16AcylCa	arCYT, C16Acyl
2	vcactC16	vcactC16	C16 A cylCorCYT CarMAT, CarCYT, C16AcylCarCYT, C16AcylCa	arMAT, CarCYT,
2			CarMAT, CarCYT, C14AcvlCarCYT, C14AcvlCa	arMAT, CarCYT,
3	vcactC14	vcactC14	CarMAT, CarCYT, C12AcvlCarCYT, C12AcvlCa	
4	vcactC12	vcactC12	C12AcylCarCYT CarMAT, CarCYT, C10AcylCarCYT, C10AcylCarCYT	
5	vcactC10	vcactC10	C10AcylCarCYT CarMAT CarCYT C8AcylCarCYT C8AcylCarM	AT CarCVT Car
6	vcactC8	vcactC8	C8AcylCarCYT CarMAT, CarCYT, C8AcylCarCYT, C8AcylCarM	
7	vcactC6	vcactC6	C6AcylCarCYT, C6AcylCarCYT, C6AcylCarM	
8	vcactC4	vcactC4	C4AcylCarCYT CarMAT, CarCYT, C4AcylCarCYT, C4AcylCarM.	AT, CarCYT, Car
9	vcpt2C16	vcpt2C16	C16AcylCarMAT C12AcylCarMAT, C10AcylCarMAT	
10	vcpt2C14	vcpt2C14	C14AcylCarMAT, C12AcylCarMAT, C10AcylCa	rMAT, C8AcylCa
11	vcpt2C12	vcpt2C12	C12AcylCarMAT C16AcylCarMAT, C14AcylCarMAT, C10AcylCa	
12	_		C16AcylCarMAT, C14AcylCarMAT, C12AcylCa	rMAT, C8AcylCa
12	vcpt2C10	vcpt2C10	C10AcylCarMAT C16AcylCarMAT, C14AcylCarMAT, C12AcylCarMAT	MAT, C10AcylCa
13	vcpt2C8	vcpt2C8	C16AcylCarMAT, C14AcylCarMAT, C12AcylCarl	
14	vcpt2C6	vcpt2C6	C6AcylCarMAT	.,

N₀	Id	Name	Reaction Equation	SBO
15	vcpt2C4	vcpt2C4	C4AcylCarMAT C16AcylCarMAT, C14AcylCarMA	
13	_	•	C4AcylCarMAT C14AcylCoAMAT, C12AcylCo	AMAT, FADtMAT, C14EnoylCoA
16	vvlcadC16	vvlcadC16	C16AcylCoAMAT	
			FADHMAT C16AcylCoAMAT, C12AcylCo C14AcylCoAMAT	AMAT FADtMAT C16FnovlCo4
17	vvlcadC14	vvlcadC14		Turin, Triburin, Crobino, Cor
			FADHMAT	AMAT FADAMAT CIGEncelCo
18	vvlcadC12	vvlcadC12	C12AcylCoAMAT C14AcylCo	AMAI, FADIMAI, CIBEROVICOA
			EADIMAT	
19	vlcadC16	vlcadC16	C16AcylCoAMAT C12AcylCo	AMAT, C10AcylCoAMAT, C8Ac
20	vlcadC14	vlcadC14	C14AcylCoAMAT C12AcylCo	AMAT, C10AcylCoAMAT, C8Ac
20	VIOGGOTT	violate i i	FADHMAT	
21	vlcadC12	vlcadC12	C12AcylCoAMAT C14AcylCo	AMAT, C10AcylCoAMAT, C8Ac
21	VICAUCIZ	vicauc 12	FADHMAT	
22	1 1040	11010	C10AcylCoAMAT C16AcylCoAMAT, C14AcylCo	AMAT, C12AcylCoAMAT, C8Ac
22	vlcadC10	vlcadC10		
			C12AcylCoAMAT, C8AcylCoA	MAT, C6AcylCoAMAT, C4Acyl
23	vmcadC12	vmcadC12	C12AcylCoAMAT ———————————————————————————————————	
			C12AcvlCoAMAT, C8AcvlCoA	MAT. C6AcvlCoAMAT. C4Acvl
24	vmcadC10	vmcadC10	C10AcylCoAMAT C12AcylCoAMAT, C8AcylCoA	
			FADHMAT C12AcylCoAMAT C10AcylCoA	MAT C6A cylCoAMAT C4A cyl
25	vmcadC8	vmcadC8	C8AcylCoAMAT C12AcylCoAMAT, C10AcylCoA	
			FADHMAT	

30	No	Id	Name	Reaction Equation SBO
	26		rum and C4	C6AcylCoAMAT C10AcylCoAMAT, C8AcylCoAMAT, C4AcylCoAMAT, C4AcylCoAMAT
	26	vmcadC6	vmcadC6	
	27	104	104	C4AcylCoAMAT C4AcylCoAMAT, FADtMAT, C6EnoylCoAMAT, C4AcylCoAMAT
	27	vscadC4	vscadC4	C4AcylCoAMAT ===================================
Produced by SBML2LEX	20		1.00	C16KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCo
	28	vmckatC6	vmckatC6	C6KetoacylCoAMAT
				AcetylCoAMAT
	29	vmckatC4	vmckatC4	C4AcetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCoAMAT, C12KetoacylCo
				C4AcetoacylCoAMAT C14EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C C16EnoylCoAMAT
	30	vmtpC16	vmtpC16	C16EnoylCoAMAI =
				AcetylCoAMAT + NADHMAT
ed t	31	vmtpC14	vmtpC14	C14EnoylCoAMAT C12EnoylCoAMAT, C10EnoylCoAMAT, C
)y (_	_	AcetylCoAMAT + NADHMAT
S	32	rm+nC10	vmtpC12	C12EnoylCoAMAT C14EnoylCoAMAT, C10EnoylCoAMAT, C
<u> </u>	32	vmtpC12	VIIIIpC12	AcetylCoAMAT + NADHMAT
Ű.				C16EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C
×	33	vmtpC10	vmtpC10	C10EnoylCoAMAT C10EnoylCoAMAT, C17EnoylCoAMAT, C17EnoylCoAMAT
				AcetylCoAMAT + NADHMAT
	2.4			C8EnoylCoAMAT C14EnoylCoAMAT, C12EnoylCoAMAT, C1 C8EnoylCoAMAT
	34	vmtpC8	vmtpC8	CSENOVICOAMAI
				AcetylCoAMAT + NADHMAT
	35	vacesink	vacesink	$AcetylCoAMAT \emptyset$
	36	reaction_1	vcrmsC6	C6EnoylCoAMAT +
				C4AcetoacylCoAMAT, C4EnoylCoAMAT, C6EnoylCoAMAT, species_1, C
				species_1 =
				NADHMAT

Nº Id	Name	Reaction Equation	SBO	
37 reaction_2	vcrmsC4	C4EnoylCoAMAT C6KetoacylCoAMAT, C6Enoyl species_1 NADHMAT	+ ICoAMAT, C4EnoylCoA	AMAT, species_1, C

8.1 Reaction vcpt1C16

This is a reversible reaction of no reactant forming one product influenced by nine modifiers.

Name vcpt1C16

Reaction equation

© C16AcylCoACYT, CarCYT, CoACYT, MalCoACYT, C16AcylCarCYT, C16AcylCoACYT, CarCYT, CoACYT

(51)

Modifiers

Table 6: Properties of each modifier.

Id	Name	SBO
C16AcylCoACYT	C16AcylCoACYT	
CarCYT	CarCYT	
CoACYT	CoACYT	
MalCoACYT	MalCoACYT	
C16AcylCarCYT	C16AcylCarCYT	
C16AcylCoACYT	C16AcylCoACYT	
CarCYT	CarCYT	
CoACYT	CoACYT	
MalCoACYT	MalCoACYT	

Product

Table 7: Properties of each product.

Id	Name	SBO
C16AcylCarCYT	C16AcylCarCYT	

Kinetic Law

Derived unit contains undeclared units

function_4_vcpt1C16_1 ([C16AcylCarCYT], [C16AcylCoACYT], [CarCYT], [CarCYT], [CoACYT], Keqcpt1, Kicpt1MalCoACYT, Kmcpt1C16AcylCarCYT, Kmcpt1C16AcylCarCYT, Kmcpt1CarCYT, Kmcpt1CarCYT, Kmcpt1CarCYT, Kmcpt1CoACYT, [MalCoACYT], vol (VCYT), Vcpt1, ncpt1, sfcpt1C16)

 $= \frac{\text{CPT1} (\text{sfcpt1C16}, \text{Vcpt1}, \text{Kmcpt1C16AcylCoACYT}, \text{Kmcpt1CarCYT}, \text{Kmcpt1C16AcylCarCYT}, \text{Kmcpt1CoACY}, \text{Kmcp$

function_4_vcpt1C16_1 ([C16AcylCarCYT], [C16AcylCoACYT], [CarCYT], [CoACYT], Keqcpt1, Kicpt1MalCoACYT, Kmcpt1C16AcylCarCYT, Kmcpt1C16AcylCoACYT, Kmcpt1CarCYT, Kmcpt1CoACYT, [MalCoACYT], vol (VCYT), Vcpt1, ncpt1, sfcpt1C16)

= CPT1 (sfcpt1C16, Vcpt1, Kmcpt1C16AcylCoACYT, Kmcpt1CarCYT, Kmcpt1C16AcylCarCYT, Kmcpt1CoACY

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Keqcpt1	Keqcpt1		0.450		Ø
Kicpt1MalCoAC	Y Kicptl MalCoACYT		9.100		
Kmcpt1C16Acyl	Cakettypt1C16AcylCarC	CYT	136.000		
Kmcpt1C16Acyl	CdAftYpt1C16AcylCoA	CYT	13.800		$ \overline{\checkmark} $
Kmcpt1CarCYT	Kmcpt1CarCYT		125.000		$\overline{\mathbf{Z}}$
Kmcpt1CoACYT	Kmcpt1CoACYT		40.700		$\overline{\checkmark}$
Vcpt1	Vcpt1		0.012		$\overline{\checkmark}$
ncpt1	ncpt1		2.480		$\overline{\checkmark}$
sfcpt1C16	sfcpt1C16		1.000		$\overline{\mathbf{Z}}$

8.2 Reaction vcactC16

This is a reversible reaction of one reactant forming one product influenced by six modifiers.

Name vcactC16

Reaction equation

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
C16AcylCarCYT	C16AcylCarCYT	

Modifiers

Table 10: Properties of each modifier.

rable 10. I repetites of each mounter.			
Id	Name	SBO	
CarMAT	CarMAT		
CarCYT	CarCYT		
C16AcylCarCYT	C16AcylCarCYT		
C16AcylCarMAT	C16AcylCarMAT		
CarCYT	CarCYT		
CarMAT	CarMAT		

Product

Table 11: Properties of each product.

Id	Name	SBO
C16AcylCarMAT	C16AcylCarMAT	

Kinetic Law

Derived unit contains undeclared units

 $\begin{aligned} v_2 &= \text{function_4_vcactC16_1} \left([\text{C16AcylCarCYT}], [\text{C16AcylCarMAT}], [\text{CarCYT}], [\text{CarMAT}], \\ &\quad \text{Keqcact}, \text{KicactC16AcylCarCYT}, \text{KicactCarCYT}, \text{KmcactC16AcylCarCYT}, \\ &\quad \text{KmcactC16AcylCarMAT}, \text{KmcactCarCYT}, \text{KmcactCarMAT}, \text{Vfcact}, \text{Vrcact} \right) \end{aligned} \tag{56}$

function_4_vcactC16_1 ([C16AcylCarCYT], [C16AcylCarMAT], [CarCYT], [CarMAT], (57) Keqcact, KicactC16AcylCarCYT, KicactCarCYT, KmcactC16AcylCarCYT, KmcactC16AcylCarMAT, KmcactCarCYT, KmcactCarMAT, Vfcact, Vrcact)

Vfcac

 $[C16AcylCarCYT] \cdot [CarMAT] + KmcactCarMAT \cdot [C16AcylCarCYT] + KmcactC16AcylCarCYT \cdot [CarMAT] \cdot [C16AcylCarCYT] + (C16AcylCarCYT) + (C16Acyl$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KicactC	16AcylC #cCMT tC16AcylC	CarCYT	56.0		
KmcactC	16AcylCakcovcactC16Acyl	ICarCYT	15.0		
KmcactC	16AcylCaKemAcTetC16Acyl	lCarMAT	15.0		

8.3 Reaction vcactC14

This is a reversible reaction of one reactant forming one product influenced by six modifiers.

Name vcactC14

Reaction equation

$$C14AcylCarCYT \xleftarrow{CarMAT, CarCYT, C14AcylCarCYT, C14AcylCarMAT, CarCYT, CarMAT}_{(58)} C14AcylCarMAT$$

Reactant

Table 13: Properties of each reactant.

There is a repersion of chemical residuals.				
Id	Name	SBO		
C14AcylCarCYT	C14AcylCarCYT			

Modifiers

Table 14: Properties of each modifier.

Id	Name	SBO
CarMAT	CarMAT	
CarCYT	CarCYT	
C14AcylCarCYT	C14AcylCarCYT	
C14AcylCarMAT	C14AcylCarMAT	
CarCYT	CarCYT	
CarMAT	CarMAT	

Product

Table 15: Properties of each product.

Id	Name	SBO
C14AcylCarMAT	C14AcylCarMAT	

Kinetic Law

Derived unit contains undeclared units

$$\begin{split} v_3 &= \text{function_4_vcactC14_1} \, ([\text{C14AcylCarCYT}], [\text{C14AcylCarMAT}], [\text{CarCYT}], [\text{CarMAT}], \\ &\quad \text{Keqcact}, \text{KicactC14AcylCarCYT}, \text{KicactCarCYT}, \text{KmcactC14AcylCarCYT}, \\ &\quad \text{KmcactC14AcylCarMAT}, \text{KmcactCarCYT}, \text{KmcactCarMAT}, \text{Vfcact}, \text{Vrcact}) \\ &\quad (59) \end{split}$$

function_4_vcactC14_1 ([C14AcylCarCYT], [C14AcylCarMAT], [CarCYT], [CarMAT], (60) Keqcact, KicactC14AcylCarCYT, KicactCarCYT, KmcactC14AcylCarCYT, KmcactC14AcylCarMAT, KmcactCarCYT, KmcactCarMAT, Vfcact, Vrcact)

Vfcac

 $[C14AcylCarCYT] \cdot [CarMAT] + KmcactCarMAT \cdot [C14AcylCarCYT] + KmcactC14AcylCarCYT \cdot [CarMAT] \cdot [C14AcylCarCYT] + KmcactC14AcylCarCYT \cdot [C14AcylCarCYT] + (C14AcylCarCYT) + (C14AcylCarCY$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kicact(C14AcylC akricYiT tC14AcylC	CarCYT	56.0		
KmcactC	C14AcylC aknova ctC14Acyl	CarCYT	15.0		\square
KmcactC	C14AcylC ax-maca ctC14Acyl	CarMAT	15.0		

8.4 Reaction vcactC12

This is a reversible reaction of one reactant forming one product influenced by six modifiers.

Name vcactC12

Reaction equation

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
C12AcylCarCYT	C12AcylCarCYT	

Modifiers

Table 18: Properties of each modifier.

Tuble 10. I roperties of each modifier.			
Id	Name	SBO	
CarMAT	CarMAT		
CarCYT	CarCYT		
C12AcylCarCYT	C12AcylCarCYT		
C12AcylCarMAT	C12AcylCarMAT		
CarCYT	CarCYT		
CarMAT	CarMAT		

Product

Table 19: Properties of each product.

Id	Name	SBO
C12AcylCarMAT	C12AcylCarMAT	

Kinetic Law

Derived unit contains undeclared units

 $\begin{aligned} \nu_4 &= \text{function_4_vcactC12_1} \left([\text{C12AcylCarCYT}], [\text{C12AcylCarMAT}], [\text{CarCYT}], [\text{CarMAT}], \\ &\quad \text{Keqcact}, \text{KicactC12AcylCarCYT}, \text{KicactCarCYT}, \text{KmcactC12AcylCarCYT}, \\ &\quad \text{KmcactC12AcylCarMAT}, \text{KmcactCarCYT}, \text{KmcactCarMAT}, \text{Vfcact}, \text{Vrcact} \right) \end{aligned}$

function_4_vcactC12_1 ([C12AcylCarCYT], [C12AcylCarMAT], [CarCYT], [CarMAT], (63) Keqcact, KicactC12AcylCarCYT, KicactCarCYT, KmcactC12AcylCarCYT, KmcactC12AcylCarMAT, KmcactCarCYT, KmcactCarMAT, Vfcact, Vrcact)

Vfcac

 $[C12AcylCarCYT] \cdot [CarMAT] + KmcactCarMAT \cdot [C12AcylCarCYT] + KmcactC12AcylCarCYT \cdot [CarMAT] \cdot [C12AcylCarCYT] + KmcactC12AcylCarCYT \cdot [C12AcylCarCYT] + KmcactC12Acy$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KicactC	12AcylC akricVit tC12AcylC	CarCYT	56.0		
${\tt KmcactC}$	12AcylCakcovactC12Acy	lCarCYT	15.0		
KmcactC	12AcylCakemAcactC12Acy	lCarMAT	15.0		

8.5 Reaction vcactC10

This is a reversible reaction of one reactant forming one product influenced by six modifiers.

Name vcactC10

Reaction equation

$$C10AcylCarCYT \xleftarrow{CarMAT, CarCYT, C10AcylCarCYT, C10AcylCarMAT, CarCYT, CarMAT} C10AcylCarMAT (64)$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
C10AcylCarCYT	C10AcylCarCYT	

Modifiers

Table 22: Properties of each modifier.

Name	SBO
CarMAT	
CarCYT	
C10AcylCarCYT	
C10AcylCarMAT	
CarCYT	
CarMAT	
	CarMAT CarCYT C10AcylCarCYT C10AcylCarMAT CarCYT

Product

Table 23: Properties of each product.

Id	Name	SBO
C10AcylCarMAT	C10AcylCarMAT	

Kinetic Law

Derived unit contains undeclared units

$$v_{5} = \text{function_4_vcactC10_1} ([\text{C10AcylCarCYT}], [\text{C10AcylCarMAT}], [\text{CarCYT}], [\text{CarMAT}], \\ \text{Keqcact}, \text{KicactC10AcylCarCYT}, \text{KicactCarCYT}, \text{KmcactC10AcylCarCYT}, \\ \text{KmcactC10AcylCarMAT}, \text{KmcactCarCYT}, \text{KmcactCarMAT}, \text{Vfcact}, \text{Vrcact}) \\ (65)$$

function_4_vcactC10_1 ([C10AcylCarCYT], [C10AcylCarMAT], [CarCYT], [CarMAT], (66) Keqcact, KicactC10AcylCarCYT, KicactCarCYT, KmcactC10AcylCarCYT, KmcactC10AcylCarMAT, KmcactCarCYT, KmcactCarMAT, Vfcact, Vrcact)

Vfcac

 $[C10AcylCarCYT] \cdot [CarMAT] + KmcactCarMAT \cdot [C10AcylCarCYT] + KmcactC10AcylCarCYT \cdot [CarMAT] \cdot [C10AcylCarCYT] + KmcactC10AcylCarCYT \cdot [C10AcylCarCYT] + KmcactC10AcylCar$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KicactC	10Acy1CakricVittC10AcylC	CarCYT	56.0		\square
KmcactC	10AcylCakronenctC10Acyl	CarCYT	15.0		
KmcactC	10AcylCakemAcTctC10Acyl	CarMAT	15.0		\checkmark

8.6 Reaction vcactC8

This is a reversible reaction of one reactant forming one product influenced by six modifiers.

Name vcactC8

Reaction equation

Reactant

Table 25: Properties of each reactant.

rusic 25. Troperties of each reactant.			
Id	Name	SBO	
C8AcylCarCYT	C8AcylCarCYT		

Modifiers

Table 26: Properties of each modifier.

rable 20. Froperties of each mounter.		
Id	Name	SBO
CarMAT	CarMAT	
CarCYT	CarCYT	
C8AcylCarCYT	C8AcylCarCYT	
C8AcylCarMAT	C8AcylCarMAT	
CarCYT	CarCYT	
CarMAT	CarMAT	

Product

Table 27: Properties of each product.

Id	Name	SBO
C8AcylCarMAT	C8AcylCarMAT	

Kinetic Law

Derived unit contains undeclared units

function_4_vcactC8_1 ([C8AcylCarCYT], [C8AcylCarMAT], [CarCYT], [CarMAT], Keqcact, KicactC8AcylCarCYT, KicactCarCYT, KmcactC8AcylCarCYT, KmcactC8AcylCarMAT, KmcactCarMAT, Vfcact, Vrcact) (69)

 $= \frac{\text{Vfcact} \cdot \left(\text{C8AcylCarCYT} \right) \cdot \left[\text{CarMAT} \right] + \text{KmcactCarMAT} \cdot \left[\text{C8AcylCarCYT} \right] + \text{KmcactC8AcylCarCYT} \cdot \left[\text{CarMAT} \right] \cdot \left(1 + \frac{1}{2} \right) \cdot \left[\frac{1}{2} \right] \cdot \left[\frac{1}{2}$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KicactC	C8AcylCarkCYTactC8AcylCa	arCYT	56.0		\square
KmcactC8AcylCarCYT		15.0			
KmcactC	C8AcylCa rkMa nEactC8AcylC	CarMAT	15.0		\mathbf{Z}

8.7 Reaction vcactC6

This is a reversible reaction of one reactant forming one product influenced by six modifiers.

Name vcactC6

Reaction equation

$$C6AcylCarCYT \xleftarrow{CarMAT, CarCYT, C6AcylCarCYT, C6AcylCarMAT, CarCYT, CarMAT} C6AcylCarMAT (70)$$

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO	
C6AcylCarCYT	C6AcylCarCYT		

Modifiers

Table 30: Properties of each modifier.

Id	Name	SBO
CarMAT	CarMAT	
CarCYT	CarCYT	
C6AcylCarCYT	C6AcylCarCYT	
C6AcylCarMAT	C6AcylCarMAT	
CarCYT	CarCYT	
${\tt CarMAT}$	CarMAT	

Product

Table 31: Properties of each product.

Id	Name	SBO
C6AcylCarMAT	C6AcylCarMAT	

Kinetic Law

Derived unit contains undeclared units

 $\overline{\left[\text{C6AcylCarCYT}\right] \cdot \left[\text{CarMAT}\right] + \text{KmcactCarMAT} \cdot \left[\text{C6AcylCarCYT}\right] + \text{KmcactC6AcylCarCYT} \cdot \left[\text{CarMAT}\right] \cdot \left(1 + \frac{1}{2}\right) \cdot \left(1 +$

Vfcact ·

Table 32: Properties of each parameter.

		1			
Id	Name	SBO	Value	Unit	Constant
Ki	cactC6AcylCarKWTctC6AcylCarC	CYT	56.0		
Kn	cactC6Acy1CarKiYiEactC6Acy1Car	rCYT	15.0		\mathbf{Z}
Kn	cactC6AcylCarMnAteactC6AcylCar	rMAT	15.0		\square

8.8 Reaction vcactC4

This is a reversible reaction of one reactant forming one product influenced by six modifiers.

Name vcactC4

Reaction equation

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
C4AcylCarCYT	C4AcylCarCYT	

Modifiers

Table 34: Properties of each modifier.

Id Name SBO		
CarMAT	CarMAT	
CarCYT	CarCYT	
C4AcylCarCYT	C4AcylCarCYT	
C4AcylCarMAT	C4AcylCarMAT	
CarCYT	CarCYT	
${\tt CarMAT}$	CarMAT	

Product

Table 35: Properties of each product.

Id	Name	SBO
C4AcylCarMAT	C4AcylCarMAT	

Kinetic Law

Derived unit contains undeclared units

$$\begin{array}{l} \nu_8 = function_4_vcactC4_1 \left([C4AcylCarCYT], [C4AcylCarMAT], [CarCYT], [CarMAT], \\ Keqcact, KicactC4AcylCarCYT, KicactCarCYT, KmcactC4AcylCarCYT, \\ KmcactC4AcylCarMAT, KmcactCarCYT, KmcactCarMAT, Vfcact, Vrcact) \end{array}$$

function_4_vcactC4_1 ([C4AcylCarCYT], [C4AcylCarMAT], [CarCYT], [CarMAT], (75) Keqcact, KicactC4AcylCarCYT, KicactCarCYT, KmcactC4AcylCarCYT, KmcactC4AcylCarMAT, Vfcact, Vrcact)

 $= \frac{}{[\text{C4AcylCarCYT}] \cdot [\text{CarMAT}] + \text{KmcactCarMAT} \cdot [\text{C4AcylCarCYT}] + \text{KmcactC4AcylCarCYT} \cdot [\text{CarMAT}] \cdot \left(1 + \frac{1}{2} + \frac{$

Vfcact · (

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KicactC	C4Acy1Ca rCiv TictC4AcylCa	arCYT	56.0		$ \mathbf{Z} $
KmcactC4AcylCarKYTEactC4AcylCarCYT		15.0		\square	
KmcactC	C4AcylCa rKnA rEactC4AcylC	CarMAT	15.0		\checkmark

8.9 Reaction vcpt2C16

This is a reversible reaction of one reactant forming one product influenced by 30 modifiers.

Name vcpt2C16

Reaction equation

C16AcylCarMAT, C12AcylCarMAT, C10AcylCarMAT, C8AcylCarMAT, C6AcylCarMAT, C4AcylCarMAT, C76)

Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
C16AcylCarMAT	C16AcylCarMAT	

Table 38: Properties of each modifier.

There is a repersion of the minute.			
Id	Name	SBO	
C14AcylCarMAT	C14AcylCarMAT		
C12AcylCarMAT	C12AcylCarMAT		
C10AcylCarMAT	C10AcylCarMAT		
C8AcylCarMAT	C8AcylCarMAT		
C6AcylCarMAT	C6AcylCarMAT		
C4AcylCarMAT	C4AcylCarMAT		
CoAMAT	CoAMAT		
C14AcylCoAMAT	C14AcylCoAMAT		
C12AcylCoAMAT	C12AcylCoAMAT		
C10AcylCoAMAT	C10AcylCoAMAT		
C8AcylCoAMAT	C8AcylCoAMAT		
C6AcylCoAMAT	C6AcylCoAMAT		

Id	Name	SBO
C4AcylCoAMAT	C4AcylCoAMAT	
CarMAT	CarMAT	
C10AcylCarMAT	C10AcylCarMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C12AcylCarMAT	C12AcylCarMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C14AcylCarMAT	C14AcylCarMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C16AcylCarMAT	C16AcylCarMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C4AcylCarMAT	C4AcylCarMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
C6AcylCarMAT	C6AcylCarMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C8AcylCarMAT	C8AcylCarMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
${\tt CarMAT}$	CarMAT	
CoAMAT	CoAMAT	

Product

Table 39: Properties of each product.

Id	Name	SBO
C16AcylCoAMAT	C16AcylCoAMAT	

Kinetic Law

Derived unit contains undeclared units

 $\begin{aligned} \nu_9 &= \text{vol}\left(\text{VMAT}\right) \cdot \text{function_4_vcpt2C16_1}\left([\text{C10AcylCarMAT}],[\text{C10AcylCoAMAT}],\\ & [\text{C12AcylCarMAT}],[\text{C12AcylCoAMAT}],[\text{C14AcylCarMAT}],[\text{C14AcylCoAMAT}],\\ & [\text{C16AcylCarMAT}],[\text{C16AcylCoAMAT}],[\text{C4AcylCarMAT}],[\text{C4AcylCoAMAT}],\\ & [\text{C6AcylCarMAT}],[\text{C6AcylCoAMAT}],[\text{C8AcylCarMAT}],[\text{C8AcylCoAMAT}],[\text{CarMAT}],\\ & [\text{CoAMAT}],\text{Keqcpt2},\text{Kmcpt2C10AcylCarMAT},\text{Kmcpt2C10AcylCoAMAT},\\ & \text{Kmcpt2C12AcylCarMAT},\text{Kmcpt2C12AcylCoAMAT},\text{Kmcpt2C14AcylCarMAT},\\ & \text{Kmcpt2C14AcylCoAMAT},\text{Kmcpt2C16AcylCarMAT},\text{Kmcpt2C16AcylCoAMAT},\\ & \text{Kmcpt2C4AcylCarMAT},\text{Kmcpt2C4AcylCoAMAT},\text{Kmcpt2C6AcylCarMAT},\\ & \text{Kmcpt2C6AcylCoAMAT},\text{Kmcpt2C8AcylCarMAT},\text{Kmcpt2C8AcylCoAMAT},\\ & \text{Kmcpt2CarMAT},\text{Kmcpt2CoAMAT},\text{Vol}\left(\text{VMAT}\right),\text{Vcpt2},\text{sfcpt2C16}) \end{aligned}$

function_4_vcpt2C16_1 ([C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], (78)

[C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCoAMAT], [C16AcylCarMAT],

[C16AcylCoAMAT], [C4AcylCarMAT], [C4AcylCoAMAT], [C6AcylCarMAT],

[C6AcylCoAMAT], [C8AcylCarMAT], [C8AcylCoAMAT], [CarMAT],

[CoAMAT], Keqcpt2, Kmcpt2C10AcylCarMAT, Kmcpt2C10AcylCoAMAT,

Kmcpt2C12AcylCarMAT, Kmcpt2C12AcylCoAMAT, Kmcpt2C14AcylCarMAT,

Kmcpt2C14AcylCoAMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C16AcylCoAMAT,

Kmcpt2C4AcylCarMAT, Kmcpt2C4AcylCoAMAT, Kmcpt2C6AcylCarMAT,

Kmcpt2C6AcylCoAMAT, Kmcpt2C8AcylCarMAT, Kmcpt2C8AcylCoAMAT,

Kmcpt2CarMAT, Kmcpt2CoAMAT, vol (VMAT), Vcpt2, sfcpt2C16)

 $CPT2 \\ (sfcpt2C16, Vcpt2, Kmcpt2C16AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C12AcylCarMAT, Kmcpt2C14AcylCarMAT, Km$

function_4_vcpt2C16_1 ([C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], (79)

[C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCoAMAT], [C16AcylCarMAT],

[C16AcylCoAMAT], [C4AcylCarMAT], [C4AcylCoAMAT], [C6AcylCarMAT],

[C6AcylCoAMAT], [C8AcylCarMAT], [C8AcylCoAMAT], [CarMAT],

[CoAMAT], Keqcpt2, Kmcpt2C10AcylCarMAT, Kmcpt2C10AcylCoAMAT,

Kmcpt2C12AcylCarMAT, Kmcpt2C12AcylCoAMAT, Kmcpt2C14AcylCarMAT,

Kmcpt2C14AcylCoAMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C16AcylCoAMAT,

Kmcpt2C4AcylCarMAT, Kmcpt2C4AcylCoAMAT, Kmcpt2C6AcylCarMAT,

Kmcpt2C6AcylCoAMAT, Kmcpt2C8AcylCarMAT, Kmcpt2C8AcylCoAMAT, Kmcp

Kmcpt2CarMAT, Kmcpt2CoAMAT, vol (VMAT), Vcpt2, sfcpt2C16)

 $CPT2 \left(sfcpt2C16, Vcpt2, Kmcpt2C16AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C12AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmc$

Table 40: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfcpt2C16	sfcpt2C16	0.85	

8.10 Reaction vcpt2C14

This is a reversible reaction of one reactant forming one product influenced by 30 modifiers.

Name vcpt2C14

Reaction equation

C14AcylCarMAT C16AcylCarMAT, C12AcylCarMAT, C10AcylCarMAT, C8AcylCarMAT, C6AcylCarMAT, C4AcylCarMAT

(80)

Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
C14AcylCarMAT	C14AcylCarMAT	

Table 42: Properties of each modifier.

Id	Name	SBO
C16AcylCarMAT	C16AcylCarMAT	
C12AcylCarMAT	C12AcylCarMAT	
C10AcylCarMAT	C10AcylCarMAT	
C8AcylCarMAT	C8AcylCarMAT	
C6AcylCarMAT	C6AcylCarMAT	
C4AcylCarMAT	C4AcylCarMAT	
CoAMAT	CoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
CarMAT	CarMAT	
C10AcylCarMAT	C10AcylCarMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C12AcylCarMAT	C12AcylCarMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C14AcylCarMAT	C14AcylCarMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C16AcylCarMAT	C16AcylCarMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C4AcylCarMAT	C4AcylCarMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
C6AcylCarMAT	C6AcylCarMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C8AcylCarMAT	C8AcylCarMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
CarMAT	CarMAT	
CoAMAT	CoAMAT	

Product

Table 43: Properties of each product.

Id	Name	SBO
C14AcylCoAMAT	C14AcylCoAMAT	

Kinetic Law

Derived unit contains undeclared units

```
function_4_vcpt2C14_1 ([C10AcylCarMAT], [C10AcylCoAMAT], (82)
[C12AcylCarMAT], [C12AcylCoAMAT], [C14AcylCarMAT],
[C14AcylCoAMAT], [C16AcylCarMAT], [C16AcylCoAMAT], [C4AcylCarMAT],
[C4AcylCoAMAT], [C6AcylCarMAT], [C6AcylCoAMAT], [C8AcylCarMAT],
[C8AcylCoAMAT], [CarMAT], [CoAMAT], Keqcpt2, Kmcpt2C10AcylCarMAT,
Kmcpt2C10AcylCoAMAT, Kmcpt2C12AcylCarMAT, Kmcpt2C12AcylCoAMAT,
Kmcpt2C14AcylCarMAT, Kmcpt2C14AcylCoAMAT, Kmcpt2C16AcylCarMAT,
Kmcpt2C16AcylCoAMAT, Kmcpt2C4AcylCoAMAT, Kmcpt2C6AcylCarMAT,
Kmcpt2C6AcylCoAMAT, Kmcpt2C8AcylCarMAT, Kmcpt2C8AcylCarMAT,
Kmcpt2CarMAT, Kmcpt2C8AcylCarMAT, Kmcpt2C8AcylCarMAT,
Kmcpt2CarMAT, Kmcpt2CarMAT, Vol (VMAT), Vcpt2, sfcpt2C14)

CPT2 (sfcpt2C14, Vcpt2, Kmcpt2C14AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C12AcylCarMAT, Kmcpt2C1
```

function_4_vcpt2C14_1 ([C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], [C12AcylCarMAT], [C12AcylCarMAT], [C14AcylCarMAT], [C14AcylCoAMAT], [C16AcylCarMAT], [C16AcylCarMAT], [C4AcylCarMAT], [C4AcylCarMAT], [C6AcylCarMAT], [C6AcylCarMAT], [C8AcylCarMAT], [C8AcylCarMAT], [C8AcylCarMAT], [C8AcylCarMAT], [C8AcylCarMAT], [C9AMAT], [C9AMA

CPT2 (sfcpt2C14, Vcpt2, Kmcpt2C14AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C12AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2

Table 44: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfcpt2C14	sfcpt2C14	1.0	

8.11 Reaction vcpt2C12

This is a reversible reaction of one reactant forming one product influenced by 30 modifiers.

Name vcpt2C12

Reaction equation

Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
C12AcylCarMAT	C12AcylCarMAT	

Table 46: Properties of each modifier.

Id	Name	SBO
C16AcylCarMAT	C16AcylCarMAT	
C14AcylCarMAT	C14AcylCarMAT	
C10AcylCarMAT	C10AcylCarMAT	
C8AcylCarMAT	C8AcylCarMAT	
C6AcylCarMAT	C6AcylCarMAT	
${\tt C4AcylCarMAT}$	C4AcylCarMAT	
CoAMAT	CoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
CarMAT	CarMAT	
C10AcylCarMAT	C10AcylCarMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C12AcylCarMAT	C12AcylCarMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C14AcylCarMAT	C14AcylCarMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C16AcylCarMAT	C16AcylCarMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C4AcylCarMAT	C4AcylCarMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
C6AcylCarMAT	C6AcylCarMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C8AcylCarMAT	C8AcylCarMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
CarMAT	CarMAT	
CoAMAT	CoAMAT	

Product

Table 47: Properties of each product.

Id	Name	SBO
C12AcylCoAMAT	C12AcylCoAMAT	

Kinetic Law

Derived unit contains undeclared units

```
v_{11} = \text{vol}(VMAT) \cdot \text{function\_4\_vcpt2C12\_1}([C10AcylCarMAT], [C10AcylCoAMAT],
                                      [C12AcylCarMAT], [C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCoAMAT],
                                              [C16AcylCarMAT], [C16AcylCoAMAT], [C4AcylCarMAT], [C4AcylCoAMAT],
                                                      [C6AcylCarMAT], [C6AcylCoAMAT], [C8AcylCarMAT], [C8AcylCoAMAT],
                        [CarMAT], [CoAMAT], Keqcpt2, Kmcpt2C10AcylCarMAT, Kmcpt2C10AcylCoAMAT,
                                          Kmcpt2C12AcylCarMAT, Kmcpt2C12AcylCoAMAT, Kmcpt2C14AcylCarMAT,
                                      Kmcpt2C14AcylCoAMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C16AcylCoAMAT,
                                                      Kmcpt2C4AcylCarMAT, Kmcpt2C4AcylCoAMAT, Kmcpt2C6AcylCarMAT,
                                                  Kmcpt2C6AcylCoAMAT, Kmcpt2C8AcylCarMAT, Kmcpt2C8AcylCoAMAT,
                                                                                Kmcpt2CarMAT, Kmcpt2CoAMAT, vol (VMAT), Vcpt2, sfcpt2C12)
                                                                                                                                                                                                                                                                                      (85)
function_4_vcpt2C12_1 ([C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT],
                                                                                                                                                                                                                                                                                      (86)
[C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCoAMAT], [C16AcylCarMAT],
[C16AcylCoAMAT], [C4AcylCarMAT], [C4AcylCoAMAT], [C6AcylCarMAT],
[C6AcylCoAMAT], [C8AcylCarMAT], [C8AcylCoAMAT], [CarMAT],
[CoAMAT], Keqcpt2, Kmcpt2C10AcylCarMAT, Kmcpt2C10AcylCoAMAT,
Kmcpt2C12AcylCarMAT, Kmcpt2C12AcylCoAMAT, Kmcpt2C14AcylCarMAT,
Kmcpt2C14AcylCoAMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C16AcylCoAMAT,
Kmcpt2C4AcylCarMAT, Kmcpt2C4AcylCoAMAT, Kmcpt2C6AcylCarMAT,
Kmcpt2C6AcylCoAMAT, Kmcpt2C8AcylCarMAT, Kmcpt2C8AcylCoAMAT,
Kmcpt2CarMAT, Kmcpt2CoAMAT, vol (VMAT), Vcpt2, sfcpt2C12)
       CPT2 \left(sfcpt2C12, Vcpt2, Kmcpt2C12AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmc
function\_4\_vcpt2C12\_1 ([C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], [C10AcylCoAMAT], [C10AcylCarMAT], [C10AcylCarMAT]
                                                                                                                                                                                                                                                                                      (87)
[C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCoAMAT], [C16AcylCarMAT],
[C16AcylCoAMAT], [C4AcylCarMAT], [C4AcylCoAMAT], [C6AcylCarMAT], \\
[C6AcylCoAMAT], [C8AcylCarMAT], [C8AcylCoAMAT], [CarMAT],
[CoAMAT], Keqcpt2, Kmcpt2C10AcylCarMAT, Kmcpt2C10AcylCoAMAT,
Kmcpt2C12AcylCarMAT, Kmcpt2C12AcylCoAMAT, Kmcpt2C14AcylCarMAT,
Kmcpt2C14AcylCoAMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C16AcylCoAMAT,
Kmcpt2C4AcylCarMAT, Kmcpt2C4AcylCoAMAT, Kmcpt2C6AcylCarMAT,
Kmcpt2C6AcylCoAMAT, Kmcpt2C8AcylCarMAT, Kmcpt2C8AcylCoAMAT,
Kmcpt2CarMAT, Kmcpt2CoAMAT, vol (VMAT), Vcpt2, sfcpt2C12)
       CPT2 \left(sfcpt2C12, Vcpt2, Kmcpt2C12AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmc
```

Table 48: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfcpt2C12	sfcpt2C12	0.95	

8.12 Reaction vcpt2C10

This is a reversible reaction of one reactant forming one product influenced by 30 modifiers.

Name vcpt2C10

Reaction equation

C10AcylCarMAT, C14AcylCarMAT, C12AcylCarMAT, C8AcylCarMAT, C6AcylCarMAT, C4AcylCarMAT, C4AcylCarMAT,

Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
C10AcylCarMAT	C10AcylCarMAT	

Table 50: Properties of each modifier.

Id	Name	SBO
C16AcylCarMAT	C16AcylCarMAT	-
C14AcylCarMAT	C14AcylCarMAT	
C12AcylCarMAT	C12AcylCarMAT	
C8AcylCarMAT	C8AcylCarMAT	
C6AcylCarMAT	C6AcylCarMAT	
${\tt C4AcylCarMAT}$	C4AcylCarMAT	
CoAMAT	CoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
${\tt CarMAT}$	CarMAT	

Id	Name	SBO
C10AcylCarMAT	C10AcylCarMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C12AcylCarMAT	C12AcylCarMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C14AcylCarMAT	C14AcylCarMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C16AcylCarMAT	C16AcylCarMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
${\tt C4AcylCarMAT}$	C4AcylCarMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
C6AcylCarMAT	C6AcylCarMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C8AcylCarMAT	C8AcylCarMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
CarMAT	CarMAT	
CoAMAT	CoAMAT	

Product

Table 51: Properties of each product.

Id	Name	SBO
C10AcylCoAMAT	C10AcylCoAMAT	

Kinetic Law

Derived unit contains undeclared units

```
v_{12} = vol\left(VMAT\right) \cdot function\_4\_vcpt2C10\_1\left([C10AcylCarMAT],[C10AcylCoAMAT],\\ [C12AcylCarMAT],[C12AcylCoAMAT],[C14AcylCarMAT],[C14AcylCoAMAT],\\ [C16AcylCarMAT],[C16AcylCoAMAT],[C4AcylCarMAT],[C4AcylCoAMAT],\\ [C6AcylCarMAT],[C6AcylCoAMAT],[C8AcylCarMAT],[C8AcylCoAMAT],\\ [CarMAT],[CoAMAT],Keqcpt2,Kmcpt2C10AcylCarMAT,Kmcpt2C10AcylCoAMAT,\\ Kmcpt2C12AcylCarMAT,Kmcpt2C12AcylCoAMAT,Kmcpt2C14AcylCarMAT,\\ Kmcpt2C14AcylCoAMAT,Kmcpt2C16AcylCarMAT,Kmcpt2C16AcylCarMAT,\\ Kmcpt2C4AcylCarMAT,Kmcpt2C4AcylCoAMAT,Kmcpt2C6AcylCarMAT,\\ Kmcpt2C6AcylCoAMAT,Kmcpt2C8AcylCarMAT,Kmcpt2C8AcylCoAMAT,\\ Kmcpt2C6AcylCoAMAT,Kmcpt2C0AMAT,Vol\left(VMAT\right),Vcpt2,sfcpt2C10\right)\\ (89)
```

 $function_4_vcpt2C10_1 ([C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], \qquad (90)$

[C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCoAMAT], [C16AcylCarMAT],

[C16AcylCoAMAT], [C4AcylCarMAT], [C4AcylCoAMAT], [C6AcylCarMAT],

[C6AcylCoAMAT], [C8AcylCarMAT], [C8AcylCoAMAT], [CarMAT],

[CoAMAT], Keqcpt2, Kmcpt2C10AcylCarMAT, Kmcpt2C10AcylCoAMAT,

Kmcpt2C12AcylCarMAT, Kmcpt2C12AcylCoAMAT, Kmcpt2C14AcylCarMAT,

Kmcpt2C14AcylCoAMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C16AcylCoAMAT,

Kmcpt2C4AcylCarMAT, Kmcpt2C4AcylCoAMAT, Kmcpt2C6AcylCarMAT,

Kmcpt2C6AcylCoAMAT, Kmcpt2C8AcylCarMAT, Kmcpt2C8AcylCoAMAT,

Kmcpt2CarMAT, Kmcpt2CoAMAT, vol (VMAT), Vcpt2, sfcpt2C10)

CPT2 (sfept2C10, Vept2, Kmept2C10AcylCarMAT, Kmept2C16AcylCarMAT, Kmept2C14AcylCarMAT, Kmept2C16AcylCarMAT, Kmep

function_4_vcpt2C10_1 ([C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], (91)

[C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCoAMAT], [C16AcylCarMAT],

[C16AcylCoAMAT], [C4AcylCarMAT], [C4AcylCoAMAT], [C6AcylCarMAT],

[C6AcylCoAMAT], [C8AcylCarMAT], [C8AcylCoAMAT], [CarMAT],

[CoAMAT], Keqcpt2, Kmcpt2C10AcylCarMAT, Kmcpt2C10AcylCoAMAT,

Kmcpt2C12AcylCarMAT, Kmcpt2C12AcylCoAMAT, Kmcpt2C14AcylCarMAT,

Kmcpt2C14AcylCoAMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C16AcylCoAMAT,

Kmcpt2C4AcylCarMAT, Kmcpt2C4AcylCoAMAT, Kmcpt2C6AcylCarMAT,

Kmcpt2C6AcylCoAMAT, Kmcpt2C8AcylCarMAT, Kmcpt2C8AcylCoAMAT,

Kmcpt2CarMAT, Kmcpt2CoAMAT, vol (VMAT), Vcpt2, sfcpt2C10)

CPT2 (sfcpt2C10, Vcpt2, Kmcpt2C10AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcp

Table 52: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfcpt2C10	sfcpt2C10	0.95	$\overline{\hspace{1cm}}$

8.13 Reaction vcpt2C8

This is a reversible reaction of one reactant forming one product influenced by 30 modifiers.

Name vcpt2C8

Reaction equation

C8 A cylCarMAT C16AcylCarMAT, C14AcylCarMAT, C12AcylCarMAT, C10AcylCarMAT, C6AcylCarMAT, C4A

(92)

Reactant

Table 53: Properties of each reactant.

Tuble 33. Troperties of each reactant.			
Id	Name	SBO	
C8AcylCarMAT	C8AcylCarMAT		

Table 54: Properties of each modifier.

Id	Name	SBO
C16AcylCarMAT	C16AcylCarMAT	
C14AcylCarMAT	C14AcylCarMAT	
C12AcylCarMAT	C12AcylCarMAT	
C10AcylCarMAT	C10AcylCarMAT	
C6AcylCarMAT	C6AcylCarMAT	
${\tt C4AcylCarMAT}$	C4AcylCarMAT	
CoAMAT	CoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
CarMAT	CarMAT	
C10AcylCarMAT	C10AcylCarMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C12AcylCarMAT	C12AcylCarMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C14AcylCarMAT	C14AcylCarMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C16AcylCarMAT	C16AcylCarMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
${\tt C4AcylCarMAT}$	C4AcylCarMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
C6AcylCarMAT	C6AcylCarMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C8AcylCarMAT	C8AcylCarMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
CarMAT	CarMAT	
CoAMAT	CoAMAT	

Product

Table 55: Properties of each product

Id	Name	SBO
C8AcylCoAMAT	C8AcylCoAMAT	

Kinetic Law

Derived unit contains undeclared units

```
v<sub>13</sub> = vol (VMAT) · function_4_vcpt2C8_1 ([C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], [C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCoAMAT], [C16AcylCarMAT], [C16AcylCarMAT], [C4AcylCarMAT], [C4AcylCarMAT], [C4AcylCarMAT], [C6AcylCarMAT], [C6AcylCarMAT], [C8AcylCarMAT], [C9AcylCarMAT], [C9AcylC
```

```
function_4_vcpt2C8_1 ([C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], (94)

[C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCoAMAT], [C16AcylCarMAT],

[C16AcylCoAMAT], [C4AcylCarMAT], [C4AcylCoAMAT], [C6AcylCarMAT],

[C6AcylCoAMAT], [C8AcylCarMAT], [C8AcylCoAMAT], [CarMAT],

[C0AMAT], Keqcpt2, Kmcpt2C10AcylCarMAT, Kmcpt2C10AcylCoAMAT,

Kmcpt2C12AcylCarMAT, Kmcpt2C12AcylCoAMAT, Kmcpt2C14AcylCarMAT,

Kmcpt2C14AcylCoAMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C16AcylCoAMAT,

Kmcpt2C4AcylCarMAT, Kmcpt2C4AcylCoAMAT, Kmcpt2C6AcylCarMAT,

Kmcpt2C6AcylCoAMAT, Kmcpt2C8AcylCarMAT, Kmcpt2C8AcylCoAMAT,

Kmcpt2CarMAT, Kmcpt2CoAMAT, vol (VMAT), Vcpt2, sfcpt2C8)

_ CPT2 (sfcpt2C8, Vcpt2, Kmcpt2C8AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C14AcylC
```

function_4_vcpt2C8_1 ([C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], [C12AcylCarMAT], [C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCoAMAT], [C16AcylCarMAT], [C16AcylCoAMAT], [C16AcylCarMAT], [C4AcylCarMAT], [C4AcylCoAMAT], [C6AcylCarMAT], [C6AcylCarMAT], [C8AcylCarMAT], [CarMAT], [Car

CPT2 (sfcpt2C8, Vcpt2, Kmcpt2C8AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C

Table 56: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfcpt2C8	sfcpt2C8	0.35	

8.14 Reaction vcpt2C6

This is a reversible reaction of one reactant forming one product influenced by 30 modifiers.

Name vcpt2C6

Reaction equation

C6AcylCarMAT, C14AcylCarMAT, C12AcylCarMAT, C10AcylCarMAT, C8AcylCarMAT, C4AcylCarMAT, C96)

Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
C6AcylCarMAT	C6AcylCarMAT	

Table 58: Properties of each modifier.

Id	Name	SBO
C16AcylCarMAT	C16AcylCarMAT	
C14AcylCarMAT	C14AcylCarMAT	
C12AcylCarMAT	C12AcylCarMAT	
C10AcylCarMAT	C10AcylCarMAT	
C8AcylCarMAT	C8AcylCarMAT	
C4AcylCarMAT	C4AcylCarMAT	
CoAMAT	CoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
CarMAT	CarMAT	
C10AcylCarMAT	C10AcylCarMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C12AcylCarMAT	C12AcylCarMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C14AcylCarMAT	C14AcylCarMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C16AcylCarMAT	C16AcylCarMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
${\tt C4AcylCarMAT}$	C4AcylCarMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
C6AcylCarMAT	C6AcylCarMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C8AcylCarMAT	C8AcylCarMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
CarMAT	CarMAT	
CoAMAT	CoAMAT	

Product

Table 59: Properties of each product.

Id	Name	SBO
C6AcylCoAMAT	C6AcylCoAMAT	

Kinetic Law

Derived unit contains undeclared units

```
v_{14} = \text{vol}(VMAT) \cdot \text{function\_4\_vcpt2C6\_1}([C10AcylCarMAT], [C10AcylCoAMAT],
                                      [C12AcylCarMAT], [C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCoAMAT],
                                              [C16AcylCarMAT], [C16AcylCoAMAT], [C4AcylCarMAT], [C4AcylCoAMAT],
                                                      [C6AcylCarMAT], [C6AcylCoAMAT], [C8AcylCarMAT], [C8AcylCoAMAT],
                        [CarMAT], [CoAMAT], Keqcpt2, Kmcpt2C10AcylCarMAT, Kmcpt2C10AcylCoAMAT,
                                          Kmcpt2C12AcylCarMAT, Kmcpt2C12AcylCoAMAT, Kmcpt2C14AcylCarMAT,
                                      Kmcpt2C14AcylCoAMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C16AcylCoAMAT,
                                                      Kmcpt2C4AcylCarMAT, Kmcpt2C4AcylCoAMAT, Kmcpt2C6AcylCarMAT,
                                                  Kmcpt2C6AcylCoAMAT, Kmcpt2C8AcylCarMAT, Kmcpt2C8AcylCoAMAT,
                                                                                    Kmcpt2CarMAT, Kmcpt2CoAMAT, vol (VMAT), Vcpt2, sfcpt2C6)
                                                                                                                                                                                                                                                                                       (97)
function_4_vcpt2C6_1 ([C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT],
                                                                                                                                                                                                                                                                                       (98)
[C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCoAMAT], [C16AcylCarMAT],
[C16AcylCoAMAT], [C4AcylCarMAT], [C4AcylCoAMAT], [C6AcylCarMAT],
[C6AcylCoAMAT], [C8AcylCarMAT], [C8AcylCoAMAT], [CarMAT],
[CoAMAT], Keqcpt2, Kmcpt2C10AcylCarMAT, Kmcpt2C10AcylCoAMAT,
Kmcpt2C12AcylCarMAT, Kmcpt2C12AcylCoAMAT, Kmcpt2C14AcylCarMAT,
Kmcpt2C14AcylCoAMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C16AcylCoAMAT,
Kmcpt2C4AcylCarMAT, Kmcpt2C4AcylCoAMAT, Kmcpt2C6AcylCarMAT,
Kmcpt2C6AcylCoAMAT, Kmcpt2C8AcylCarMAT, Kmcpt2C8AcylCoAMAT,
Kmcpt2CarMAT, Kmcpt2CoAMAT, vol (VMAT), Vcpt2, sfcpt2C6)
       CPT2 \left(sfcpt2C6, Vcpt2, Kmcpt2C6AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt
function\_4\_vcpt2C6\_1 ([C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], [C10AcylCoAMAT], [C10AcylCarMAT], [C10AcylCarMAT],
                                                                                                                                                                                                                                                                                       (99)
[C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCoAMAT], [C16AcylCarMAT],
[C16AcylCoAMAT], [C4AcylCarMAT], [C4AcylCoAMAT], [C6AcylCarMAT], \\
[C6AcylCoAMAT], [C8AcylCarMAT], [C8AcylCoAMAT], [CarMAT],
[CoAMAT], Keqcpt2, Kmcpt2C10AcylCarMAT, Kmcpt2C10AcylCoAMAT,
Kmcpt2C12AcylCarMAT, Kmcpt2C12AcylCoAMAT, Kmcpt2C14AcylCarMAT,
Kmcpt2C14AcylCoAMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C16AcylCoAMAT,
Kmcpt2C4AcylCarMAT, Kmcpt2C4AcylCoAMAT, Kmcpt2C6AcylCarMAT,
Kmcpt2C6AcylCoAMAT, Kmcpt2C8AcylCarMAT, Kmcpt2C8AcylCoAMAT,
Kmcpt2CarMAT, Kmcpt2CoAMAT, vol (VMAT), Vcpt2, sfcpt2C6)
       CPT2 (sfcpt2C6, Vcpt2, Kmcpt2C6AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2
```

Table 60: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfcpt2C6	sfcpt2C6	0.15	

8.15 Reaction vcpt2C4

This is a reversible reaction of one reactant forming one product influenced by 30 modifiers.

Name vcpt2C4

Reaction equation

C4AcylCarMAT, C14AcylCarMAT, C12AcylCarMAT, C10AcylCarMAT, C8AcylCarMAT, C6AcylCarMAT, C6AcylCarMAT, C6AcylCarMAT, C100)

Reactant

Table 61: Properties of each reactant.

Id	Name	SBO
C4AcylCarMAT	C4AcylCarMAT	

Table 62: Properties of each modifier.

Id	Name	SBO
C16AcylCarMAT	C16AcylCarMAT	
C14AcylCarMAT	C14AcylCarMAT	
C12AcylCarMAT	C12AcylCarMAT	
C10AcylCarMAT	C10AcylCarMAT	
C8AcylCarMAT	C8AcylCarMAT	
C6AcylCarMAT	C6AcylCarMAT	
CoAMAT	CoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
CarMAT	CarMAT	

Id	Name	SBO
C10AcylCarMAT	C10AcylCarMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C12AcylCarMAT	C12AcylCarMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C14AcylCarMAT	C14AcylCarMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C16AcylCarMAT	C16AcylCarMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
${\tt C4AcylCarMAT}$	C4AcylCarMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
C6AcylCarMAT	C6AcylCarMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C8AcylCarMAT	C8AcylCarMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
${\tt CarMAT}$	CarMAT	
CoAMAT	CoAMAT	

Product

Table 63: Properties of each product.

Id	Name	SBO
C4AcylCoAMAT	C4AcylCoAMAT	

Kinetic Law

Derived unit contains undeclared units

```
v_{15} = vol\left(VMAT\right) \cdot function\_4\_vept2C4\_1\left([C10AcylCarMAT],[C10AcylCoAMAT],\\ [C12AcylCarMAT],[C12AcylCoAMAT],[C14AcylCarMAT],[C14AcylCoAMAT],\\ [C16AcylCarMAT],[C16AcylCoAMAT],[C4AcylCarMAT],[C4AcylCoAMAT],\\ [C6AcylCarMAT],[C6AcylCoAMAT],[C8AcylCarMAT],[C8AcylCoAMAT],\\ [CarMAT],[CoAMAT],Keqcpt2,Kmcpt2C10AcylCarMAT,Kmcpt2C10AcylCoAMAT,\\ Kmcpt2C12AcylCarMAT,Kmcpt2C12AcylCoAMAT,Kmcpt2C14AcylCarMAT,\\ Kmcpt2C14AcylCoAMAT,Kmcpt2C16AcylCarMAT,Kmcpt2C16AcylCarMAT,\\ Kmcpt2C4AcylCarMAT,Kmcpt2C4AcylCoAMAT,Kmcpt2C6AcylCarMAT,\\ Kmcpt2C6AcylCoAMAT,Kmcpt2C8AcylCarMAT,Kmcpt2C8AcylCoAMAT,\\ Kmcpt2C6AcylCoAMAT,Kmcpt2C8AcylCarMAT,Kmcpt2C8AcylCoAMAT,\\ Kmcpt2CarMAT,Kmcpt2C0AMAT,Vol\left(VMAT\right),Vcpt2,sfcpt2C4\right) \equiv (101)
```

function_4_vcpt2C4_1 ([C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], (102)

[C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCoAMAT], [C16AcylCarMAT],

[C16AcylCoAMAT], [C4AcylCarMAT], [C4AcylCoAMAT], [C6AcylCarMAT],

[C6AcylCoAMAT], [C8AcylCarMAT], [C8AcylCoAMAT], [CarMAT],

[CoAMAT], Keqcpt2, Kmcpt2C10AcylCarMAT, Kmcpt2C10AcylCoAMAT,

Kmept 2C12 Acyl Car MAT, Kmept 2C12 Acyl CoAMAT, Kmept 2C14 Acyl Car MAT, Kmept 2C14 Acyl Car

Kmcpt2C14AcylCoAMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C16AcylCoAMAT,

Kmcpt2C4AcylCarMAT, Kmcpt2C4AcylCoAMAT, Kmcpt2C6AcylCarMAT,

Kmcpt2C6AcylCoAMAT, Kmcpt2C8AcylCarMAT, Kmcpt2C8AcylCoAMAT, Kmcp

Kmcpt2CarMAT, Kmcpt2CoAMAT, vol (VMAT), Vcpt2, sfcpt2C4)

CPT2 (sfept2C4, Vept2, Kmept2C4AcylCarMAT, Kmept2C16AcylCarMAT, Kmept2C14AcylCarMAT, Kmept2C16AcylCarMAT, Kmept2

function_4_vcpt2C4_1 ([C10AcylCarMAT], [C10AcylCoAMAT], [C12AcylCarMAT], (103)

[C12AcylCoAMAT], [C14AcylCarMAT], [C14AcylCoAMAT], [C16AcylCarMAT],

[C16AcylCoAMAT], [C4AcylCarMAT], [C4AcylCoAMAT], [C6AcylCarMAT],

[C6AcylCoAMAT], [C8AcylCarMAT], [C8AcylCoAMAT], [CarMAT],

[CoAMAT], Keqcpt2, Kmcpt2C10AcylCarMAT, Kmcpt2C10AcylCoAMAT,

Kmcpt2C12AcylCarMAT, Kmcpt2C12AcylCoAMAT, Kmcpt2C14AcylCarMAT,

Kmcpt2C14AcylCoAMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C16AcylCoAMAT,

Kmcpt2C4AcylCarMAT, Kmcpt2C4AcylCoAMAT, Kmcpt2C6AcylCarMAT,

Kmcpt2C6AcylCoAMAT, Kmcpt2C8AcylCarMAT, Kmcpt2C8AcylCoAMAT,

Kmcpt2CarMAT, Kmcpt2CoAMAT, vol (VMAT), Vcpt2, sfcpt2C4)

CPT2 (sfcpt2C4, Vcpt2, Kmcpt2C4AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C16AcylCarMAT, Kmcpt2

Table 64: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfcpt2C4	sfcpt2C4	0.01	

8.16 Reaction vvlcadC16

This is a reversible reaction of one reactant forming two products influenced by 13 modifiers.

Name vvlcadC16

Reaction equation

C16AcylCoAMAT C14AcylCoAMAT, C12AcylCoAMAT, FADtMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C

(104)

Reactant

Table 65: Properties of each reactant.

Id	Name	SBO
C16AcylCoAMAT	C16AcylCoAMAT	

Modifiers

Table 66: Properties of each modifier.

Id	Name	SBO
C14AcylCoAMAT	C14AcylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
FADtMAT	FADtMAT	
C14EnoylCoAMAT	C14EnoylCoAMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C14EnoylCoAMAT	C14EnoylCoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C16EnoylCoAMAT	C16EnoylCoAMAT	
FADHMAT	FADHMAT	
FADtMAT	FADtMAT	

Products

Table 67: Properties of each product.

Id	Name	SBO
C16EnoylCoAMAT FADHMAT	C16EnoylCoAMAT FADHMAT	

Kinetic Law

Derived unit contains undeclared units

```
v_{16} = \text{vol}(\text{VMAT}) \cdot \text{function\_4\_vvlcadC16\_1}([\text{C12AcylCoAMAT}], [\text{C12EnoylCoAMAT}],
      [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT],
                         [FADHMAT], [FADtMAT], Keqvlcad, KmvlcadC12AcylCoAMAT,
                                KmvlcadC12EnoylCoAMAT, KmvlcadC14AcylCoAMAT,
                                KmvlcadC14EnoylCoAMAT, KmvlcadC16AcylCoAMAT,
          KmvlcadC16EnoylCoAMAT, KmvlcadFAD, KmvlcadFADH, vol (VMAT), Vvlcad,
                                                                          sfvlcadC16)
                                                                                (105)
```

function_4_vvlcadC16_1 ([C12AcylCoAMAT], [C12EnoylCoAMAT], (106)[C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqvlcad,

KmvlcadC12AcylCoAMAT, KmvlcadC12EnoylCoAMAT,

KmvlcadC14AcylCoAMAT, KmvlcadC14EnoylCoAMAT,

KmvlcadC16AcylCoAMAT, KmvlcadC16EnoylCoAMAT,

KmvlcadFAD, KmvlcadFADH, vol (VMAT), Vvlcad, sfvlcadC16)

VLCAD (sfvlcadC16, Vvlcad, KmvlcadC16AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC14AcylCoA

function_4_vvlcadC16_1 ([C12AcylCoAMAT], [C12EnoylCoAMAT], (107)[C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqvlcad, KmvlcadC12AcylCoAMAT, KmvlcadC12EnoylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC14EnoylCoAMAT,

KmvlcadC16AcylCoAMAT, KmvlcadC16EnoylCoAMAT,

KmvlcadFAD, KmvlcadFADH, vol (VMAT), Vvlcad, sfvlcadC16)

VLCAD (sfvlcadC16, Vvlcad, KmvlcadC16AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC12AcylC

Table 68: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfvlcadC16	sfvlcadC16	1.0	

8.17 Reaction vvlcadC14

This is a reversible reaction of one reactant forming two products influenced by 13 modifiers.

Name vvlcadC14

Reaction equation

C14AcylCoAMAT, C12AcylCoAMAT, FADtMAT, C16EnoylCoAMAT, C12EnoylCoAMAT, C12AcylCoAMAT, C16EnoylCoAMAT, C12EnoylCoAMAT, C16EnoylCoAMAT, C16Enoyl

(108)

Reactant

Table 69: Properties of each reactant.

Id	Name	SBO
C14AcylCoAMAT	C14AcylCoAMAT	

Modifiers

Table 70: Properties of each modifier.

Id	Name	SBO
C16AcylCoAMAT	C16AcylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
FADtMAT	FADtMAT	
C16EnoylCoAMAT	C16EnoylCoAMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C14EnoylCoAMAT	C14EnoylCoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C16EnoylCoAMAT	C16EnoylCoAMAT	
FADHMAT	FADHMAT	
FADtMAT	FADtMAT	

Products

Table 71: Properties of each product.

Id	Name	SBO
C14EnoylCoAMAT FADHMAT	C14EnoylCoAMAT FADHMAT	

Kinetic Law

Derived unit contains undeclared units

```
v_{17} = \text{vol}(\text{VMAT}) \cdot \text{function\_4\_vvlcadC14\_1}([\text{C12AcylCoAMAT}], [\text{C12EnoylCoAMAT}],
      [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT],
                         [FADHMAT], [FADtMAT], Keqvlcad, KmvlcadC12AcylCoAMAT,
                                KmvlcadC12EnoylCoAMAT, KmvlcadC14AcylCoAMAT,
                                KmvlcadC14EnoylCoAMAT, KmvlcadC16AcylCoAMAT,
          KmvlcadC16EnoylCoAMAT, KmvlcadFAD, KmvlcadFADH, vol (VMAT), Vvlcad,
                                                                          sfvlcadC14)
                                                                                (109)
```

function_4_vvlcadC14_1 ([C12AcylCoAMAT], [C12EnoylCoAMAT], (110)[C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqvlcad, KmvlcadC12AcylCoAMAT, KmvlcadC12EnoylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC14EnoylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC16EnoylCoAMAT, KmvlcadFAD, KmvlcadFADH, vol (VMAT), Vvlcad, sfvlcadC14)

 $VLCAD \\ (sfvlcadC14, Vvlcad, KmvlcadC14AcylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC12Acy$

```
function_4_vvlcadC14_1 ([C12AcylCoAMAT], [C12EnoylCoAMAT],
                                                                          (111)
[C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT],
[C16EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqvlcad,
KmvlcadC12AcylCoAMAT, KmvlcadC12EnoylCoAMAT,
KmvlcadC14AcylCoAMAT, KmvlcadC14EnoylCoAMAT,
KmvlcadC16AcylCoAMAT, KmvlcadC16EnoylCoAMAT,
KmvlcadFAD, KmvlcadFADH, vol\left(VMAT\right), Vvlcad, sfvlcadC14)
```

VLCAD (sfvlcadC14, Vvlcad, KmvlcadC14AcylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC16AcylCoA

Table 72: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfvlcadC14	sfvlcadC14	0.42	\checkmark

8.18 Reaction vvlcadC12

This is a reversible reaction of one reactant forming two products influenced by 13 modifiers.

Name vvlcadC12

Reaction equation

C12AcylCoAMAT, C14AcylCoAMAT, FADtMAT, C16EnoylCoAMAT, C14EnoylCoAMAT, C12AcylCoAMAT, C16EnoylCoAMAT, C16Enoyl

(112)

Reactant

Table 73: Properties of each reactant.

Id	Name	SBO
C12AcylCoAMAT	C12AcylCoAMAT	

Modifiers

Table 74: Properties of each modifier.

Id	Name	SBO
C16AcylCoAMAT	C16AcylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
FADtMAT	FADtMAT	
C16EnoylCoAMAT	C16EnoylCoAMAT	
C14EnoylCoAMAT	C14EnoylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C14EnoylCoAMAT	C14EnoylCoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C16EnoylCoAMAT	C16EnoylCoAMAT	
FADHMAT	FADHMAT	
FADtMAT	FADtMAT	

Products

Table 75: Properties of each product.

Id	Name	SBO
C12EnoylCoAMAT FADHMAT	C12EnoylCoAMAT FADHMAT	

Kinetic Law

Derived unit contains undeclared units

```
\begin{split} \nu_{18} &= vol\left(VMAT\right) \cdot function\_4\_vvlcadC12\_1\left([C12AcylCoAMAT],[C12EnoylCoAMAT],\\ &[C14AcylCoAMAT],[C14EnoylCoAMAT],[C16AcylCoAMAT],[C16EnoylCoAMAT],\\ &[FADHMAT],[FADtMAT],Keqvlcad,KmvlcadC12AcylCoAMAT,\\ &KmvlcadC12EnoylCoAMAT,KmvlcadC14AcylCoAMAT,\\ &KmvlcadC14EnoylCoAMAT,KmvlcadC16AcylCoAMAT,\\ &KmvlcadC16EnoylCoAMAT,KmvlcadFADH,vol\left(VMAT\right),Vvlcad,\\ &sfvlcadC12\right) \end{split}
```

function_4_vvlcadC12_1 ([C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqvlcad, KmvlcadC12AcylCoAMAT, KmvlcadC12EnoylCoAMAT, KmvlcadC14EnoylCoAMAT, KmvlcadC14EnoylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC16EnoylCoAMAT, K

 $KmvlcadFAD, KmvlcadFADH, vol\left(VMAT\right), Vvlcad, sfvlcadC12)$

 $\underline{VLCAD (sfvlcadC12, Vvlcad, KmvlcadC12AcylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC14Acy$

```
function_4_vvlcadC12_1 ([C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqvlcad, KmvlcadC12AcylCoAMAT, KmvlcadC12EnoylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC14EnoylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC16EnoylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC16EnoylCoAMAT, KmvlcadFAD, KmvlcadFADH, vol (VMAT), Vvlcad, sfvlcadC12) VLCAD (sfvlcadC12, Vvlcad, KmvlcadC12AcvlCoAMAT, KmvlcadC16AcvlCoAMAT, KmvlcadC16AcvlC
```

VLCAD (sfvlcadC12, Vvlcad, KmvlcadC12AcylCoAMAT, KmvlcadC16AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC14AcylCoA

Table 76: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfvlcadC12	sfvlcadC12	0.11	\checkmark

8.19 Reaction vlcadC16

This is a reversible reaction of one reactant forming two products influenced by 21 modifiers.

Name vlcadC16

Reaction equation

C16AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, FADtMAT, C14

(116)

Reactant

Table 77: Properties of each reactant.

Id	Name	SBO
C16AcylCoAMAT	C16AcylCoAMAT	

Table 78: Properties of each modifier.

Id	Name	SBO
C14AcylCoAMAT	C14AcylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
FADtMAT	FADtMAT	
C14EnoylCoAMAT	C14EnoylCoAMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C10EnoylCoAMAT	C10EnoylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C10EnoylCoAMAT	C10EnoylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C14EnoylCoAMAT	C14EnoylCoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C16EnoylCoAMAT	C16EnoylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
FADHMAT	FADHMAT	
FADtMAT	FADtMAT	

Products

Table 79: Properties of each product.

Id	Name	SBO
C16EnoylCoAMAT FADHMAT	C16EnoylCoAMAT FADHMAT	

Kinetic Law

Derived unit contains undeclared units

```
v_{19} = \text{vol}(VMAT) \cdot \text{function\_4\_vlcadC16\_1}([C10AcylCoAMAT], [C10EnoylCoAMAT],
      [C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT],
        [C16AcylCoAMAT], [C16EnoylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT],
                         [FADHMAT], [FADtMAT], Keqlcad, KmlcadC10AcylCoAMAT,
        KmlcadC10EnoylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12EnoylCoAMAT,
        KmlcadC14AcylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC16AcylCoAMAT,
         KmlcadC16EnoylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC8EnoylCoAMAT,
                            KmlcadFAD, KmlcadFADH, vol (VMAT), Vlcad, sflcadC16)
                                                                         (117)
function_4_vlcadC16_1 ([C10AcylCoAMAT], [C10EnoylCoAMAT],
                                                                         (118)
[C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT],
[C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [C8AcylCoAMAT],
[C8EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqlcad, KmlcadC10AcylCoAMAT,
KmlcadC10EnoylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12EnoylCoAMAT,
KmlcadC14AcylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC16AcylCoAMAT,
KmlcadC16EnoylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC8EnoylCoAMAT, \\
KmlcadFAD, KmlcadFADH, vol (VMAT), Vlcad, sflcadC16)
```

LCAD (sflcadC16, Vlcad, KmlcadC16AcylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC16AcylCoAMAT, Kmlc

```
function_4_vlcadC16_1 ([C10AcylCoAMAT], [C10EnoylCoAMAT], (119)
[C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16EnoylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [C8EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqlcad, KmlcadC10AcylCoAMAT, KmlcadC10EnoylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12EnoylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFAD, KmlcadFADH, vol (VMAT), Vlcad, sflcadC16
```

 $\underline{LCAD\,(sfleadC16,Vlead,KmleadC16AcylCoAMAT,KmleadC14AcylCoAMAT,KmleadC12AcylCoAMAT,KmleadC12AcylCoAMAT,KmleadC16ACylCoAMAT,KmleadC16AcylCoAMAT,KmleadC16AcylCoAMAT,KmleadC16AcylCoAMAT,KmleadC16AcylCoAMAT,$

Table 80: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sflcadC16	sflcadC16	0.9	

8.20 Reaction vlcadC14

This is a reversible reaction of one reactant forming two products influenced by 21 modifiers.

Name vlcadC14

Reaction equation

C14AcylCoAMAT, C16AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, FADtMAT, C16
(120)

Reactant

Table 81: Properties of each reactant.

Id	Name	SBO
C14AcylCoAMAT	C14AcylCoAMAT	

Table 82: Properties of each modifier.

Id		Name	SBO
C16AcylCoA	MAT	C16AcylCoAMAT	
C12AcylCoA	MAT	C12AcylCoAMAT	
C10AcylCoA	MAT	C10AcylCoAMAT	
C8AcylCoAM	AT	C8AcylCoAMAT	
FADtMAT		FADtMAT	
C16EnoylCo	AMAT	C16EnoylCoAMAT	
C12EnoylCo	AMAT	C12EnoylCoAMAT	
C10EnoylCo	AMAT	C10EnoylCoAMAT	
C8EnoylCoA	MAT	C8EnoylCoAMAT	
C10AcylCoA	MAT	C10AcylCoAMAT	
C10EnoylCo	AMAT	C10EnoylCoAMAT	
C12AcylCoA	MAT	C12AcylCoAMAT	
C12EnoylCo	AMAT	C12EnoylCoAMAT	
C14AcylCoA	MAT	C14AcylCoAMAT	

Id	Name	SBO
C14EnoylCoAMAT	C14EnoylCoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C16EnoylCoAMAT	C16EnoylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
FADHMAT	FADHMAT	
FADtMAT	FADtMAT	

Products

Table 83: Properties of each product.

product.			
Id	Name	SBO	
C14EnoylCoAMAT FADHMAT	C14EnoylCoAMAT FADHMAT		

Kinetic Law

Derived unit contains undeclared units

```
\begin{aligned} v_{20} &= \text{vol}\left(\text{VMAT}\right) \cdot \text{function\_4\_vlcadC14\_1}\left([\text{C10AcylCoAMAT}], [\text{C10EnoylCoAMAT}], \\ &[\text{C12AcylCoAMAT}], [\text{C12EnoylCoAMAT}], [\text{C14AcylCoAMAT}], [\text{C14EnoylCoAMAT}], \\ &[\text{C16AcylCoAMAT}], [\text{C16EnoylCoAMAT}], [\text{C8AcylCoAMAT}], [\text{C8EnoylCoAMAT}], \\ &[\text{FADHMAT}], [\text{FADtMAT}], \text{Keqlcad}, \text{KmlcadC10AcylCoAMAT}, \\ &[\text{KmlcadC10EnoylCoAMAT}, \text{KmlcadC12AcylCoAMAT}, \text{KmlcadC12EnoylCoAMAT}, \\ &[\text{KmlcadC14AcylCoAMAT}, \text{KmlcadC14EnoylCoAMAT}, \text{KmlcadC16AcylCoAMAT}, \\ &[\text{KmlcadC16EnoylCoAMAT}, \text{KmlcadC8AcylCoAMAT}, \text{KmlcadC8EnoylCoAMAT}, \\ &[\text{KmlcadFAD}, \text{KmlcadFADH}, \text{vol}\left(\text{VMAT}\right), \text{Vlcad}, \text{sflcadC14}\right) \end{aligned} \tag{121}
```

```
function_4_vlcadC14_1 ([C10AcylCoAMAT], [C10EnoylCoAMAT], (122) [C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16EnoylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqlcad, KmlcadC10AcylCoAMAT, KmlcadC10EnoylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12EnoylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFAD, KmlcadFADH, vol (VMAT), Vlcad, sflcadC14)
```

LCAD (sflcadC14, Vlcad, KmlcadC14AcylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC16AcylCoAMAT, Kmlc

 $function_4_vlcadC14_1 ([C10AcylCoAMAT], [C10EnoylCoAMAT], \\ (123)$

[C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT],

[C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [C8AcylCoAMAT],

[C8EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqlcad, KmlcadC10AcylCoAMAT,

KmlcadC10EnoylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12EnoylCoAMAT,

KmlcadC14AcylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC16AcylCoAMAT, Kmlcad

KmlcadC16EnoylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC8EnoylCoAMAT,

KmlcadFAD, KmlcadFADH, vol (VMAT), Vlcad, sflcadC14)

 $\underline{LCAD}(sflcadC14, Vlcad, KmlcadC14AcylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC16AcylCoAMAT, Km$

Table 84: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sflcadC14	sflcadC14	1.0	\overline{Z}

8.21 Reaction vlcadC12

This is a reversible reaction of one reactant forming two products influenced by 20 modifiers.

Name vlcadC12

Reaction equation

C12AcylCoAMAT, C14AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, FADtMAT, C14

(124)

Reactant

Table 85: Properties of each reactant.

Id	Name	SBO
C12AcylCoAMAT	C12AcylCoAMAT	

Table 86: Properties of each modifier.

Id	Name	SBO
C16AcylCoAMAT	C16AcylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	

Id	Name	SBO
C10AcylCoAMAT	C10AcylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
FADtMAT	FADtMAT	
C14EnoylCoAMAT	C14EnoylCoAMAT	
C16EnoylCoAMAT	C16EnoylCoAMAT	
C10EnoylCoAMAT	C10EnoylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C10EnoylCoAMAT	C10EnoylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C14EnoylCoAMAT	C14EnoylCoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C16EnoylCoAMAT	C16EnoylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
FADHMAT	FADHMAT	
FADtMAT	FADtMAT	

Table 87: Properties of each product.

Id	Name	SBO
C12EnoylCoAMAT FADHMAT	C12EnoylCoAMAT FADHMAT	

Kinetic Law

```
\begin{split} v_{21} &= vol\left(VMAT\right) \cdot function\_4\_vlcadC12\_1\left([C10AcylCoAMAT], [C10EnoylCoAMAT], \\ & [C12AcylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], \\ & [C16EnoylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [FADHMAT], \\ & [FADtMAT], Keqlcad, KmlcadC10AcylCoAMAT, KmlcadC10EnoylCoAMAT, \\ & KmlcadC12AcylCoAMAT, KmlcadC12EnoylCoAMAT, KmlcadC14AcylCoAMAT, \\ & KmlcadC14EnoylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC16EnoylCoAMAT, \\ & KmlcadC8AcylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFAD, KmlcadFADH, \\ & vol\left(VMAT\right), Vlcad, sflcadC12\right) \end{split}
```

function_4_vlcadC12_1 ([C10AcylCoAMAT], [C10EnoylCoAMAT], (126)

[C12AcylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT],

[C16AcylCoAMAT], [C16EnoylCoAMAT], [C8AcylCoAMAT],

[C8EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqlcad, KmlcadC10AcylCoAMAT,

KmlcadC10EnoylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12EnoylCoAMAT,

KmlcadC14AcylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC16AcylCoAMAT,

KmlcadC16EnoylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC8EnoylCoAMAT,

KmlcadFAD, KmlcadFADH, vol (VMAT), Vlcad, sflcadC12)

ECAD (sflcadC12, Vlcad, KmlcadC12AcylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC16AcylCoAMAT, Kmlcad

function_4_vlcadC12_1 ([C10AcylCoAMAT], [C10EnoylCoAMAT], (127)

[C12AcylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT],

[C16AcylCoAMAT], [C16EnoylCoAMAT], [C8AcylCoAMAT],

[C8EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqlcad, KmlcadC10AcylCoAMAT,

KmlcadC10EnoylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12EnoylCoAMAT,

KmlcadC14AcylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC16AcylCoAMAT,

KmlcadC16EnoylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC8EnoylCoAMAT,

KmlcadFAD, KmlcadFADH, vol (VMAT), Vlcad, sflcadC12)

 $\underline{\quad LCAD\left(sflcadC12,Vlcad,KmlcadC12AcylCoAMAT,KmlcadC16AcylCoAMAT,KmlcadC14AcylCoAMAT,KmlcadC14AcylCoAMAT,KmlcadC16AcylCoAMAT,KmlcadC14AcylCoAMAT,KmlcadC16AcylCoAMA$

Table 88: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sflcadC12	sflcadC12	0.9	\checkmark

8.22 Reaction vlcadC10

This is a reversible reaction of one reactant forming two products influenced by 21 modifiers.

Name vlcadC10

Reaction equation

C10AcylCoAMAT, C14AcylCoAMAT, C12AcylCoAMAT, C8AcylCoAMAT, FADtMAT, C16
(128)

Reactant

Table 89: Properties of each reactant.

Id	Name	SBO
C10AcylCoAMAT	C10AcylCoAMAT	

Modifiers

Table 90: Properties of each modifier.

Id	Name	SBO
C16AcylCoAMAT	C16AcylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
FADtMAT	FADtMAT	
C16EnoylCoAMAT	C16EnoylCoAMAT	
C14EnoylCoAMAT	C14EnoylCoAMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C10EnoylCoAMAT	C10EnoylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C14EnoylCoAMAT	C14EnoylCoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C16EnoylCoAMAT	C16EnoylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
FADHMAT	FADHMAT	
FADtMAT	FADtMAT	

Products

Table 91: Properties of each product.

Id	Name	SBO
C10EnoylCoAMAT FADHMAT	C10EnoylCoAMAT FADHMAT	

Kinetic Law

Derived unit contains undeclared units

```
v_{22} = \text{vol}(VMAT) \cdot \text{function\_4\_vlcadC10\_1}([C10AcylCoAMAT], [C10EnoylCoAMAT],
      [C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT],
        [C16AcylCoAMAT], [C16EnoylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT],
                         [FADHMAT], [FADtMAT], Keqlcad, KmlcadC10AcylCoAMAT,
        KmlcadC10EnoylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12EnoylCoAMAT,
         KmlcadC14AcylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC16AcylCoAMAT,
          KmlcadC16EnoylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC8EnoylCoAMAT,
                            KmlcadFAD, KmlcadFADH, vol (VMAT), Vlcad, sflcadC10)
                                                                          (129)
function_4_vlcadC10_1 ([C10AcylCoAMAT], [C10EnoylCoAMAT],
                                                                          (130)
[C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT],
[C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [C8AcylCoAMAT],
[C8EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqlcad, KmlcadC10AcylCoAMAT,
KmlcadC10EnoylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12EnoylCoAMAT, \\
```

KmlcadFAD, KmlcadFADH, vol (VMAT), Vlcad, sflcadC10) LCAD (sflcadC10, Vlcad, KmlcadC10AcylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC10AcylCoAMAT, Kmlc

```
function_4_vlcadC10_1 ([C10AcylCoAMAT], [C10EnoylCoAMAT],
                                                                        (131)
[C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT],
[C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [C8AcylCoAMAT],
[C8EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqlcad, KmlcadC10AcylCoAMAT,
KmlcadC10EnoylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC12EnoylCoAMAT,
KmlcadC14AcylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC16AcylCoAMAT, \\
KmlcadC16EnoylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC8EnoylCoAMAT, \\
KmlcadFAD, KmlcadFADH, vol (VMAT), Vlcad, sflcadC10)
```

KmlcadC14AcylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC8EnoylCoAMAT,

LCAD (sflcad C10, Vlcad, Kmlcad C10 Acyl CoAMAT, Kmlcad C16 Acyl CoAMAT, Kmlcad C14 Acyl CoAMAT, Kmlcad C16 Acyl C0AMAT, Kml

Table 92: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sflcadC10	sflcadC10	0.75	Ø

8.23 Reaction vmcadC12

This is a reversible reaction of one reactant forming two products influenced by 21 modifiers.

Name vmcadC12

Reaction equation

C12AcylCoAMAT, C8AcylCoAMAT, C6AcylCoAMAT, C4AcylCoAMAT, FADtMAT, C10Er

(132)

Reactant

Table 93: Properties of each reactant.

Id	Name	SBO
C12AcylCoAMAT	C12AcylCoAMAT	

Table 94: Properties of each modifier.

Id	Name	SBO
C10AcylCoAMAT	C10AcylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
FADtMAT	FADtMAT	
C10EnoylCoAMAT	C10EnoylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
C6EnoylCoAMAT	C6EnoylCoAMAT	
C4EnoylCoAMAT	C4EnoylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C10EnoylCoAMAT	C10EnoylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
C4EnoylCoAMAT	C4EnoylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C6EnoylCoAMAT	C6EnoylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
FADHMAT	FADHMAT	

Id	Name	SBO
FADtMAT	FADtMAT	

Table 95: Properties of each product.

Id	Name	SBO
C12EnoylCoAMAT FADHMAT	C12EnoylCoAMAT FADHMAT	

Kinetic Law

```
v_{23} = vol\left(VMAT\right) \cdot function\_4\_vmcadC12\_1\left([C10AcylCoAMAT],[C10EnoylCoAMAT],\\ [C12AcylCoAMAT],[C12EnoylCoAMAT],[C4AcylCoAMAT],[C4EnoylCoAMAT],\\ [C6AcylCoAMAT],[C6EnoylCoAMAT],[C8AcylCoAMAT],[C8EnoylCoAMAT],\\ [FADHMAT],[FADtMAT],Keqmcad,KmmcadC10AcylCoAMAT,\\ KmmcadC10EnoylCoAMAT,KmmcadC12AcylCoAMAT,\\ KmmcadC12EnoylCoAMAT,KmmcadC4AcylCoAMAT,KmmcadC4EnoylCoAMAT,\\ KmmcadC6AcylCoAMAT,KmmcadC6EnoylCoAMAT,KmmcadC8AcylCoAMAT,\\ KmmcadC8EnoylCoAMAT,KmmcadFADH,vol\left(VMAT\right),Vmcad,\\ sfmcadC12\right)
```

```
function_4_vmcadC12_1 ([C10AcylCoAMAT], [C10EnoylCoAMAT], (134)

[C12AcylCoAMAT], [C12EnoylCoAMAT], [C4AcylCoAMAT],

[C4EnoylCoAMAT], [C6AcylCoAMAT], [C6EnoylCoAMAT],

[C8AcylCoAMAT], [C8EnoylCoAMAT], [FADHMAT], [FADtMAT],

Keqmcad, KmmcadC10AcylCoAMAT, KmmcadC10EnoylCoAMAT,

KmmcadC12AcylCoAMAT, KmmcadC12EnoylCoAMAT,

KmmcadC4AcylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadC6AcylCoAMAT,

KmmcadC6EnoylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC8EnoylCoAMAT,

KmmcadFAD, KmmcadFADH, vol (VMAT), Vmcad, sfmcadC12)

MCAD (sfmcadC12, Vmcad, KmmcadC12AcylCoAMAT, KmmcadC10AcylCoAMAT, KmmcadC8AcylCoAMAT)
```

function_4_vmcadC12_1 ([C10AcylCoAMAT], [C10EnoylCoAMAT],

(135)

[C12AcylCoAMAT], [C12EnoylCoAMAT], [C4AcylCoAMAT],

[C4EnoylCoAMAT], [C6AcylCoAMAT], [C6EnoylCoAMAT],

[C8AcylCoAMAT], [C8EnoylCoAMAT], [FADHMAT], [FADtMAT],

Keqmcad, KmmcadC10AcylCoAMAT, KmmcadC10EnoylCoAMAT,

KmmcadC12AcylCoAMAT, KmmcadC12EnoylCoAMAT,

KmmcadC4AcylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadC6AcylCoAMAT,

KmmcadC6EnoylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC8EnoylCoAMAT, KmmcadC8

KmmcadFAD, KmmcadFADH, vol (VMAT), Vmcad, sfmcadC12)

 $\underline{MCAD} (sfmcadC12, Vmcad, KmmcadC12AcylCoAMAT, KmmcadC10AcylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC10AcylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC10AcylCoAMAT, Kmmc$

Table 96: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfmcadC12	sfmcadC12	0.38	

8.24 Reaction vmcadC10

This is a reversible reaction of one reactant forming two products influenced by 21 modifiers.

Name vmcadC10

Reaction equation

C10AcylCoAMAT, C12AcylCoAMAT, C8AcylCoAMAT, C6AcylCoAMAT, C4AcylCoAMAT, FADtMAT, C12Er

Reactant

Table 97: Properties of each reactant.

Id	Name	SBO
C10AcylCoAMAT	C10AcylCoAMAT	

Table 98: Properties of each modifier.

Id	Name	SBO
C12AcylCoAMAT	C12AcylCoAMAT	-

Id	Name	SBO
C8AcylCoAMAT	C8AcylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
FADtMAT	FADtMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
C6EnoylCoAMAT	C6EnoylCoAMAT	
C4EnoylCoAMAT	C4EnoylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C10EnoylCoAMAT	C10EnoylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
C4EnoylCoAMAT	C4EnoylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C6EnoylCoAMAT	C6EnoylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
FADHMAT	FADHMAT	
FADtMAT	FADtMAT	

Table 99: Properties of each product.

Id	Name	SBO
C10EnoylCoAMAT FADHMAT	C10EnoylCoAMAT FADHMAT	

Kinetic Law

```
v_{24} = \text{vol}(\text{VMAT}) \cdot \text{function\_4\_vmcadC10\_1}([\text{C10AcylCoAMAT}], [\text{C10EnoylCoAMAT}],
        [C12AcylCoAMAT], [C12EnoylCoAMAT], [C4AcylCoAMAT], [C4EnoylCoAMAT],
           [C6AcylCoAMAT], [C6EnoylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT],
                        [FADHMAT], [FADtMAT], Keqmcad, KmmcadC10AcylCoAMAT,
                              KmmcadC10EnoylCoAMAT, KmmcadC12AcylCoAMAT,
       KmmcadC12EnoylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadC4EnoylCoAMAT,
         KmmcadC6AcylCoAMAT, KmmcadC6EnoylCoAMAT, KmmcadC8AcylCoAMAT,
           KmmcadC8EnoylCoAMAT, KmmcadFAD, KmmcadFADH, vol (VMAT), Vmcad,
                                                                     sfmcadC10)
                                                                           (137)
function_4_vmcadC10_1 ([C10AcylCoAMAT], [C10EnoylCoAMAT],
                                                                           (138)
```

[C12AcylCoAMAT], [C12EnoylCoAMAT], [C4AcylCoAMAT], [C4EnoylCoAMAT], [C6AcylCoAMAT], [C6EnoylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqmcad, KmmcadC10AcylCoAMAT, KmmcadC10EnoylCoAMAT, KmmcadC12AcylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadC6AcylCoAMAT,

KmmcadC6EnoylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC8EnoylCoAMAT,

KmmcadFAD, KmmcadFADH, vol (VMAT), Vmcad, sfmcadC10)

MCAD (sfmcadC10, Vmcad, KmmcadC10AcylCoAMAT, KmmcadC12AcylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC10AcylCoAMAT, Kmmcad

```
function_4_vmcadC10_1 ([C10AcylCoAMAT], [C10EnoylCoAMAT],
                                                                       (139)
[C12AcylCoAMAT], [C12EnoylCoAMAT], [C4AcylCoAMAT],
[C4EnoylCoAMAT], [C6AcylCoAMAT], [C6EnoylCoAMAT],
[C8AcylCoAMAT], [C8EnoylCoAMAT], [FADHMAT], [FADtMAT],
Keqmcad, KmmcadC10AcylCoAMAT, KmmcadC10EnoylCoAMAT,
KmmcadC12AcylCoAMAT, KmmcadC12EnoylCoAMAT,
```

KmmcadC4AcylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadC6AcylCoAMAT,

KmmcadC6EnoylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC8EnoylCoAMAT, KmmcadC8

KmmcadFAD, KmmcadFADH, vol (VMAT), Vmcad, sfmcadC10)

MCAD (sfmcadC10, Vmcad, KmmcadC10AcylCoAMAT, KmmcadC12AcylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC10AcylCoAMAT, Kmmcad

Table 100: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfmcadC10	sfmcadC10	0.8	\square

8.25 Reaction vmcadC8

This is a reversible reaction of one reactant forming two products influenced by 21 modifiers.

Name vmcadC8

Reaction equation

C8AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT, C6AcylCoAMAT, C4AcylCoAMAT, FADtMAT, C12Er

Reactant

Table 101: Properties of each reactant.

Id	Name	SBO
C8AcylCoAMAT	C8AcylCoAMAT	

Table 102: Properties of each modifier.

Id	Name	SBO
C12AcylCoAMAT	C12AcylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
FADtMAT	FADtMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C10EnoylCoAMAT	C10EnoylCoAMAT	
C6EnoylCoAMAT	C6EnoylCoAMAT	
C4EnoylCoAMAT	C4EnoylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C10EnoylCoAMAT	C10EnoylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
C4EnoylCoAMAT	C4EnoylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C6EnoylCoAMAT	C6EnoylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
FADHMAT	FADHMAT	

Id	Name	SBO
FADtMAT	FADtMAT	

Table 103: Properties of each product.

Id	Name	SBO
C8EnoylCoAMAT FADHMAT	C8EnoylCoAMAT FADHMAT	

Kinetic Law

```
v_{25} = vol\left(VMAT\right) \cdot function\_4\_vmcadC8\_1\left([C10AcylCoAMAT],[C10EnoylCoAMAT],\\ [C12AcylCoAMAT],[C12EnoylCoAMAT],[C4AcylCoAMAT],[C4EnoylCoAMAT],\\ [C6AcylCoAMAT],[C6EnoylCoAMAT],[C8AcylCoAMAT],[C8EnoylCoAMAT],\\ [FADHMAT],[FADtMAT],Keqmcad,KmmcadC10AcylCoAMAT,\\ KmmcadC10EnoylCoAMAT,KmmcadC12AcylCoAMAT,\\ KmmcadC12EnoylCoAMAT,KmmcadC4AcylCoAMAT,KmmcadC4EnoylCoAMAT,\\ KmmcadC6AcylCoAMAT,KmmcadC6EnoylCoAMAT,KmmcadC8AcylCoAMAT,\\ KmmcadC8EnoylCoAMAT,KmmcadFADH,vol\left(VMAT\right),Vmcad,\\ sfmcadC8\right) \\ (141)
```

```
function_4_vmcadC8_1 ([C10AcylCoAMAT], [C10EnoylCoAMAT], (142)

[C12AcylCoAMAT], [C12EnoylCoAMAT], [C4AcylCoAMAT],

[C4EnoylCoAMAT], [C6AcylCoAMAT], [C6EnoylCoAMAT],

[C8AcylCoAMAT], [C8EnoylCoAMAT], [FADHMAT], [FADtMAT],

Keqmcad, KmmcadC10AcylCoAMAT, KmmcadC10EnoylCoAMAT,

KmmcadC12AcylCoAMAT, KmmcadC12EnoylCoAMAT,

KmmcadC4AcylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadC6AcylCoAMAT,

KmmcadC6EnoylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC8EnoylCoAMAT,

KmmcadFAD, KmmcadFADH, vol (VMAT), Vmcad, sfmcadC8)

MCAD (sfmcadC8, Vmcad, KmmcadC8AcylCoAMAT, KmmcadC12AcylCoAMAT, KmmcadC10AcylCoAMAT
```

function_4_vmcadC8_1 ([C10AcylCoAMAT], [C10EnoylCoAMAT],

(143)

[C12AcylCoAMAT], [C12EnoylCoAMAT], [C4AcylCoAMAT],

[C4EnoylCoAMAT], [C6AcylCoAMAT], [C6EnoylCoAMAT],

[C8AcylCoAMAT], [C8EnoylCoAMAT], [FADHMAT], [FADtMAT],

Keqmcad, KmmcadC10AcylCoAMAT, KmmcadC10EnoylCoAMAT,

KmmcadC12AcylCoAMAT, KmmcadC12EnoylCoAMAT,

KmmcadC4AcylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadC6AcylCoAMAT,

KmmcadC6EnoylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC8EnoylCoAMAT, KmmcadC8

KmmcadFAD, KmmcadFADH, vol (VMAT), Vmcad, sfmcadC8)

MCAD (sfmcadC8, Vmcad, KmmcadC8AcylCoAMAT, KmmcadC12AcylCoAMAT, KmmcadC10AcylCoAMAT, Kmmcad

Table 104: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfmcadC8	sfmcadC8	0.87	

8.26 Reaction vmcadC6

This is a reversible reaction of one reactant forming two products influenced by 21 modifiers.

Name vmcadC6

Reaction equation

C6AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, C4AcylCoAMAT, FADtMAT, C12Er

Reactant

Table 105: Properties of each reactant.

Id	Name	SBO
C6AcylCoAMAT	C6AcylCoAMAT	

Table 106: Properties of each modifier.

Id	Name	SBO
C12AcylCoAMAT	C12AcylCoAMAT	

Id	Name	SBO
C10AcylCoAMAT	C10AcylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
FADtMAT	FADtMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C10EnoylCoAMAT	C10EnoylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
C4EnoylCoAMAT	C4EnoylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C10EnoylCoAMAT	C10EnoylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
C4EnoylCoAMAT	C4EnoylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C6EnoylCoAMAT	C6EnoylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
FADHMAT	FADHMAT	
FADtMAT	FADtMAT	

Table 107: Properties of each product.

Table 107. Troperties of each product.		
Id	Name	SBO
C6EnoylCoAMAT FADHMAT	C6EnoylCoAMAT FADHMAT	

Kinetic Law

```
v_{26} = \text{vol}(VMAT) \cdot \text{function\_4\_vmcadC6\_1}([C10AcylCoAMAT], [C10EnoylCoAMAT],
        [C12AcylCoAMAT], [C12EnoylCoAMAT], [C4AcylCoAMAT], [C4EnoylCoAMAT],
          [C6AcylCoAMAT], [C6EnoylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT],
                       [FADHMAT], [FADtMAT], Keqmcad, KmmcadC10AcylCoAMAT,
                             KmmcadC10EnoylCoAMAT, KmmcadC12AcylCoAMAT,
      KmmcadC12EnoylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadC4EnoylCoAMAT,
        KmmcadC6AcylCoAMAT, KmmcadC6EnoylCoAMAT, KmmcadC8AcylCoAMAT,
          KmmcadC8EnoylCoAMAT, KmmcadFAD, KmmcadFADH, vol (VMAT), Vmcad,
                                                                   sfmcadC6)
                                                                        (145)
function_4_vmcadC6_1 ([C10AcylCoAMAT], [C10EnoylCoAMAT],
                                                                        (146)
[C12AcylCoAMAT], [C12EnoylCoAMAT], [C4AcylCoAMAT],
[C4EnoylCoAMAT], [C6AcylCoAMAT], [C6EnoylCoAMAT],
[C8AcylCoAMAT], [C8EnoylCoAMAT], [FADHMAT], [FADtMAT],
Keqmcad, KmmcadC10AcylCoAMAT, KmmcadC10EnoylCoAMAT,
```

KmmcadC12AcylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadC6AcylCoAMAT, Km

KmmcadC6EnoylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC8EnoylCoAMAT, KmmcadC8

KmmcadFAD, KmmcadFADH, vol (VMAT), Vmcad, sfmcadC6)

 $\label{eq:mcad} \\ MCAD (sfmcadC6, Vmcad, KmmcadC6AcylCoAMAT, KmmcadC12AcylCoAMAT, KmmcadC10AcylCoAMAT, KmmcadC10$

```
function_4_vmcadC6_1 ([C10AcylCoAMAT], [C10EnoylCoAMAT], [C12AcylCoAMAT], [C12EnoylCoAMAT], [C4AcylCoAMAT], [C4EnoylCoAMAT], [C6EnoylCoAMAT], [C6EnoylCoAMAT], [C6EnoylCoAMAT], [C8AcylCoAMAT], [FADHMAT], [FADHMAT], [FADtMAT], [FADtMAT], Keqmcad, KmmcadC10AcylCoAMAT, KmmcadC10EnoylCoAMAT, KmmcadC12AcylCoAMAT, KmmcadC12EnoylCoAMAT,
```

KmmcadC4AcylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadC6AcylCoAMAT, Kmm

KmmcadC6EnoylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC8EnoylCoAMAT,

KmmcadFAD, KmmcadFADH, vol (VMAT), Vmcad, sfmcadC6)

 $\label{eq:mcad} \underline{\mathsf{MCAD}}(\mathsf{sfmcadC6}, \mathsf{Vmcad}, \mathsf{KmmcadC6} \mathsf{AcylCoAMAT}, \mathsf{KmmcadC12} \mathsf{AcylCoAMAT}, \mathsf{KmmcadC10} \mathsf{AcylCoAMAT})$

Table 108: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfmcadC6	sfmcadC6	1.0	\square

8.27 Reaction vscadC4

This is a reversible reaction of one reactant forming two products influenced by nine modifiers.

Name vscadC4

Reaction equation

C4AcylCoAMAT, C6EnoylCoAMAT, C4AcylCoAMAT, C4EnoylCoAMAT, C6AcylCoAMAT, C4EnoylCoAMAT, C6AcylCoAMAT, C6AcylCoAMAT,

Reactant

Table 109: Properties of each reactant.

Id	Name	SBO
C4AcylCoAMAT	C4AcylCoAMAT	

Modifiers

Table 110: Properties of each modifier.

rable 110. 110perties of each mounter.			
Id	Name	SBO	
C6AcylCoAMAT	C6AcylCoAMAT		
FADtMAT	FADtMAT		
C6EnoylCoAMAT	C6EnoylCoAMAT		
C4AcylCoAMAT	C4AcylCoAMAT		
C4EnoylCoAMAT	C4EnoylCoAMAT		
C6AcylCoAMAT	C6AcylCoAMAT		
C6EnoylCoAMAT	C6EnoylCoAMAT		
FADHMAT	FADHMAT		
FADtMAT	FADtMAT		

Products

Table 111: Properties of each product.

Id	Name	SBO
C4EnoylCoAMAT FADHMAT	C4EnoylCoAMAT FADHMAT	

Kinetic Law

Derived unit contains undeclared units

```
\begin{split} v_{27} &= vol\left(VMAT\right) \\ &\cdot function\_4\_vscadC4\_1\left([C4AcylCoAMAT],[C4EnoylCoAMAT],[C6AcylCoAMAT], \\ &\left[C6EnoylCoAMAT\right],[FADHMAT],[FADtMAT],Keqscad,KmscadC4AcylCoAMAT, \\ &KmscadC4EnoylCoAMAT,KmscadC6AcylCoAMAT,KmscadC6EnoylCoAMAT, \\ &KmscadFAD,KmscadFADH,vol\left(VMAT\right),Vscad,sfscadC4\right) \end{aligned} \tag{149}
```

function_4_vscadC4_1 ([C4AcylCoAMAT], [C4EnoylCoAMAT], [C6AcylCoAMAT], [C6EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqscad, KmscadC4AcylCoAMAT, KmscadC4EnoylCoAMAT, KmscadC6AcylCoAMAT, KmscadC6EnoylCoAMAT, KmscadFAD, KmscadFADH, vol (VMAT), Vscad, sfscadC4)

 $\underline{\quad SCAD\left(sfscadC4,Vscad,KmscadC4AcylCoAMAT,KmscadC6AcylCoAMAT,KmscadFAD,KmscadC4EnoylCoAMAT,KmscadFAD,KmscadC4EnoylCoAMAT,KmscadFAD,KmscadC4EnoylCoAMAT,KmscadFAD,KmscadC4EnoylCoAMAT,KmscadFAD,KmscadC4EnoylCoAMAT,KmscadFAD,KmscadC4EnoylCoAMAT,KmscadFAD,KmscadC4EnoylCoAMAT,KmscadFAD,KmscadC4EnoylCoAMAT,KmscadFAD,KmscadC4EnoylCoAMAT,KmscadFAD,KmscadC4EnoylCoAMAT,KmscadFAD,KmscadC4EnoylCoAMAT,KmscadFAD,KmscadC4EnoylCoAMAT,KmscadFAD,KmscadC4EnoylCoAMAT,KmscadFAD,KmscadC4EnoylCoAMAT,KmscadFAD,KmscadC4EnoylCoAMAT,KmscadFAD,KmscadC4EnoylCoAMAT,KmscadFAD,KmscadC4EnoylCoAMAT,KmscadFAD,KmscadC4EnoylCoAMAT,KmscadFAD,K$

```
function_4_vscadC4_1 ([C4AcylCoAMAT], [C4EnoylCoAMAT], [C6AcylCoAMAT], [C6EnoylCoAMAT], [FADHMAT], [FADtMAT], Keqscad, KmscadC4AcylCoAMAT, KmscadC4EnoylCoAMAT, KmscadC6AcylCoAMAT, KmscadC6EnoylCoAMAT, KmscadFAD, KmscadFADH, vol (VMAT), Vscad, sfscadC4)
```

 $\underline{\quad SCAD \left(sfscadC4, Vscad, KmscadC4AcylCoAMAT, KmscadC6AcylCoAMAT, KmscadFAD, KmscadC4EnoylCoAMAT, KmscadC4Enoy$

Table 112: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfscadC4	sfscadC4	1.0	\checkmark

8.28 Reaction vmckatC6

This is a reversible reaction of one reactant forming two products influenced by 29 modifiers.

Name vmckatC6

Reaction equation

C6KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCoAMAT, C10KetoacylCoAM
(152)

Reactant

Table 113: Properties of each reactant.

Id	Name	SBO
14	Turne	550
C6KetoacvlCoAMAT	C6KetoacylCoAMAT	
0011000000	001100000000001111111111111111111111111	

Table 114: Properties of each modifier.

Id	Name	SBO
C16KetoacylCoAMAT	C16KetoacylCoAMAT	
C14KetoacylCoAMAT	C14KetoacylCoAMAT	
C12KetoacylCoAMAT	C12KetoacylCoAMAT	
C10KetoacylCoAMAT	C10KetoacylCoAMAT	
C8KetoacylCoAMAT	C8KetoacylCoAMAT	
C4AcetoacylCoAMAT	C4AcetoacylCoAMAT	
CoAMAT	CoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
AcetylCoAMAT	AcetylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C10KetoacylCoAMAT	C10KetoacylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C12KetoacylCoAMAT	C12KetoacylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C14KetoacylCoAMAT	C14KetoacylCoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C16KetoacylCoAMAT	C16KetoacylCoAMAT	
C4AcetoacylCoAMAT	C4AcetoacylCoAMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C6KetoacylCoAMAT	C6KetoacylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C8KetoacylCoAMAT	C8KetoacylCoAMAT	
CoAMAT	CoAMAT	

Table 115: Properties of each product.

ruste 115. 110perties of each product.		
Id	Name	SBO
C4AcylCoAMAT AcetylCoAMAT	C4AcylCoAMAT AcetylCoAMAT	

 $v_{28} = \text{vol}(\text{VMAT}) \cdot \text{function_4_vmckatC6_1}([\text{AcetylCoAMAT}], [\text{C10AcylCoAMAT}],$

Kinetic Law

```
[C10KetoacylCoAMAT], [C12AcylCoAMAT], [C12KetoacylCoAMAT], [C12Ketoacy
                                                   [C14AcylCoAMAT], [C14KetoacylCoAMAT], [C16AcylCoAMAT],
                                              [C16Ke to a cyl CoAMAT], [C4Aceto a cyl CoAMAT], [C4Acyl CoAMAT], \\
             [C6AcylCoAMAT], [C6KetoacylCoAMAT], [C8AcylCoAMAT], [C8KetoacylCoAMAT],
                           [CoAMAT], Keqmckat, KmmckatAcetylCoAMAT, KmmckatC10AcylCoAMAT,
                                                           KmmckatC10KetoacylCoAMAT, KmmckatC12AcylCoAMAT,
                                                           KmmckatC12KetoacylCoAMAT, KmmckatC14AcylCoAMAT,
                                                           KmmckatC14KetoacylCoAMAT, KmmckatC16AcylCoAMAT,
                                                   Kmmck at C16 Ke to a cyl CoAMAT, Kmmck at C4 Aceto a cyl CoAMAT, \\
                                                                       KmmckatC4AcylCoAMAT, KmmckatC6AcylCoAMAT,
                                                                KmmckatC6KetoacylCoAMAT, KmmckatC8AcylCoAMAT,
              KmmckatC8KetoacylCoAMAT, KmmckatCoAMAT, vol (VMAT), Vmckat, sfmckatC6)
                                                                                                                                                                      (153)
function_4_vmckatC6_1 ([AcetylCoAMAT], [C10AcylCoAMAT],
                                                                                                                                                                      (154)
[C10KetoacylCoAMAT], [C12AcylCoAMAT], [C12KetoacylCoAMAT],
[C14AcylCoAMAT], [C14KetoacylCoAMAT], [C16AcylCoAMAT],
[C16KetoacylCoAMAT], [C4AcetoacylCoAMAT], [C4AcylCoAMAT],
[C6AcylCoAMAT], [C6KetoacylCoAMAT], [C8AcylCoAMAT],
[C8KetoacylCoAMAT], [CoAMAT], Kegmckat, KmmckatAcetylCoAMAT,
KmmckatC10AcylCoAMAT, KmmckatC10KetoacylCoAMAT,
KmmckatC12AcylCoAMAT, KmmckatC12KetoacylCoAMAT,
KmmckatC14AcylCoAMAT, KmmckatC14KetoacylCoAMAT,
KmmckatC16AcylCoAMAT, KmmckatC16KetoacylCoAMAT,
KmmckatC4AcetoacylCoAMAT, KmmckatC4AcylCoAMAT,
KmmckatC6AcylCoAMAT, KmmckatC6KetoacylCoAMAT,
KmmckatC8AcylCoAMAT, KmmckatC8KetoacylCoAMAT,
KmmckatCoAMAT, vol (VMAT), Vmckat, sfmckatC6)
    MCKATA (sfmckatC6, Vmckat, KmmckatC6KetoacylCoAMAT, KmmckatC16KetoacylCoAMAT, KmmckatC14E
```

function_4_vmckatC6_1 ([AcetylCoAMAT], [C10AcylCoAMAT],

(155)

[C10KetoacylCoAMAT], [C12AcylCoAMAT], [C12KetoacylCoAMAT],

[C14AcylCoAMAT], [C14KetoacylCoAMAT], [C16AcylCoAMAT],

[C16KetoacylCoAMAT], [C4AcetoacylCoAMAT], [C4AcylCoAMAT],

[C6AcylCoAMAT], [C6KetoacylCoAMAT], [C8AcylCoAMAT],

[C8KetoacylCoAMAT], [CoAMAT], Keqmckat, KmmckatAcetylCoAMAT,

KmmckatC10AcylCoAMAT, KmmckatC10KetoacylCoAMAT,

KmmckatC12AcylCoAMAT, KmmckatC12KetoacylCoAMAT,

KmmckatC14AcylCoAMAT, KmmckatC14KetoacylCoAMAT,

KmmckatC16AcylCoAMAT, KmmckatC16KetoacylCoAMAT,

KmmckatC4AcetoacylCoAMAT, KmmckatC4AcylCoAMAT,

KmmckatC6AcylCoAMAT, KmmckatC6KetoacylCoAMAT,

KmmckatC8AcylCoAMAT, KmmckatC8KetoacylCoAMAT,

KmmckatCoAMAT, vol (VMAT), Vmckat, sfmckatC6)

MCKATA (sfmckatC6, Vmckat, KmmckatC6KetoacylCoAMAT, KmmckatC16KetoacylCoAMAT, KmmckatC14EMAT, KmmckatC14EMAT

Table 116: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfmckatC6	sfmckatC6	1.0	

8.29 Reaction vmckatC4

This is a reversible reaction of one reactant forming one product influenced by 30 modifiers.

Name vmckatC4

Reaction equation

C4AcetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCoAMAT, C10KetoacylCoAM
(156)

Reactant

Table 117: Properties of each reactant.

Id	Name	SBO
C4AcetoacylCoAMAT	C4AcetoacylCoAMAT	

Modifiers

Table 118: Properties of each modifier.

Table 118: Properties of each modifier.		
Id	Name	SBO
C16KetoacylCoAMAT	C16KetoacylCoAMAT	
C14KetoacylCoAMAT	C14KetoacylCoAMAT	
C12KetoacylCoAMAT	C12KetoacylCoAMAT	
C10KetoacylCoAMAT	C10KetoacylCoAMAT	
C8KetoacylCoAMAT	C8KetoacylCoAMAT	
C6KetoacylCoAMAT	C6KetoacylCoAMAT	
CoAMAT	CoAMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
AcetylCoAMAT	AcetylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C10KetoacylCoAMAT	C10KetoacylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C12KetoacylCoAMAT	C12KetoacylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C14KetoacylCoAMAT	C14KetoacylCoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C16KetoacylCoAMAT	C16KetoacylCoAMAT	
C4AcetoacylCoAMAT	C4AcetoacylCoAMAT	
C4AcylCoAMAT	C4AcylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C6KetoacylCoAMAT	C6KetoacylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C8KetoacylCoAMAT	C8KetoacylCoAMAT	
CoAMAT	CoAMAT	

Product

Table 119: Properties of each product.

Id	Name	SBO
AcetylCoAMAT	AcetylCoAMAT	

Kinetic Law

```
v_{29} = \text{vol}(VMAT) \cdot \text{function\_4\_vmckatC4\_1}([AcetylCoAMAT], [C10AcylCoAMAT],
                   [C10KetoacylCoAMAT], [C12AcylCoAMAT], [C12KetoacylCoAMAT],
                      [C14AcylCoAMAT], [C14KetoacylCoAMAT], [C16AcylCoAMAT],
                    [C16KetoacylCoAMAT], [C4AcetoacylCoAMAT], [C4AcylCoAMAT],
      [C6AcylCoAMAT], [C6KetoacylCoAMAT], [C8AcylCoAMAT], [C8KetoacylCoAMAT],
            [CoAMAT], Keqmckat, KmmckatAcetylCoAMAT, KmmckatC10AcylCoAMAT,
                          KmmckatC10KetoacylCoAMAT, KmmckatC12AcylCoAMAT,
                          KmmckatC12KetoacylCoAMAT, KmmckatC14AcylCoAMAT,
                          KmmckatC14KetoacylCoAMAT, KmmckatC16AcylCoAMAT,
                      KmmckatC16KetoacylCoAMAT, KmmckatC4AcetoacylCoAMAT,
                               KmmckatC4AcylCoAMAT, KmmckatC6AcylCoAMAT,
                            KmmckatC6KetoacylCoAMAT, KmmckatC8AcylCoAMAT,
      KmmckatC8KetoacylCoAMAT, KmmckatCoAMAT, vol (VMAT), Vmckat, sfmckatC4)
                                                                         (157)
function_4_vmckatC4_1 ([AcetylCoAMAT], [C10AcylCoAMAT],
                                                                         (158)
[C10KetoacylCoAMAT], [C12AcylCoAMAT], [C12KetoacylCoAMAT],
```

```
[C10KetoacylCoAMAT], [C12AcylCoAMAT], [C12KetoacylCoAMAT],
[C14AcylCoAMAT], [C14KetoacylCoAMAT], [C16AcylCoAMAT],
[C16KetoacylCoAMAT], [C4AcetoacylCoAMAT], [C4AcylCoAMAT],
[C6AcylCoAMAT], [C6KetoacylCoAMAT], [C8AcylCoAMAT],
[C8KetoacylCoAMAT], [C6KetoacylCoAMAT], [C8AcylCoAMAT],
[C8KetoacylCoAMAT], [C0AMAT], Keqmckat, KmmckatAcetylCoAMAT,
KmmckatC10AcylCoAMAT, KmmckatC10KetoacylCoAMAT,
KmmckatC12AcylCoAMAT, KmmckatC12KetoacylCoAMAT,
KmmckatC14AcylCoAMAT, KmmckatC14KetoacylCoAMAT,
KmmckatC16AcylCoAMAT, KmmckatC16KetoacylCoAMAT,
KmmckatC4AcetoacylCoAMAT, KmmckatC4AcylCoAMAT,
KmmckatC6AcylCoAMAT, KmmckatC6KetoacylCoAMAT,
KmmckatC6AcylCoAMAT, KmmckatC6KetoacylCoAMAT,
KmmckatC8AcylCoAMAT, KmmckatC8KetoacylCoAMAT,
KmmckatC8AcylCoAMAT, KmmckatC8KetoacylCoAMAT,
KmmckatC0AMAT, vol (VMAT), Vmckat, sfmckatC4)
MCKATB (sfmckatC4, Vmckat, KmmckatC4AcetoacylCoAMAT, KmmckatC16KetoacylCoAMAT, KmmckatC4AcetoacylCoAMAT, KmmckatC16KetoacylCoAMAT, KmmckatC16Ket
```

 $function_4_vmckatC4_1 ([AcetylCoAMAT], [C10AcylCoAMAT],$

(159)

[C10KetoacylCoAMAT], [C12AcylCoAMAT], [C12KetoacylCoAMAT],

[C14AcylCoAMAT], [C14KetoacylCoAMAT], [C16AcylCoAMAT],

[C16KetoacylCoAMAT], [C4AcetoacylCoAMAT], [C4AcylCoAMAT],

[C6AcylCoAMAT], [C6KetoacylCoAMAT], [C8AcylCoAMAT],

[C8KetoacylCoAMAT], [CoAMAT], Keqmckat, KmmckatAcetylCoAMAT,

KmmckatC10AcylCoAMAT, KmmckatC10KetoacylCoAMAT,

Kmmckat C12 Acyl CoAMAT, Kmmckat C12 Ketoacyl CoAMAT,

KmmckatC14AcylCoAMAT, KmmckatC14KetoacylCoAMAT,

KmmckatC16AcylCoAMAT, KmmckatC16KetoacylCoAMAT,

KmmckatC4AcetoacylCoAMAT, KmmckatC4AcylCoAMAT,

KmmckatC6AcylCoAMAT, KmmckatC6KetoacylCoAMAT,

KmmckatC8AcylCoAMAT, KmmckatC8KetoacylCoAMAT,

KmmckatCoAMAT, vol (VMAT), Vmckat, sfmckatC4)

MCKATB (sfmckatC4, Vmckat, KmmckatC4AcetoacylCoAMAT, KmmckatC16KetoacylCoAMAT, KmmckatC14

Table 120: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfmckatC4	sfmckatC4	0.49	

8.30 Reaction vmtpC16

This is a reversible reaction of one reactant forming three products influenced by 28 modifiers.

Name vmtpC16

Reaction equation

C16EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C8EnoylCoAMAT, NADtMAT

Reactant

Table 121: Properties of each reactant.

Id	Name	SBO
C16EnoylCoAMAT	C16EnoylCoAMAT	

Modifiers

Table 122: Properties of each modifier.

Table 122: Properties of each modifier.			
Id	Name	SBO	
C14EnoylCoAMAT	C14EnoylCoAMAT		
C12EnoylCoAMAT	C12EnoylCoAMAT		
C10EnoylCoAMAT	C10EnoylCoAMAT		
C8EnoylCoAMAT	C8EnoylCoAMAT		
NADtMAT	NADtMAT		
CoAMAT	CoAMAT		
C16AcylCoAMAT	C16AcylCoAMAT		
C12AcylCoAMAT	C12AcylCoAMAT		
C10AcylCoAMAT	C10AcylCoAMAT		
C8AcylCoAMAT	C8AcylCoAMAT		
C6AcylCoAMAT	C6AcylCoAMAT		
C4AcetoacylCoAMAT	C4AcetoacylCoAMAT		
AcetylCoAMAT	AcetylCoAMAT		
C10AcylCoAMAT	C10AcylCoAMAT		
C10EnoylCoAMAT	C10EnoylCoAMAT		
C12AcylCoAMAT	C12AcylCoAMAT		
C12EnoylCoAMAT	C12EnoylCoAMAT		
C14AcylCoAMAT	C14AcylCoAMAT		
C14EnoylCoAMAT	C14EnoylCoAMAT		
C16AcylCoAMAT	C16AcylCoAMAT		
C16EnoylCoAMAT	C16EnoylCoAMAT		
C4AcetoacylCoAMAT	C4AcetoacylCoAMAT		
C6AcylCoAMAT	C6AcylCoAMAT		
C8AcylCoAMAT	C8AcylCoAMAT		
C8EnoylCoAMAT	C8EnoylCoAMAT		
CoAMAT	CoAMAT		
NADHMAT	NADHMAT		
NADtMAT	NADtMAT		

Products

Table 123: Properties of each product.

Id	Name	SBO
C14AcylCoAMAT AcetylCoAMAT NADHMAT	C14AcylCoAMAT AcetylCoAMAT NADHMAT	

Kinetic Law

Derived unit contains undeclared units

```
v_{30} = \text{vol}(VMAT)
          · function_4_vmtpC16_1 ([AcetylCoAMAT], [C10AcylCoAMAT], [C10EnoylCoAMAT],
            [C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT],
                                         [C16AcylCoAMAT], [C16EnoylCoAMAT], [C4AcetoacylCoAMAT],
                    [C6AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [CoAMAT], Keqmtp,
                           KicrotC4AcetoacylCoA, KmmtpAcetylCoAMAT, KmmtpC10AcylCoAMAT,
                KmmtpC10EnoylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC12
                  KmmtpC14AcylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16AcylCoAMAT,
                      KmmtpC16EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT,
               KmmtpC8EnoylCoAMAT, KmmtpCoAMAT, KmmtpNADHMAT, KmmtpNADMAT,
                                                        [NADHMAT], [NADtMAT], vol (VMAT), Vmtp, sfmtpC16)
                                                                                                                                             (161)
function_4_vmtpC16_1 ([AcetylCoAMAT], [C10AcylCoAMAT], [C10EnoylCoAMAT],
                                                                                                                                             (162)
[C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT],
[C16AcylCoAMAT], [C16EnoylCoAMAT], [C4AcetoacylCoAMAT],
[C6AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [CoAMAT], Keqmtp,
KicrotC4AcetoacylCoA, KmmtpAcetylCoAMAT, KmmtpC10AcylCoAMAT,
KmmtpC10EnoylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC12EnoylCoAMAT,
KmmtpC14AcylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16AcylCoAMAT,
KmmtpC16EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT,
KmmtpC8EnoylCoAMAT, KmmtpCoAMAT, KmmtpNADHMAT,
KmmtpNADMAT, [NADHMAT], [NADtMAT], vol (VMAT), Vmtp, sfmtpC16)
    MTP (sfmtpC16, Vmtp, KmmtpC16EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC12EnoylCoAMAT, Km
function_4_vmtpC16_1 ([AcetylCoAMAT], [C10AcylCoAMAT], [C10EnoylCoAMAT],
                                                                                                                                             (163)
[C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT],
[C16AcylCoAMAT], [C16EnoylCoAMAT], [C4AcetoacylCoAMAT],
[C6AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [CoAMAT], Keqmtp,
KicrotC4AcetoacylCoA, KmmtpAcetylCoAMAT, KmmtpC10AcylCoAMAT,
KmmtpC10EnoylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC12EnoylCoAMAT,
KmmtpC14AcylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16AcylCoAMAT,
KmmtpC16EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT,
KmmtpC8EnoylCoAMAT, KmmtpCoAMAT, KmmtpNADHMAT,
```

MTP (sfmtpC16, Vmtp, KmmtpC16EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC1

KmmtpNADMAT, [NADHMAT], [NADtMAT], vol (VMAT), Vmtp, sfmtpC16)

Table 124: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfmtpC16	sfmtpC16	1.0	

8.31 Reaction vmtpC14

This is a reversible reaction of one reactant forming three products influenced by 28 modifiers.

Name vmtpC14

Reaction equation

C14EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C8EnoylCoAMAT, NADtMAT
(164)

Reactant

Table 125: Properties of each reactant.

Id	Name	SBO
C14EnoylCoAMAT	C14EnoylCoAMAT	

Table 126: Properties of each modifier.

<u> </u>	
Name	SBO
C16EnoylCoAMAT	
C12EnoylCoAMAT	
C10EnoylCoAMAT	
C8EnoylCoAMAT	
NADtMAT	
CoAMAT	
C16AcylCoAMAT	
C14AcylCoAMAT	
C10AcylCoAMAT	
C8AcylCoAMAT	
C6AcylCoAMAT	
C4AcetoacylCoAMAT	
AcetylCoAMAT	
C10AcylCoAMAT	
	C16EnoylCoAMAT C12EnoylCoAMAT C10EnoylCoAMAT C8EnoylCoAMAT NADtMAT CoAMAT C16AcylCoAMAT C14AcylCoAMAT C10AcylCoAMAT C8AcylCoAMAT C8AcylCoAMAT C4AcetoacylCoAMAT AcetylCoAMAT

Id	Name	SBO
C10EnoylCoAMAT	C10EnoylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C14EnoylCoAMAT	C14EnoylCoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C16EnoylCoAMAT	C16EnoylCoAMAT	
C4AcetoacylCoAMAT	C4AcetoacylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
CoAMAT	CoAMAT	
NADHMAT	NADHMAT	
NADtMAT	NADtMAT	

Table 127: Properties of each product.

Id	Name	SBO
C12AcylCoAMAT	C12AcylCoAMAT	
AcetylCoAMAT	AcetylCoAMAT	
NADHMAT	NADHMAT	

Kinetic Law

```
v_{31} = vol\left(VMAT\right) \\ \cdot function\_4\_vmtpC14\_1\left([AcetylCoAMAT],[C10AcylCoAMAT],[C10EnoylCoAMAT],\\ [C12AcylCoAMAT],[C12EnoylCoAMAT],[C14AcylCoAMAT],[C14EnoylCoAMAT],\\ [C16AcylCoAMAT],[C16EnoylCoAMAT],[C4AcetoacylCoAMAT],\\ [C6AcylCoAMAT],[C8AcylCoAMAT],[C8EnoylCoAMAT],[CoAMAT],Keqmtp,\\ KicrotC4AcetoacylCoA,KmmtpAcetylCoAMAT,KmmtpC10AcylCoAMAT,\\ KmmtpC10EnoylCoAMAT,KmmtpC12AcylCoAMAT,KmmtpC12EnoylCoAMAT,\\ KmmtpC14AcylCoAMAT,KmmtpC14EnoylCoAMAT,KmmtpC16AcylCoAMAT,\\ KmmtpC16EnoylCoAMAT,KmmtpC6AcylCoAMAT,KmmtpC8AcylCoAMAT,\\ KmmtpC8EnoylCoAMAT,KmmtpCoAMAT,KmmtpNADHMAT,KmmtpNADMAT,\\ [NADHMAT],[NADtMAT],vol\left(VMAT\right),Vmtp,sfmtpC14\right) \equiv{(165)}
```

function_4_vmtpC14_1 ([AcetylCoAMAT], [C10AcylCoAMAT], [C10EnoylCoAMAT], (166)

[C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT],

[C16AcylCoAMAT], [C16EnoylCoAMAT], [C4AcetoacylCoAMAT],

[C6AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [CoAMAT], Keqmtp,

KicrotC4AcetoacylCoA, KmmtpAcetylCoAMAT, KmmtpC10AcylCoAMAT,

KmmtpC10EnoylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC12EnoylCoAMAT,

KmmtpC14AcylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16AcylCoAMAT,

KmmtpC16EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT,

KmmtpC8EnoylCoAMAT, KmmtpCoAMAT, KmmtpNADHMAT,

KmmtpNADMAT, [NADHMAT], [NADtMAT], vol (VMAT), Vmtp, sfmtpC14)

MTP (sfmtpC14, Vmtp, KmmtpC14EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC1

function_4_vmtpC14_1 ([AcetylCoAMAT], [C10AcylCoAMAT], [C10EnoylCoAMAT], (167)

[C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT],

[C16AcylCoAMAT], [C16EnoylCoAMAT], [C4AcetoacylCoAMAT],

[C6AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [CoAMAT], Keqmtp,

KicrotC4AcetoacylCoA, KmmtpAcetylCoAMAT, KmmtpC10AcylCoAMAT,

KmmtpC10EnoylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC12

KmmtpC14AcylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16AcylCoAMAT,

KmmtpC16EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT,

KmmtpC8EnoylCoAMAT, KmmtpCoAMAT, KmmtpNADHMAT,

KmmtpNADMAT, [NADHMAT], [NADtMAT], vol (VMAT), Vmtp, sfmtpC14)

MTP (sfmtpC14, Vmtp, KmmtpC14EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC1

Table 128: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfmtpC14	sfmtpC14	0.9	

8.32 Reaction vmtpC12

This is a reversible reaction of one reactant forming three products influenced by 28 modifiers.

Name vmtpC12

Reaction equation

C12EnoylCoAMAT, C14EnoylCoAMAT, C10EnoylCoAMAT, C8EnoylCoAMAT, NADtMAT

(168)

Reactant

Table 129: Properties of each reactant.

Id	Name	SBO
C12EnoylCoAMAT	C12EnoylCoAMAT	

Table 130: Properties of each modifier.

Table 130: Properties of each modifier.		
Id	Name	SBO
C16EnoylCoAMAT	C16EnoylCoAMAT	
C14EnoylCoAMAT	C14EnoylCoAMAT	
C10EnoylCoAMAT	C10EnoylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
NADtMAT	NADtMAT	
CoAMAT	CoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
${\tt C4AcetoacylCoAMAT}$	C4AcetoacylCoAMAT	
AcetylCoAMAT	AcetylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C10EnoylCoAMAT	C10EnoylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C14EnoylCoAMAT	C14EnoylCoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C16EnoylCoAMAT	C16EnoylCoAMAT	
C4AcetoacylCoAMAT	C4AcetoacylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
CoAMAT	CoAMAT	
NADHMAT	NADHMAT	
NADtMAT	NADtMAT	

Table 131: Properties of each product.

Id	Name	SBO
C10AcylCoAMAT AcetylCoAMAT NADHMAT	C10AcylCoAMAT AcetylCoAMAT NADHMAT	

Kinetic Law

```
function_4_vmtpC12_1 ([AcetylCoAMAT], [C10AcylCoAMAT], [C10EnoylCoAMAT], (170)
[C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT],
[C16AcylCoAMAT], [C16EnoylCoAMAT], [C4AcetoacylCoAMAT],
[C6AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [CoAMAT], Keqmtp,
KicrotC4AcetoacylCoA, KmmtpAcetylCoAMAT, KmmtpC10AcylCoAMAT,
KmmtpC10EnoylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC12EnoylCoAMAT,
KmmtpC14AcylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16AcylCoAMAT,
KmmtpC16EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT,
KmmtpC8EnoylCoAMAT, KmmtpCoAMAT, KmmtpNADHMAT,
KmmtpNADMAT, [NADHMAT], [NADtMAT], vol (VMAT), Vmtp, sfmtpC12

MTP(sfmtpC12, Vmtp, KmmtpC12EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC14EnoylCoAMAT, Km

MTP(sfmtpC12, Vmtp, KmmtpC12EnoylCoAMAT, KmmtpC16EnoylCoAMAT, Km

MTP(sfmtpC12, Vmtp, KmmtpC12EnoylCoAMAT, KmmtpC16EnoylCoAMAT, Km

MTP(sfmtpC12, Vmtp, KmmtpC12EnoylCoAMAT, Km

MTP(sfmtpC12, Vmtp, KmmtpC12EnoylCoAMAT, Km

MTP(sfmtpC12, Vmtp, Vmt
```

function_4_vmtpC12_1 ([AcetylCoAMAT], [C10AcylCoAMAT], [C10EnoylCoAMAT], (171)

[C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT],

[C16AcylCoAMAT], [C16EnoylCoAMAT], [C4AcetoacylCoAMAT],

[C6AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [CoAMAT], Keqmtp,

KicrotC4AcetoacylCoA, KmmtpAcetylCoAMAT, KmmtpC10AcylCoAMAT,

KmmtpC10EnoylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC12

KmmtpC14AcylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16AcylCoAMAT,

KmmtpC16EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT,

KmmtpC8EnoylCoAMAT, KmmtpCoAMAT, KmmtpNADHMAT,

KmmtpNADMAT, [NADHMAT], [NADtMAT], vol (VMAT), Vmtp, sfmtpC12)

MTP (sfmtpC12, Vmtp, KmmtpC12EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC1

Table 132: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfmtpC12	sfmtpC12	0.81	$ \overline{\checkmark} $

8.33 Reaction vmtpC10

This is a reversible reaction of one reactant forming three products influenced by 28 modifiers.

Name vmtpC10

Reaction equation

C10EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C8EnoylCoAMAT, NADtMAT

Reactant

Table 133: Properties of each reactant.

Id	Name	SBO
C10EnoylCoAMAT	C10EnoylCoAMAT	

Table 134: Properties of each modifier.

Id	Name	SBO
C16EnoylCoAMAT	C16EnoylCoAMAT	
C14EnoylCoAMAT	C14EnoylCoAMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
NADtMAT	NADtMAT	
CoAMAT	CoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C4AcetoacylCoAMAT	C4AcetoacylCoAMAT	
AcetylCoAMAT	AcetylCoAMAT	
C10AcylCoAMAT	C10AcylCoAMAT	
C10EnoylCoAMAT	C10EnoylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C14EnoylCoAMAT	C14EnoylCoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C16EnoylCoAMAT	C16EnoylCoAMAT	
C4AcetoacylCoAMAT	C4AcetoacylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
CoAMAT	CoAMAT	
NADHMAT	NADHMAT	
NADtMAT	NADtMAT	

Table 135: Properties of each product.

Id	Name	SBO
C8AcylCoAMAT AcetylCoAMAT NADHMAT	C8AcylCoAMAT AcetylCoAMAT NADHMAT	

Kinetic Law

Derived unit contains undeclared units

```
v_{33} = \text{vol}(VMAT)
          · function_4_vmtpC10_1 ([AcetylCoAMAT], [C10AcylCoAMAT], [C10EnoylCoAMAT],
            [C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT],
                                        [C16AcylCoAMAT], [C16EnoylCoAMAT], [C4AcetoacylCoAMAT],
                    [C6AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [CoAMAT], Keqmtp,
                           KicrotC4AcetoacylCoA, KmmtpAcetylCoAMAT, KmmtpC10AcylCoAMAT,
                KmmtpC10EnoylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC12
                  KmmtpC14AcylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16AcylCoAMAT,
                      KmmtpC16EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT,
              KmmtpC8EnoylCoAMAT, KmmtpCoAMAT, KmmtpNADHMAT, KmmtpNADMAT,
                                                       [NADHMAT], [NADtMAT], vol (VMAT), Vmtp, sfmtpC10)
                                                                                                                                           (173)
function_4_vmtpC10_1 ([AcetylCoAMAT], [C10AcylCoAMAT], [C10EnoylCoAMAT],
                                                                                                                                           (174)
[C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT],
[C16AcylCoAMAT], [C16EnoylCoAMAT], [C4AcetoacylCoAMAT],
[C6AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [CoAMAT], Keqmtp,
KicrotC4AcetoacylCoA, KmmtpAcetylCoAMAT, KmmtpC10AcylCoAMAT,
KmmtpC10EnoylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC12EnoylCoAMAT,
KmmtpC14AcylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16AcylCoAMAT,
KmmtpC16EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT,
KmmtpC8EnoylCoAMAT, KmmtpCoAMAT, KmmtpNADHMAT,
KmmtpNADMAT, [NADHMAT], [NADtMAT], vol (VMAT), Vmtp, sfmtpC10)
    MTP (sfmtpC10, Vmtp, KmmtpC10EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC14EnoylCoAMAT, Km
function_4_vmtpC10_1 ([AcetylCoAMAT], [C10AcylCoAMAT], [C10EnoylCoAMAT],
                                                                                                                                           (175)
[C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT],
[C16AcylCoAMAT], [C16EnoylCoAMAT], [C4AcetoacylCoAMAT],
[C6AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [CoAMAT], Keqmtp,
KicrotC4AcetoacylCoA, KmmtpAcetylCoAMAT, KmmtpC10AcylCoAMAT,
KmmtpC10EnoylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC12EnoylCoAMAT,
KmmtpC14AcylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16AcylCoAMAT,
KmmtpC16EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT,
KmmtpC8EnoylCoAMAT, KmmtpCoAMAT, KmmtpNADHMAT,
KmmtpNADMAT, [NADHMAT], [NADtMAT], vol (VMAT), Vmtp, sfmtpC10)
```

MTP (sfmtpC10, Vmtp, KmmtpC10EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC1

Table 136: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfmtpC10	sfmtpC10	0.73	

8.34 Reaction vmtpC8

This is a reversible reaction of one reactant forming three products influenced by 28 modifiers.

Name vmtpC8

Reaction equation

C8EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, NADtMAT (176)

Reactant

Table 137: Properties of each reactant.

Id	Name	SBO
C8EnoylCoAMAT	C8EnoylCoAMAT	

Table 138: Properties of each modifier.

<u> </u>	
Name	SBO
C16EnoylCoAMAT	
C14EnoylCoAMAT	
C12EnoylCoAMAT	
C10EnoylCoAMAT	
NADtMAT	
CoAMAT	
C16AcylCoAMAT	
C14AcylCoAMAT	
C12AcylCoAMAT	
C10AcylCoAMAT	
C8AcylCoAMAT	
C4AcetoacylCoAMAT	
AcetylCoAMAT	
C10AcylCoAMAT	
	C16EnoylCoAMAT C14EnoylCoAMAT C12EnoylCoAMAT C10EnoylCoAMAT NADtMAT CoAMAT C16AcylCoAMAT C14AcylCoAMAT C12AcylCoAMAT C10AcylCoAMAT C10AcylCoAMAT C4AcetoacylCoAMAT AcetylCoAMAT

Id	Name	SBO
C10EnoylCoAMAT	C10EnoylCoAMAT	
C12AcylCoAMAT	C12AcylCoAMAT	
C12EnoylCoAMAT	C12EnoylCoAMAT	
C14AcylCoAMAT	C14AcylCoAMAT	
C14EnoylCoAMAT	C14EnoylCoAMAT	
C16AcylCoAMAT	C16AcylCoAMAT	
C16EnoylCoAMAT	C16EnoylCoAMAT	
C4AcetoacylCoAMAT	C4AcetoacylCoAMAT	
C6AcylCoAMAT	C6AcylCoAMAT	
C8AcylCoAMAT	C8AcylCoAMAT	
C8EnoylCoAMAT	C8EnoylCoAMAT	
CoAMAT	CoAMAT	
NADHMAT	NADHMAT	
NADtMAT	NADtMAT	

Table 139: Properties of each product.

Id	Name	SBO
C6AcylCoAMAT	C6AcylCoAMAT	
AcetylCoAMAT	AcetylCoAMAT	
NADHMAT	NADHMAT	

Kinetic Law

```
v_{34} = vol\left(VMAT\right) \\ \cdot function\_4\_vmtpC8\_1\left([AcetylCoAMAT], [C10AcylCoAMAT], [C10EnoylCoAMAT], [C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT], [C16AcylCoAMAT], [C16EnoylCoAMAT], [C4AcetoacylCoAMAT], [C6AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [C0AMAT], Keqmtp, KicrotC4AcetoacylCoA, KmmtpAcetylCoAMAT, KmmtpC10AcylCoAMAT, KmmtpC10EnoylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC14AcylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16AcylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT, KmmtpC8EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT, KmmtpC8EnoylCoAMAT, KmmtpC0AMAT, KmmtpNADHMAT, KmmtpNADMAT, [NADHMAT], [NADHMAT], vol (VMAT), Vmtp, sfmtpC8) (177)
```

function_4_vmtpC8_1 ([AcetylCoAMAT], [C10AcylCoAMAT], [C10EnoylCoAMAT], (178)

[C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT],

[C16AcylCoAMAT], [C16EnoylCoAMAT], [C4AcetoacylCoAMAT],

[C6AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [CoAMAT], Keqmtp,

KicrotC4AcetoacylCoA, KmmtpAcetylCoAMAT, KmmtpC10AcylCoAMAT,

KmmtpC10EnoylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC12EnoylCoAMAT,

KmmtpC14AcylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16AcylCoAMAT,

KmmtpC16EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT,

KmmtpC8EnoylCoAMAT, KmmtpCoAMAT, KmmtpNADHMAT,

KmmtpNADMAT, [NADHMAT], [NADtMAT], vol (VMAT), Vmtp, sfmtpC8)

MTP (sfmtpC8, Vmtp, KmmtpC8EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC16E

function_4_vmtpC8_1 ([AcetylCoAMAT], [C10AcylCoAMAT], [C10EnoylCoAMAT], (179)

[C12AcylCoAMAT], [C12EnoylCoAMAT], [C14AcylCoAMAT], [C14EnoylCoAMAT],

[C16AcylCoAMAT], [C16EnoylCoAMAT], [C4AcetoacylCoAMAT],

[C6AcylCoAMAT], [C8AcylCoAMAT], [C8EnoylCoAMAT], [CoAMAT], Keqmtp,

KicrotC4AcetoacylCoA, KmmtpAcetylCoAMAT, KmmtpC10AcylCoAMAT,

KmmtpC10EnoylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC12

KmmtpC14AcylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16AcylCoAMAT,

KmmtpC16EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC8AcylCoAMAT,

KmmtpC8EnoylCoAMAT, KmmtpCoAMAT, KmmtpNADHMAT,

KmmtpNADMAT, [NADHMAT], [NADtMAT], vol (VMAT), Vmtp, sfmtpC8)

MTP (sfmtpC8, Vmtp, KmmtpC8EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC14E

Table 140: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
sfmtpC8	sfmtpC8	0.34	

8.35 Reaction vacesink

This is a reversible reaction of one reactant forming no product influenced by one modifier.

Name vacesink

Reaction equation

$$AcetylCoAMAT \xrightarrow{AcetylCoAMAT} \emptyset$$
 (180)

Reactant

Table 141: Properties of each reactant.

Id	Name	SBO
	AcetylCoAMAT	

Modifier

Table 142: Properties of each modifier.

Id	Name	SBO
AcetylCoAMAT	AcetylCoAMAT	

Kinetic Law

Derived unit contains undeclared units

 $v_{35} = \text{vol}(VMAT) \cdot \text{function_4_vacesink_1}([AcetylCoAMAT], K1acesink, Ksacesink, vol(VMAT))$

$$\begin{aligned} & \text{function_4_vacesink_1} \left([\text{AcetylCoAMAT}], \text{K1acesink}, \text{Ksacesink}, \text{vol} \left(\text{VMAT} \right) \right) \\ &= \frac{\text{RES} \left(\text{Ksacesink}, [\text{AcetylCoAMAT}], \text{K1acesink} \right)}{\text{vol} \left(\text{VMAT} \right)} \end{aligned} \tag{182}$$

$$\begin{aligned} & \text{function_4_vacesink_1} \left([\text{AcetylCoAMAT}], \text{K1acesink}, \text{Ksacesink}, \text{vol}\left(\text{VMAT} \right) \right) \\ &= \frac{\text{RES}\left(\text{Ksacesink}, [\text{AcetylCoAMAT}], \text{K1acesink} \right)}{\text{vol}\left(\text{VMAT} \right)} \end{aligned} \tag{183}$$

Table 143: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K1acesink Ksacesink	K1acesink Ksacesink		30.0 6000000.0		Z

8.36 Reaction reaction_1

This is a reversible reaction of two reactants forming two products influenced by eight modifiers.

Name vcrmsC6

Reaction equation

C6EnoylCoAMAT + species_1 C4AcetoacylCoAMAT, C4EnoylCoAMAT, C6EnoylCoAMAT, species_1, C6Ketoa

(184)

Reactants

Table 144: Properties of each reactant.

Id	Name	SBO
C6EnoylCoAMAT species_1	C6EnoylCoAMAT NAD	

Modifiers

Table 145: Properties of each modifier.

rusic 115.11 operates of each mounter.		
Id	Name	SBO
C4AcetoacylCoAMAT	C4AcetoacylCoAMAT	
C4EnoylCoAMAT	C4EnoylCoAMAT	
C6EnoylCoAMAT	C6EnoylCoAMAT	
${ t species}_{ extsf{-}}1$	NAD	
C6KetoacylCoAMAT	C6KetoacylCoAMAT	
NADHMAT	NADHMAT	
${\tt C4AcetoacylCoAMAT}$	C4AcetoacylCoAMAT	
C4EnoylCoAMAT	C4EnoylCoAMAT	

Products

Table 146: Properties of each product.

Id	Name	SBO
C6KetoacylCoAMAT NADHMAT	C6KetoacylCoAMAT NADHMAT	

Kinetic Law

Derived unit contains undeclared units

```
\begin{aligned} v_{36} &= \text{vol}\left(\text{VMAT}\right) \cdot \text{CRMS\_C6}\left(\text{sfcrotC6}, \text{Vcrot}, \text{sfmschadC6}, \text{Vmschad}, [\text{C6EnoylCoAMAT}], \\ & [\text{species\_1}], \text{KmcrotC6EnoylCoAMAT}, \text{KmmschadC6HydroxyacylCoAMAT}, \\ & \text{KmmschadNADMAT}, [\text{C6KetoacylCoAMAT}], [\text{NADHMAT}], \text{Keqcrot}, \text{Keqmschad}, \\ & \text{KmmschadC6KetoacylCoAMAT}, [\text{C4AcetoacylCoAMAT}], \\ & \text{KmmschadC4AcetoacylCoAMAT}, \text{KmmschadNADHMAT}, [\text{C4EnoylCoAMAT}], \\ & \text{KmcrotC4EnoylCoAMAT}, \text{KicrotC4AcetoacylCoA}, \text{vol}\left(\text{VMAT}\right)\right) \end{aligned} \tag{185}
```

CRMS_C6 (sfcrotC6, Vcrot, sfmschadC6, Vmschad, [C6EnoylCoAMAT], (186)
NAD, KmcrotC6EnoylCoAMAT, KmmschadC6HydroxyacylCoAMAT,
KmmschadNADMAT, [C6KetoacylCoAMAT], [NADHMAT], Keqcrot,
Keqmschad, KmmschadC6KetoacylCoAMAT, [C4AcetoacylCoAMAT],
KmmschadC4AcetoacylCoAMAT, KmmschadNADHMAT, [C4EnoylCoAMAT],
KmmschadC4FnoylCoAMAT, KinrotC4AcetoacylCoA, ycl (YMAT))

KmcrotC4EnoylCoAMAT, KicrotC4AcetoacylCoA, vol (VMAT))

 $\underline{CRMS} (sfcrotC6, Vcrot, sfmschadC6, Vmschad, [C6EnoylCoAMAT], NAD, KmcrotC6EnoylCoAMAT, KmmschadC6, Vmschad, [C6EnoylCoAMAT], NAD, Vmschad, [C6En$

CRMS_C6 (sfcrotC6, Vcrot, sfmschadC6, Vmschad, [C6EnoylCoAMAT],
NAD, KmcrotC6EnoylCoAMAT, KmmschadC6HydroxyacylCoAMAT,
KmmschadNADMAT, [C6KetoacylCoAMAT], [NADHMAT], Keqcrot,
Keqmschad, KmmschadC6KetoacylCoAMAT, [C4AcetoacylCoAMAT],
KmmschadC4AcetoacylCoAMAT, KmmschadNADHMAT, [C4EnoylCoAMAT],
KmcrotC4EnoylCoAMAT, KicrotC4AcetoacylCoA, vol (VMAT))

CRMS (sfcrotC6, Vcrot, sfmschadC6, Vmschad, [C6EnoylCoAMAT], NAD, KmcrotC6EnoylCoAMAT, KmmschadC6, Vmschad, [C6EnoylCoAMAT], NAD, KmcrotC6EnoylCoAMAT, KmmschadC6, Vmschad, [C6EnoylCoAMAT], NAD, Vmschad, [C6EnoylCoAM

Table 147: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
	Tunic	SBO varac Cint	Constant
sfcrotC6	sfcrotC6	0.83	\square
${\tt sfmschadC6}$	sfmschadC6	1.00	

8.37 Reaction reaction_2

This is a reversible reaction of two reactants forming two products influenced by eight modifiers.

Name vcrmsC4

Reaction equation

(188)

Reactants

Table 148: Properties of each reactant.

Id	Name	SBO
C4EnoylCoAMAT species_1	C4EnoylCoAMAT NAD	

Modifiers

Table 149: Properties of each modifier.

rable 119. 11operates of each mounter.		
Id	Name	SBO
C6KetoacylCoAMAT	C6KetoacylCoAMAT	
C6EnoylCoAMAT	C6EnoylCoAMAT	
C4EnoylCoAMAT	C4EnoylCoAMAT	
${ t species}_{ extsf{-}}1$	NAD	
C4AcetoacylCoAMAT	C4AcetoacylCoAMAT	
NADHMAT	NADHMAT	
C6KetoacylCoAMAT	C6KetoacylCoAMAT	
C6EnoylCoAMAT	C6EnoylCoAMAT	

Products

Table 150: Properties of each product.

	F F	
Id	Name	SBO
C4AcetoacylCoAMAT NADHMAT	C4AcetoacylCoAMAT NADHMAT	

Kinetic Law

Derived unit contains undeclared units

```
v_{37} = \text{vol}(\text{VMAT}) \cdot \text{CRMS\_C4}(\text{sfcrotC4}, \text{Vcrot}, \text{sfmschadC4}, \text{Vmschad}, [\text{C4EnoylCoAMAT}],
                                                                                         [species_1], KmcrotC4EnoylCoAMAT, KmmschadC4HydroxyacylCoAMAT,
                                                   KmmschadNADMAT, [C4AcetoacylCoAMAT], [NADHMAT], Keqcrot, Keqmschad, Albert Cambridge (Management of the Cambridge (Management of t
                                                                                                                                                                                     KmmschadC4AcetoacylCoAMAT, [C6KetoacylCoAMAT],
                                                                           KmmschadC6KetoacylCoAMAT, KmmschadNADHMAT, [C6EnoylCoAMAT],
                                                                                                                                                  KmcrotC6EnoylCoAMAT, KicrotC4AcetoacylCoA, vol (VMAT))
                                                                                                                                                                                                                                                                                                                                                                                                                                                                           (189)
```

```
(190)
CRMS_C4 (sfcrotC4, Vcrot, sfmschadC4, Vmschad, [C4EnoylCoAMAT],
NAD, KmcrotC4EnoylCoAMAT, KmmschadC4HydroxyacylCoAMAT,
KmmschadNADMAT, [C4AcetoacylCoAMAT], [NADHMAT], Keqcrot,
Keqmschad, KmmschadC4AcetoacylCoAMAT, [C6KetoacylCoAMAT],
KmmschadC6KetoacylCoAMAT, KmmschadNADHMAT, [C6EnoylCoAMAT],
```

KmcrotC6EnoylCoAMAT, KicrotC4AcetoacylCoA, vol (VMAT))

 $CRMS \ (sfcrotC4, Vcrot, sfmschadC4, Vmschad, [C4EnoylCoAMAT], NAD, KmcrotC4EnoylCoAMAT, KmmschadC4, Vmschad, [C4EnoylCoAMAT], NAD, KmcrotC4EnoylCoAMAT, KmmschadC4, Vmschad, [C4EnoylCoAMAT], NAD, Vmschad, [C4EnoylCo$

```
(191)
CRMS_C4 (sfcrotC4, Vcrot, sfmschadC4, Vmschad, [C4EnoylCoAMAT],
NAD, KmcrotC4EnoylCoAMAT, KmmschadC4HydroxyacylCoAMAT,
KmmschadNADMAT, [C4AcetoacylCoAMAT], [NADHMAT], Keqcrot,\\
Keqmschad, KmmschadC4AcetoacylCoAMAT, [C6KetoacylCoAMAT],
KmmschadC6KetoacylCoAMAT, KmmschadNADHMAT, [C6EnoylCoAMAT],
KmcrotC6EnoylCoAMAT, KicrotC4AcetoacylCoA, vol (VMAT))
```

CRMS (sfcrotC4, Vcrot, sfmschadC4, Vmschad, [C4EnoylCoAMAT], NAD, KmcrotC4EnoylCoAMAT, Kmmscha

	14010 131.1	roperties of each parameter.	
Id	Name	SBO Value Unit	Constant
sfcrotC4	sfcrotC4	1.00	\overline{Z}
sfmschadC4	sfmschadC4	0.67	

Table 151: Properties of each parameter

9 Derived Rate Equations

When interpreted as an ordinary differential equation framework, this model implies the following set of equations for the rates of change of each species.

Identifiers for kinetic laws highlighted in gray cannot be verified to evaluate to units of SBML substance per time. As a result, some SBML interpreters may not be able to verify the consistency of the units on quantities in the model. Please check if

• parameters without an unit definition are involved or

• volume correction is necessary because the hasOnlySubstanceUnits flag may be set to false and spacialDimensions> 0 for certain species.

9.1 Species C16AcylCarCYT

Name C16AcylCarCYT

Initial concentration $0.171 \, \mu mol \cdot l^{-1}$

This species takes part in four reactions (as a reactant in vcactC16 and as a product in vcpt1C16 and as a modifier in vcpt1C16, vcactC16).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}16\mathrm{AcylCarCYT} = |v_1| - |v_2| \tag{192}$$

9.2 Species C14AcylCarCYT

Name C14AcylCarCYT

Initial concentration $0.023~\mu mol \cdot l^{-1}$

This species takes part in two reactions (as a reactant in vcactC14 and as a modifier in vcactC14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}14\mathrm{AcylCarCYT} = -v_3 \tag{193}$$

9.3 Species C12AcylCarCYT

Name C12AcylCarCYT

Initial concentration $0.11 \ \mu mol \cdot l^{-1}$

This species takes part in two reactions (as a reactant in vcactC12 and as a modifier in vcactC12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}12\mathrm{A}\mathrm{c}\mathrm{y}\mathrm{l}\mathrm{C}\mathrm{a}\mathrm{r}\mathrm{C}\mathrm{Y}\mathrm{T} = -\nu_4 \tag{194}$$

9.4 Species C10AcylCarCYT

Name C10AcylCarCYT

Initial concentration $0.019 \, \mu \text{mol} \cdot l^{-1}$

This species takes part in two reactions (as a reactant in vcactC10 and as a modifier in vcactC10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}10\mathrm{AcylCarCYT} = -\nu_5 \tag{195}$$

9.5 Species C8AcylCarCYT

Name C8AcylCarCYT

Initial concentration $0.052 \, \mu \text{mol} \cdot l^{-1}$

This species takes part in two reactions (as a reactant in vcactC8 and as a modifier in vcactC8).

$$\frac{\mathrm{d}}{\mathrm{d}t} C8 A \mathrm{cylCarCYT} = -v_6 \tag{196}$$

9.6 Species C6AcylCarCYT

Name C6AcylCarCYT

Initial concentration $0.017 \ \mu mol \cdot l^{-1}$

This species takes part in two reactions (as a reactant in vcactC6 and as a modifier in vcactC6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C6AcylCarCYT} = -\nu_7 \tag{197}$$

9.7 Species C4AcylCarCYT

Name C4AcylCarCYT

Initial concentration $0.0080 \ \mu mol \cdot l^{-1}$

This species takes part in two reactions (as a reactant in vcactC4 and as a modifier in vcactC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C4AcylCarCYT} = -\nu_8 \tag{198}$$

9.8 Species C16AcylCoACYT

Name C16AcylCoACYT

Initial concentration 26.8 µmol·1⁻¹

Involved in rule C16AcylCoACYT

This species takes part in two reactions (as a modifier in vcpt1C16, vcpt1C16). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

9.9 Species CarCYT

Name CarCYT

Initial concentration $400 \mu mol \cdot l^{-1}$

This species takes part in 16 reactions (as a modifier in vcpt1C16, vcactC16, vcactC16, vcactC14, vcactC14, vcactC12, vcactC12, vcactC10, vcactC10, vcactC10, vcactC8, vcactC8, vcactC6, vcactC6, vcactC4, vcactC4), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CarCYT} = 0\tag{199}$$

9.10 Species CoACYT

Name CoACYT

Initial concentration $140 \ \mu mol \cdot l^{-1}$

This species takes part in two reactions (as a modifier in vcpt1C16, vcpt1C16), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CoACYT} = 0\tag{200}$$

9.11 Species MalCoACYT

Name MalCoACYT

Initial concentration $0 \, \mu \text{mol} \cdot l^{-1}$

This species takes part in two reactions (as a modifier in vcpt1C16, vcpt1C16), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{MalCoACYT} = 0 \tag{201}$$

9.12 Species C16AcylCarMAT

Name C16AcylCarMAT

Initial concentration $0 \, \mu \text{mol} \cdot l^{-1}$

This species takes part in 16 reactions (as a reactant in vcpt2C16 and as a product in vcactC16 and as a modifier in vcactC16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}16\mathrm{AcylCarMAT} = |v_2| - |v_9| \tag{202}$$

9.13 Species C16AcylCoAMAT

Name C16AcylCoAMAT

Initial concentration $0 \ \mu mol \cdot l^{-1}$

This species takes part in 42 reactions (as a reactant in vvlcadC16, vlcadC16 and as a product in vcpt2C16 and as a modifier in vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vvlcadC16, vvlcadC14, vvlcadC14, vvlcadC12, vvlcadC12, vlcadC16, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC12, vlcadC10, vlcadC10, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC10, vmtpC10, vmtpC10, vmtpC8, vmtpC8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}16\mathrm{AcylCoAMAT} = v_9 - v_{16} - v_{19} \tag{203}$$

9.14 Species C16EnoylCoAMAT

Name C16EnoylCoAMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

This species takes part in 24 reactions (as a reactant in vmtpC16 and as a product in vvlcadC16, vlcadC16 and as a modifier in vvlcadC16, vvlcadC14, vvlcadC14, vvlcadC12, vvlcadC12, vlcadC16, vlcadC14, vlcadC14, vlcadC12, vlcadC10, vlcadC10, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC8, vmtpC8).

$$\frac{d}{dt}C16EnoylCoAMAT = |v_{16}| + |v_{19}| - |v_{30}|$$
 (204)

9.15 Species C16HydroxyacylCoAMAT

Name C16HydroxyacylCoAMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}16\mathrm{HydroxyacylCoAMAT} = 0 \tag{205}$$

9.16 Species C16KetoacylCoAMAT

Name C16KetoacylCoAMAT

Initial concentration $0 \, \mu mol \cdot l^{-1}$

This species takes part in four reactions (as a modifier in vmckatC6, vmckatC6, vmckatC4, vmckatC4), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}16\mathrm{KetoacylCoAMAT} = 0 \tag{206}$$

9.17 Species C14AcylCarMAT

Name C14AcylCarMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

This species takes part in 16 reactions (as a reactant in vcpt2C14 and as a product in vcactC14 and as a modifier in vcactC14, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}14\mathrm{AcylCarMAT} = |v_3| - |v_{10}| \tag{207}$$

9.18 Species C14AcylCoAMAT

Name C14AcylCoAMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

This species takes part in 42 reactions (as a reactant in vvlcadC14, vlcadC14 and as a product in vcpt2C14, vmtpC16 and as a modifier in vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vvlcadC16, vvlcadC16, vvlcadC14, vvlcadC12, vvlcadC12, vlcadC16, vlcadC16, vlcadC14, vlcadC12, vlcadC12, vlcadC12, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC10, vmtpC10, vmtpC10, vmtpC8, vmtpC8).

$$\frac{d}{dt}C14AcylCoAMAT = |v_{10}| + |v_{30}| - |v_{17}| - |v_{20}|$$
(208)

9.19 Species C14EnoylCoAMAT

Name C14EnoylCoAMAT

Initial concentration $0 \, \mu \text{mol} \cdot l^{-1}$

This species takes part in 24 reactions (as a reactant in vmtpC14 and as a product in vvlcadC14, vlcadC14 and as a modifier in vvlcadC16, vvlcadC16, vvlcadC14, vvlcadC12, vvlcadC12, vlcadC16, vlcadC16, vlcadC16, vlcadC16, vlcadC10, vlcadC10, vmtpC16, vmtpC16, vmtpC14, vmtpC12, vmtpC10, vmtpC10, vmtpC3, vmtpC3).

$$\frac{d}{dt}C14EnoylCoAMAT = |v_{17}| + |v_{20}| - |v_{31}|$$
 (209)

9.20 Species C14HydroxyacylCoAMAT

Name C14HydroxyacylCoAMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}14\mathrm{HydroxyacylCoAMAT} = 0 \tag{210}$$

9.21 Species C14KetoacylCoAMAT

Name C14KetoacylCoAMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

This species takes part in four reactions (as a modifier in vmckatC6, vmckatC6, vmckatC4, vmckatC4), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}14\mathrm{KetoacylCoAMAT} = 0 \tag{211}$$

9.22 Species C12AcylCarMAT

Name C12AcylCarMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

This species takes part in 16 reactions (as a reactant in vcpt2C12 and as a product in vcactC12 and as a modifier in vcactC12, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}12\mathrm{AcylCarMAT} = |v_4| - |v_{11}| \tag{212}$$

9.23 Species C12AcylCoAMAT

Name C12AcylCoAMAT

Initial concentration $0 \, \mu mol \cdot l^{-1}$

This species takes part in 50 reactions (as a reactant in vvlcadC12, vlcadC12, vmcadC12 and as a product in vcpt2C12, vmtpC14 and as a modifier in vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vvlcadC16, vvlcadC16, vvlcadC14, vvlcadC14, vvlcadC12, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC14, vlcadC12, vlcadC10, vmcadC10, vmcadC12, vmcadC10, vmcadC10, vmcadC8, vmcadC8, vmcadC6, vmcadC6, vmckatC6, vmckatC6, vmckatC4, vmtpC16, vmtpC16, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC8, vmtpC8).

$$\frac{d}{dt}C12AcylCoAMAT = |v_{11}| + |v_{31}| - |v_{18}| - |v_{21}| - |v_{23}|$$
(213)

9.24 Species C12EnoylCoAMAT

Name C12EnoylCoAMAT

Initial concentration $0 \ \mu mol \cdot l^{-1}$

This species takes part in 31 reactions (as a reactant in vmtpC12 and as a product in vvlcadC12, vlcadC12, vmcadC12 and as a modifier in vvlcadC16, vvlcadC16, vvlcadC14, vvlcadC14, vvlcadC14, vvlcadC12, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC10, vmcadC10, vmcadC10, vmcadC10, vmcadC10, vmcadC8, vmcadC6, vmcadC6, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC10, vmtpC10, vmtpC8, vmtpC8).

$$\frac{d}{dt}C12EnoylCoAMAT = |v_{18}| + |v_{21}| + |v_{23}| - |v_{32}|$$
(214)

9.25 Species C12HydroxyacylCoAMAT

Name C12HydroxyacylCoAMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

$$\frac{d}{dt}C12HydroxyacylCoAMAT = 0 (215)$$

9.26 Species C12KetoacylCoAMAT

Name C12KetoacylCoAMAT

Initial concentration $0 \, \mu \text{mol} \cdot l^{-1}$

This species takes part in four reactions (as a modifier in vmckatC6, vmckatC6, vmckatC4, vmckatC4), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}12\mathrm{KetoacylCoAMAT} = 0 \tag{216}$$

9.27 Species C10AcylCarMAT

Name C10AcylCarMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

This species takes part in 16 reactions (as a reactant in vcpt2C10 and as a product in vcactC10 and as a modifier in vcactC10, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}10\mathrm{AcylCarMAT} = |v_5| - |v_{12}| \tag{217}$$

9.28 Species C10AcylCoAMAT

Name C10AcylCoAMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

This species takes part in 44 reactions (as a reactant in vlcadC10, vmcadC10 and as a product in vcpt2C10, vmtpC12 and as a modifier in vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC10, vmcadC12, vmcadC12, vmcadC10, vmcadC8, vmcadC6, vmcadC6, vmckatC6, vmckatC6, vmckatC4, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC10, vmtpC10, vmtpC8, vmtpC8).

$$\frac{d}{dt}C10AcylCoAMAT = |v_{12}| + |v_{32}| - |v_{22}| - |v_{24}|$$
 (218)

9.29 Species C10EnoylCoAMAT

Name C10EnoylCoAMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

This species takes part in 26 reactions (as a reactant in vmtpC10 and as a product in vlcadC10, vmcadC10 and as a modifier in vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC10, vmcadC10, vmcadC12, vmcadC10, vmcadC8, vmcadC6, vmcadC6, vmtpC16, vmtpC16, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC8, vmtpC8).

$$\frac{d}{dt}C10EnoylCoAMAT = |v_{22}| + |v_{24}| - |v_{33}|$$
 (219)

9.30 Species C10HydroxyacylCoAMAT

Name C10HydroxyacylCoAMAT

Initial concentration $0 \, \mu \text{mol} \cdot l^{-1}$

$$\frac{d}{dt}C10HydroxyacylCoAMAT = 0 (220)$$

9.31 Species C10KetoacylCoAMAT

Name C10KetoacylCoAMAT

Initial concentration $0 \, \mu mol \cdot l^{-1}$

This species takes part in four reactions (as a modifier in vmckatC6, vmckatC6, vmckatC4, vmckatC4), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}10\mathrm{KetoacylCoAMAT} = 0 \tag{221}$$

9.32 Species C8AcylCarMAT

Name C8AcylCarMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

This species takes part in 16 reactions (as a reactant in vcpt2C8 and as a product in vcactC8 and as a modifier in vcactC8, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{C8AcylCarMAT} = v_6 - v_{13} \tag{222}$$

9.33 Species C8AcylCoAMAT

Name C8AcylCoAMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

This species takes part in 44 reactions (as a reactant in vmcadC8 and as a product in vcpt2C8, vmtpC10 and as a modifier in vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC10, vlcadC10, vmcadC12, vmcadC10, vmcadC10, vmcadC10, vmcadC6, vmcadC6, vmckatC6, vmckatC6, vmckatC4, vmtpC16, vmtpC16, vmtpC16, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC8, vmtpC8).

$$\frac{d}{dt}C8AcylCoAMAT = v_{13} + v_{33} - v_{25}$$
 (223)

9.34 Species C8EnoylCoAMAT

Name C8EnoylCoAMAT

Initial concentration $0 \, \mu \text{mol} \cdot l^{-1}$

This species takes part in 26 reactions (as a reactant in vmtpC8 and as a product in vmcadC8 and as a modifier in vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC10, vmcadC10, vmcadC10, vmcadC10, vmcadC10, vmcadC6, vmcadC6, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC3).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{C8EnoylCoAMAT} = v_{25} - v_{34} \tag{224}$$

9.35 Species C8HydroxyacylCoAMAT

Name C8HydroxyacylCoAMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C8HydroxyacylCoAMAT} = 0 \tag{225}$$

9.36 Species C8KetoacylCoAMAT

Name C8KetoacylCoAMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

This species takes part in four reactions (as a modifier in vmckatC6, vmckatC6, vmckatC4, vmckatC4), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t} C8 \text{KetoacylCoAMAT} = 0 \tag{226}$$

9.37 Species C6AcylCarMAT

Name C6AcylCarMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

This species takes part in 16 reactions (as a reactant in vcpt2C6 and as a product in vcactC6 and as a modifier in vcactC6, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C6AcylCarMAT} = v_7 - v_{14} \tag{227}$$

9.38 Species C6AcylCoAMAT

Name C6AcylCoAMAT

Initial concentration $0 \ \mu mol \cdot l^{-1}$

This species takes part in 38 reactions (as a reactant in vmcadC6 and as a product in vcpt2C6, vmtpC8 and as a modifier in vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC8, vmcadC8, vmcadC6, vscadC4, vscadC4, vmckatC6, vmckatC6, vmckatC4, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC10, vmtpC10, vmtpC10, vmtpC10, vmtpC3).

$$\frac{d}{dt}C6AcylCoAMAT = |v_{14}| + |v_{34}| - |v_{26}|$$
 (228)

9.39 Species C6EnoylCoAMAT

Name C6EnoylCoAMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

This species takes part in 14 reactions (as a reactant in reaction_1 and as a product in vmcadC6 and as a modifier in vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC8, vmcadC8, vmcadC6, vscadC4, vscadC4, reaction_1, reaction_2, reaction_2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C6EnoylCoAMAT} = |v_{26}| - |v_{36}| \tag{229}$$

9.40 Species C6HydroxyacylCoAMAT

Name C6HydroxyacylCoAMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C6HydroxyacylCoAMAT} = 0 \tag{230}$$

9.41 Species C6KetoacylCoAMAT

Name C6KetoacylCoAMAT

Initial concentration $0 \, \mu mol \cdot l^{-1}$

This species takes part in eight reactions (as a reactant in vmckatC6 and as a product in reaction—1 and as a modifier in vmckatC6, vmckatC4, vmckatC4, reaction—1, reaction—2, reaction—2).

$$\frac{d}{dt}C6KetoacylCoAMAT = v_{36} - v_{28}$$
 (231)

9.42 Species C4AcylCarMAT

Name C4AcylCarMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

This species takes part in 16 reactions (as a reactant in vcpt2C4 and as a product in vcactC4 and as a modifier in vcactC4, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C4AcylCarMAT} = |v_8| - |v_{15}| \tag{232}$$

9.43 Species C4AcylCoAMAT

Name C4AcylCoAMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

This species takes part in 28 reactions (as a reactant in vscadC4 and as a product in vcpt2C4, vmckatC6 and as a modifier in vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C4, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC3, vmcadC6, vmcadC6, vmcadC6, vmcadC4, vmckatC4, vmckatC4).

$$\frac{d}{dt}C4AcylCoAMAT = v_{15} + v_{28} - v_{27}$$
 (233)

9.44 Species C4EnoylCoAMAT

Name C4EnoylCoAMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

This species takes part in 14 reactions (as a reactant in reaction_2 and as a product in vscadC4 and as a modifier in vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC8, vmcadC8, vmcadC6, vmcadC4, reaction_1, reaction_1, reaction_2).

$$\frac{d}{dt}C4EnoylCoAMAT = v_{27} - v_{37}$$
 (234)

9.45 Species C4HydroxyacylCoAMAT

Name C4HydroxyacylCoAMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C4HydroxyacylCoAMAT} = 0 \tag{235}$$

9.46 Species C4AcetoacylCoAMAT

Name C4AcetoacylCoAMAT

Initial concentration $0 \mu mol \cdot l^{-1}$

This species takes part in 18 reactions (as a reactant in vmckatC4 and as a product in reaction—2 and as a modifier in vmckatC6, vmckatC6, vmckatC4, vmtpC16, vmtpC16, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC8, vmtpC8, reaction_1, reaction—2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C4AcetoacylCoAMAT} = v_{37} - v_{29} \tag{236}$$

9.47 Species AcetylCoAMAT

Name AcetylCoAMAT

Initial concentration 30 µmol·l⁻¹

This species takes part in 16 reactions (as a reactant in vacesink and as a product in vmckatC6, vmckatC4, vmtpC16, vmtpC14, vmtpC12, vmtpC10, vmtpC8 and as a modifier in vmckatC6, vmckatC4, vmtpC16, vmtpC14, vmtpC12, vmtpC10, vmtpC8, vacesink).

$$\frac{d}{dt}AcetylCoAMAT = v_{28} + 2 v_{29} + v_{30} + v_{31} + v_{32} + v_{33} + v_{34} - v_{35}$$
 (237)

9.48 Species FADHMAT

Name FADHMAT

Initial concentration $0.46 \ \mu mol \cdot l^{-1}$

This species takes part in 24 reactions (as a product in vvlcadC16, vvlcadC14, vvlcadC12, vlcadC16, vlcadC14, vlcadC12, vlcadC10, vmcadC12, vmcadC10, vmcadC10, vmcadC6, vscadC4 and as a modifier in vvlcadC16, vvlcadC14, vvlcadC12, vlcadC16, vlcadC14, vlcadC12, vlcadC10, vmcadC12, vmcadC10, vmcad

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{FADHMAT} = 0\tag{238}$$

9.49 Species NADHMAT

Name NADHMAT

Initial concentration $16 \mu mol \cdot l^{-1}$

This species takes part in 14 reactions (as a product in vmtpC16, vmtpC14, vmtpC12, vmtpC10, vmtpC8, reaction_1, reaction_2 and as a modifier in vmtpC16, vmtpC14, vmtpC12, vmtpC10, vmtpC8, reaction_1, reaction_2), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADHMAT} = 0 \tag{239}$$

9.50 Species Coamat

Name CoAMAT

Initial concentration $4970 \, \mu \text{mol} \cdot l^{-1}$

Involved in rule COAMAT

This species takes part in 28 reactions (as a modifier in vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vcpt2C4, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC8, vmtpC8). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

9.51 Species CarMAT

Name CarMAT

Initial concentration 950 µmol·1⁻¹

This species takes part in 28 reactions (as a modifier in vcactC16, vcactC16, vcactC14, vcactC14, vcactC12, vcactC12, vcactC10, vcactC10, vcactC8, vcactC8, vcactC6, vcactC6, vcactC4, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C3, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CarMAT} = 0\tag{240}$$

9.52 Species FADtMAT

Name FADtMAT

Initial concentration $0.77 \ \mu mol \cdot l^{-1}$

This species takes part in 24 reactions (as a modifier in vvlcadC16, vvlcadC16, vvlcadC14, vvlcadC14, vvlcadC12, vvlcadC12, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC12, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC10, vmcadC10, vmcadC10, vmcadC10, vmcadC3, vmcadC6, vmcadC6, vmcadC6, vmcadC4, vscadC4), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{FADtMAT} = 0\tag{241}$$

9.53 Species NADtMAT

Name NADtMAT

Initial concentration 250 µmol·l⁻¹

This species takes part in ten reactions (as a modifier in vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC8, vmtpC8), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADtMAT} = 0 \tag{242}$$

9.54 Species CoAMATt

Name CoAMATt

Initial concentration $5000 \ \mu mol \cdot l^{-1}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CoAMATt} = 0 \tag{243}$$

9.55 Species species_1

Name NAD

Initial concentration 234 μ mol·l⁻¹

This species takes part in four reactions (as a reactant in reaction_1, reaction_2 and as a modifier in reaction_1, reaction_2), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species}_{-1} = 0 \tag{244}$$

 $\mathfrak{BML2}^{d}$ was developed by Andreas Dräger^a, Hannes Planatscher^a, Dieudonné M Wouamba^a, Adrian Schröder^a, Michael Hucka^b, Lukas Endler^c, Martin Golebiewski^d and Andreas Zell^a. Please see http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX for more information.

^aCenter for Bioinformatics Tübingen (ZBIT), Germany

^bCalifornia Institute of Technology, Beckman Institute BNMC, Pasadena, United States

^cEuropean Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom

 $[^]d$ EML Research gGmbH, Heidelberg, Germany