SBML Model Report

Model name: "vanEunen2013 - Network dynamics of fatty acid -oxidation (time-course model)"



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1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah¹ and Kieran Smallbone² at January 15th 2014 at 10:56 a.m. and last time modified at March fourth 2014 at 11:24 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	54
events	0	constraints	0
reactions	59	function definitions	13
global parameters	140	unit definitions	6
rules	2	initial assignments	0

Model Notes

vanEunen2013 - Network dynamics of fatty acid -oxidation (time-course model)

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Lipid metabolism plays an important role in the development of metabolic syndrome, a major risk factor for cardiovascular disease and diabetes. This model gives insights into the response of lipid oxidation to dietart and medical interventions. The model predicts the rate of lipid oxidation and the time course of most acyl carnitines. There are two models described in the paper, (i) steady-state model [BIOMD0000000505], (ii) time-course model [BIOMD0000000506]. This model corresponds to the time-course model.

This model is described in the article:Biochemical competition makes fatty-acid -oxidation vulnerable to substrate overload.van Eunen K, Simons SM, Gerding A, Bleeker A, den Besten G, Touw CM, Houten SM, Groen BK, Krab K, Reijngoud DJ, Bakker BM.PLoS Comput Biol. 2013;9(8):e1003186.

Abstract:

Fatty-acid metabolism plays a key role in acquired and inborn metabolic diseases. To obtain insight into the network dynamics of fatty-acid -oxidation, we constructed a detailed computational model of the pathway and subjected it to a fat overload condition. The model contains reversible and saturable enzyme-kinetic equations and experimentally determined parameters for rat-liver enzymes. It was validated by adding palmitoyl CoA or palmitoyl carnitine to isolated rat-liver mitochondria: without refitting of measured parameters, the model correctly predicted the -oxidation flux as well as the time profiles of most acyl-carnitine concentrations. Subsequently, we simulated the condition of obesity by increasing the palmitoyl-CoA concentration. At a high concentration of palmitoyl CoA the -oxidation became overloaded: the flux dropped and metabolites accumulated. This behavior originated from the competition between acyl CoAs of different chain lengths for a set of acyl-CoA dehydrogenases with overlapping substrate specificity. This effectively induced competitive feedforward inhibition and thereby led to accumulation of CoA-ester intermediates and depletion of free CoA (CoASH). The mitochondrial [NAD]/[NADH] ratio modulated the sensitivity to substrate overload, revealing a tight interplay between regulation of -oxidation and mitochondrial respiration.

This model is hosted on BioModels Database and identifiedby: BIOMD000000506.

To cite BioModels Database, please use: BioModels Database: An enhanced, curated and annotated resourcefor published quantitative kinetic models .

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2 Unit Definitions

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

2.1 Unit substance

Name umol

Definition µmol

2.2 Unit time

Name min

Definition 60 s

2.3 Unit volume

Name litre per mgProtein

Definition 1

2.4 Unit uM

Name uM

Definition $\mu mol \cdot l^{-1}$

2.5 Unit uM_per_min_per_mgProtein

Name uM per min per mgProtein

Definition $\mu mol \cdot l^{-1} \cdot (60 \text{ s})^{-1}$

2.6 Unit l_per_min_per_mgProtein

Name 1 per min per mgProtein

Definition $1 \cdot (60 \text{ s})^{-1}$

2.7 Unit area

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

Definition m²

2.8 Unit length

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

 $\textbf{Definition} \ m$

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

			F			~ -	
Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
VCYT VMAT			3 3	$0.01 \\ 1.8 \cdot 10^{-6}$	1 1	1	

3.1 Compartment VCYT

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

3.2 Compartment VMAT

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

4 Species

This model contains 54 species. The boundary condition of nine 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	VCYT	μ mol·l ⁻¹		
C16AcylCarMAT	VMAT	$\mu \text{mol} \cdot l^{-1}$		
C16AcylCoAMAT	VMAT	$\mu \text{mol} \cdot l^{-1}$		
C16EnoylCoAMAT	VMAT	$\mu \text{mol} \cdot l^{-1}$		
C16HydroxyacylCoAMAT	VMAT	μ mol·l ⁻¹		
C16KetoacylCoAMAT	VMAT	$\mu \text{mol} \cdot 1^{-1}$		
C14AcylCarCYT	VCYT	μ mol·l ⁻¹		
C14AcylCarMAT	VMAT	μ mol·l ⁻¹		
C14AcylCoAMAT	VMAT	μ mol·l ⁻¹		
C14EnoylCoAMAT	VMAT	μ mol·l ⁻¹		
C14HydroxyacylCoAMAT	VMAT	μ mol·l ⁻¹		
C14KetoacylCoAMAT	VMAT	μ mol·l ⁻¹		
C12AcylCarCYT	VCYT	μ mol·l ⁻¹		\Box
C12AcylCarMAT	VMAT	$\mu mol \cdot l^{-1}$		
C12AcylCoAMAT	VMAT	$\mu mol \cdot l^{-1}$		\Box
C12EnoylCoAMAT	VMAT	$\mu mol \cdot l^{-1}$		\Box
C12HydroxyacylCoAMAT	VMAT	$\mu mol \cdot l^{-1}$		\Box
C12KetoacylCoAMAT	VMAT	$\mu mol \cdot l^{-1}$		
C10AcylCarCYT	VCYT	$\mu mol \cdot l^{-1}$		\Box
C10AcylCarMAT	VMAT	$\mu mol \cdot l^{-1}$		\Box
C10AcylCoAMAT	VMAT	$\mu mol \cdot l^{-1}$		\Box

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
C10EnoylCoA	MAT	VMAT	$\mu \text{mol} \cdot l^{-1}$		\Box
C10Hydroxya	cylCoAMAT	VMAT	μ mol·l ⁻¹		\Box
C10Ketoacyl	COAMAT	VMAT	μ mol·l ⁻¹		
C8AcylCarCY	Т	VCYT	μ mol· 1^{-1}		
C8AcylCarMA	T	VMAT	$\mu mol \cdot l^{-1}$		
C8AcylCoAMA	T	VMAT	$\mu mol \cdot l^{-1}$		\Box
C8EnoylCoAM	TAT	VMAT	μ mol · l ⁻¹		\Box
C8Hydroxyac	ylCoAMAT	VMAT	$\mu mol \cdot l^{-1}$		\Box
C8KetoacylC	OAMAT	VMAT	$\mu mol \cdot l^{-1}$		\Box
C6AcylCarCY	T	VCYT	$\mu mol \cdot l^{-1}$		\Box
C6AcylCarMA	T	VMAT	$\mu \mathrm{mol} \cdot \mathrm{l}^{-1}$		\Box
C6AcylCoAMA	T	VMAT	$\mu \mathrm{mol} \cdot \mathrm{l}^{-1}$		\Box
C6EnoylCoAM	TAT	VMAT	$\mu mol \cdot l^{-1}$		
C6Hydroxyac	ylCoAMAT	VMAT	$\mu mol \cdot l^{-1}$		\Box
C6KetoacylC	OAMAT	VMAT	$\mu mol \cdot l^{-1}$		\Box
C4AcylCarCY	T	VCYT	μ mol·l ⁻¹		
C4AcylCarMA	T	VMAT	$\mu mol \cdot l^{-1}$		\Box
C4AcylCoAMA	T	VMAT	$\mu mol \cdot l^{-1}$		\Box
C4EnoylCoAM	TAT	VMAT	$\mu \mathrm{mol} \cdot \mathrm{l}^{-1}$		
C4Hydroxyac	ylCoAMAT	VMAT	$\mu mol \cdot l^{-1}$		\Box
C4Acetoacyl	CoAMAT	VMAT	$\mu mol \cdot l^{-1}$		\Box
AcetylCoAMA	T	VMAT	$\mu mol \cdot l^{-1}$		\Box
FADHMAT		VMAT	$\mu mol \cdot l^{-1}$		
NADHMAT		VMAT	$\mu mol \cdot l^{-1}$		\Box
CoAMAT		VMAT	$\mu mol \cdot l^{-1}$		
C16AcylCoAC	YYT	VCYT	$\mu mol \cdot l^{-1}$		$ \overline{\mathcal{L}} $
CarCYT		VCYT	$\mu mol \cdot l^{-1}$		$\overline{\mathbf{Z}}$

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
CoACYT		VCYT	μ mol·l ⁻¹		
MalCoACYT		VCYT	$\mu mol \cdot l^{-1}$		\square
CarMAT		VMAT	$\mu mol \cdot l^{-1}$		\square
FADtMAT		VMAT	$\mu mol \cdot l^{-1}$		\square
NADtMAT		VMAT	$\mu mol \cdot l^{-1}$		\square
CoAMATt		VMAT	μ mol·l ⁻¹	\square	

5 Parameters

This model contains 140 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vfcact			0.420	$\mu mol \cdot l^{-1} \cdot (60 \text{ s})^{-1}$	
Vrcact			0.420	$\mu \text{mol} \cdot l^{-1} \cdot (60 \text{ s})^{-1}$	
KmcactCa	arMAT		130.000	$\mu \text{mol} \cdot l^{-1}$	
KmcactCa	arCYT		130.000	$\mu \text{mol} \cdot l^{-1}$	
KicactCa	arCYT		200.000	μ mol·l ⁻¹	
Keqcact			1.000	dimensionless	
Vcpt2			0.391	$\mu \text{mol} \cdot l^{-1} \cdot (60 \text{ s})^{-1}$	
Kmcpt2C1	.6AcylCarMAT		51.000	μ mol·l ⁻¹	
Kmcpt2C1	.4AcylCarMAT		51.000	$\mu mol \cdot l^{-1}$	
Kmcpt2C1	.2AcylCarMAT		51.000	μ mol·l ⁻¹	
Kmcpt2C1	.OAcylCarMAT		51.000	$\mu \text{mol} \cdot l^{-1}$	
Kmcpt2C8	BAcylCarMAT		51.000	μ mol·l ⁻¹	
Kmcpt2C6	SAcylCarMAT		51.000	μ mol·l ⁻¹	
Kmcpt2C4	AcylCarMAT		51.000	μ mol·l ⁻¹	
Kmcpt2Co	AMAT		30.000	μ mol·l ⁻¹	
Kmcpt2C1	.6AcylCoAMAT		38.000	μ mol·l ⁻¹	
Kmcpt2C1	.4AcylCoAMAT		38.000	μ mol·l ⁻¹	
Kmcpt2C1	.2AcylCoAMAT		38.000	μ mol·l ⁻¹	
Kmcpt2C1	.OAcylCoAMAT		38.000	μ mol·l ⁻¹	
Kmcpt2C8	BAcylCoAMAT		38.000	μ mol·l ⁻¹	
Kmcpt2C6	SAcylCoAMAT		1000.000	μ mol·l ⁻¹	
Kmcpt2C4	AcylCoAMAT		1000000.000	μ mol·l ⁻¹	
Kmcpt2Ca	arMAT		350.000	μ mol·l ⁻¹	
Keqcpt2			2.220	dimensionless	
Vvlcad			0.008	$\mu \text{mol} \cdot l^{-1} \cdot (60 \text{ s})^{-1}$	
KmvlcadC	C16AcylCoAMAT		6.500	μ mol·l ⁻¹	
KmvlcadC	C14AcylCoAMAT		4.000	μ mol·l ⁻¹	
KmvlcadC	C12AcylCoAMAT		2.700	μ mol·l ⁻¹	
KmvlcadF	AD		0.120	μ mol·l ⁻¹	
KmvlcadC	C16EnoylCoAMAT		1.080	μ mol·l ⁻¹	
KmvlcadC	C14EnoylCoAMAT		1.080	μ mol·l ⁻¹	
KmvlcadC	C12EnoylCoAMAT		1.080	μ mol·l ⁻¹	
KmvlcadF	ADH		24.200	μ mol·l ⁻¹	
Keqvlcad	l		6.000	dimensionless	
Vlcad			0.010	$\mu \text{mol} \cdot l^{-1} \cdot (60 \text{ s})^{-1}$	
KmlcadC1	.6AcylCoAMAT		2.500	μ mol·l ⁻¹	

Id	Name	SBO	Value	Unit	Constant
KmlcadC14	AcylCoAMAT		7.400	μ mol·l ⁻¹	
KmlcadC12	AcylCoAMAT		9.000	$\mu mol \cdot l^{-1}$	
KmlcadC10	AcylCoAMAT		24.300	μ mol·l ⁻¹	
KmlcadC8A	AcylCoAMAT		123.000	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmlcadFAD)		0.120	μ mol·l ⁻¹	
KmlcadC16	SEnoylCoAMAT		1.080	μ mol·l ⁻¹	
KmlcadC14	EnoylCoAMAT		1.080	$\mu mol \cdot l^{-1}$	
KmlcadC12	REnoylCoAMAT		1.080	μ mol·l ⁻¹	
KmlcadC10	EnoylCoAMAT		1.080	μ mol·l ⁻¹	
KmlcadC8E	EnoylCoAMAT		1.080	$\mu \text{mol} \cdot l^{-1}$	$\overline{\mathbf{Z}}$
KmlcadFAD	Н		24.200	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
Keqlcad			6.000	dimensionless	$\overline{\mathbf{Z}}$
Vmcad			0.081	$\mu \text{mol} \cdot l^{-1} \cdot (60 \text{ s})^{-1}$	$ \overline{\mathscr{L}} $
KmmcadC12	AcylCoAMAT		5.700	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmmcadC10	AcylCoAMAT		5.400	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
	AcylCoAMAT		4.000	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
	AcylCoAMAT		9.400	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmmcadC4A	AcylCoAMAT		135.000	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmmcadFAD	-		0.120	μ mol·l ⁻¹	Z
KmmcadC12	EnoylCoAMAT		1.080	$\mu \text{mol} \cdot l^{-1}$	$\overline{\mathbf{Z}}$
KmmcadC10	EnoylCoAMAT		1.080	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmmcadC8E	EnoylCoAMAT		1.080	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmmcadC6E	EnoylCoAMAT		1.080	$\mu mol \cdot l^{-1}$	
KmmcadC4E	EnoylCoAMAT		1.080	$\mu mol \cdot l^{-1}$	$\overline{\mathbf{Z}}$
KmmcadFAD	Н		24.200	$\mu mol \cdot l^{-1}$	
Keqmcad			6.000	dimensionless	
Vscad			0.081	$\mu \text{mol} \cdot l^{-1} \cdot (60 \text{ s})^{-1}$	$\overline{\mathbf{Z}}$
KmscadC6A	AcylCoAMAT		285.000	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmscadC4A	AcylCoAMAT		10.700	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmscadFAD)		0.120	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmscadC6E	EnoylCoAMAT		1.080	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmscadC4E	EnoylCoAMAT		1.080	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmscadFAD)H		24.200	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
Keqscad			6.000	dimensionless	$\overline{\mathbf{Z}}$
Vcrot			3.600	$\mu \text{mol} \cdot l^{-1} \cdot (60 \text{ s})^{-1}$	$\overline{\mathbf{Z}}$
	EnoylCoAMAT		150.000	μ mol·l ⁻¹	\mathbf{Z}
	EnoylCoAMAT		100.000	μ mol·l ⁻¹	
	EnoylCoAMAT		25.000	μ mol·l ⁻¹	\mathbf{Z}
	EnoylCoAMAT		25.000	μ mol·l ⁻¹	\mathbf{Z}
	EnoylCoAMAT		25.000	μ mol·l ⁻¹	\mathbf{Z}
	EnoylCoAMAT		25.000	$\mu \text{mol} \cdot l^{-1}$	\mathbf{Z}

Id	Name	SBO	Value	Unit	Constant
KmcrotC4Enoy	LCoAMAT		40.000	μ mol·l ⁻¹	
KmcrotC16Hyd	roxyacylCoAMAT		45.000	μ mol·l ⁻¹	
KmcrotC14Hyd	roxyacylCoAMAT		45.000	μ mol·l ⁻¹	$ \overline{\mathbf{Z}} $
KmcrotC12Hyd	roxyacylCoAMAT		45.000	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmcrotC10Hyd	roxyacylCoAMAT		45.000	μ mol·l ⁻¹	$ \overline{\mathbf{Z}} $
KmcrotC8Hydr	oxyacylCoAMAT		45.000	μ mol·l ⁻¹	$ \overline{\mathbf{Z}} $
KmcrotC6Hydro	oxyacylCoAMAT		45.000	μ mol·l ⁻¹	
KmcrotC4Hydro	oxyacylCoAMAT		45.000	μ mol·l ⁻¹	$ \overline{\mathbf{Z}} $
KicrotC4Acet	pacylCoA		1.600	$\mu \text{mol} \cdot l^{-1}$	$\overline{\mathbf{Z}}$
Keqcrot			3.130	dimensionless	$\overline{\mathbf{Z}}$
Vmschad			1.000	$\mu \text{mol} \cdot l^{-1} \cdot (60 \text{ s})^{-1}$	$\overline{\mathbf{Z}}$
KmmschadC16H	ydroxyacylCoAMAT		1.500	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
•	ydroxyacylCoAMAT		1.800	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
	ydroxyacylCoAMAT		3.700	μ mol·l ⁻¹	\mathbf{Z}
	ydroxyacylCoAMAT		8.800	μ mol·l ⁻¹	\mathbf{Z}
	droxyacylCoAMAT		16.300	μ mol·l ⁻¹	\mathbf{Z}
•	droxyacylCoAMAT		28.600	μ mol·l ⁻¹	\mathbf{Z}
•	droxyacylCoAMAT		69.900	μ mol·l ⁻¹	\mathbf{Z}
KmmschadNADM	• •		58.500	μ mol·l ⁻¹	Z
KmmschadC16Ke	etoacylCoAMAT		1.400	μ mol·l ⁻¹	\mathbf{Z}
	etoacylCoAMAT		1.400	μ mol·l ⁻¹	\mathbf{Z}
	etoacylCoAMAT		1.600	μ mol·l ⁻¹	Z
	etoacylCoAMAT		2.300	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmmschadC8Ke	•		4.100	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmmschadC6Ke	•		5.800	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
	etoacylCoAMAT		16.900	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmmschadNADH			5.400	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
Keqmschad			$2.17 \cdot 10^{-4}$	dimensionless	$\overline{\mathbf{Z}}$
Vmckat			0.377	$\mu \text{mol} \cdot l^{-1} \cdot (60 \text{ s})^{-1}$	\mathbf{Z}
KmmckatC16Ke	toacylCoAMAT		1.100	μ mol·l ⁻¹	\mathbf{Z}
KmmckatC14Ke	•		1.200	μ mol·l ⁻¹	\mathbf{Z}
KmmckatC12Ke	•		1.300	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmmckatC10Ke	•		2.100	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmmckatC8Ket	•		3.200	μ mol·l ⁻¹	\mathbf{Z}
KmmckatC6Ket	· ·		6.700	μ mol·l ⁻¹	\mathbf{Z}
KmmckatC4Ace	•		12.400	μ mol·l ⁻¹	\mathbf{Z}
KmmckatCoAMA'	•		26.600	μ mol·l ⁻¹	\mathbf{Z}
KmmckatC14Ac	ylCoAMAT		13.830	μ mol·l ⁻¹	\mathbf{Z}
KmmckatC16Ac			13.830	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmmckatC12Ac			13.830	μ mol·l ⁻¹	\mathbf{Z}
KmmckatC10Ac			13.830	μ mol·l ⁻¹	\mathbf{Z}
KmmckatC8Acy			13.830	μ mol·l ⁻¹	\mathbf{Z}

Id	Name	SBO	Value	Unit	Constant
KmmckatC	GAcylCoAMAT		13.830	μ mol·l ⁻¹	\overline{Z}
KmmckatC	4AcylCoAMAT		13.830	μ mol·l ⁻¹	
KmmckatA	cetylCoAMAT		30.000	μ mol·l ⁻¹	
Keqmckat	;		1051.000	dimensionless	
Vmtp			2.840	$\mu \text{mol} \cdot l^{-1} \cdot (60 \text{ s})^{-1}$	
KmmtpC16	EnoylCoAMAT		25.000	μ mol·l ⁻¹	
KmmtpC14	EnoylCoAMAT		25.000	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmmtpC12	EnoylCoAMAT		25.000	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmmtpC10	EnoylCoAMAT		25.000	μ mol·l ⁻¹	$\overline{\checkmark}$
KmmtpC8E	EnoylCoAMAT		25.000	$\mu mol \cdot l^{-1}$	$\overline{\mathbf{Z}}$
KmmtpNAD	TAM		60.000	$\mu mol \cdot l^{-1}$	$\overline{\mathbf{Z}}$
KmmtpCoA	TAM		30.000	μ mol·l ⁻¹	
KmmtpC14	AcylCoAMAT		13.830	μ mol·l ⁻¹	
KmmtpC16	SAcylCoAMAT		13.830	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmmtpC12	AcylCoAMAT		13.830	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
KmmtpC10	AcylCoAMAT		13.830	μ mol·l ⁻¹	
KmmtpC8A	cylCoAMAT		13.830	μ mol·l ⁻¹	
KmmtpC6A	cylCoAMAT		13.830	μ mol·l ⁻¹	
KmmtpNAD	TAMH		50.000	$\mu mol \cdot l^{-1}$	$\overline{\mathbf{Z}}$
KmmtpAce	tylCoAMAT		30.000	$\mu mol \cdot l^{-1}$	$\overline{\mathbf{Z}}$
Keqmtp			0.710	dimensionless	$\overline{\mathbf{Z}}$

6 Function definitions

This is an overview of 13 function definitions.

6.1 Function definition CPT1

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

Mathematical Expression

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

6.2 Function definition CACT

Arguments Vf, Vr, Kms1, Kms2, Kmp1, Kmp2, Kis1, Kip2, Keq, S1, S2, P1, P2

Mathematical Expression

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

6.3 Function definition CPT2

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

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

6.4 Function definition VLCAD

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

Mathematical Expression

$$\frac{sf \cdot V \cdot \left(\frac{S1 \cdot (S4 - P4)}{Kms1 \cdot Kms4} - \frac{P1 \cdot P4}{Kms1 \cdot Kms4 \cdot Keq}\right)}{\left(1 + \frac{S1}{Kms1} + \frac{P1}{Kmp1} + \frac{S2}{Kms2} + \frac{P2}{Kmp2} + \frac{S3}{Kms3} + \frac{P3}{Kmp3}\right) \cdot \left(1 + \frac{S4 - P4}{Kms4} + \frac{P4}{Kmp4}\right)} \left(4\right)$$

6.5 Function definition LCAD

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

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

6.6 Function definition MCAD

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 SCAD

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

Mathematical Expression

$$\frac{sf \cdot V \cdot \left(\frac{S1 \cdot (S3-P3)}{Kms1 \cdot Kms3} - \frac{P1 \cdot P3}{Kms1 \cdot Kms3 \cdot Keq}\right)}{\left(1 + \frac{S1}{Kms1} + \frac{P1}{Kmp1} + \frac{S2}{Kms2} + \frac{P2}{Kmp2}\right) \cdot \left(1 + \frac{S3-P3}{Kms3} + \frac{P3}{Kmp3}\right)}$$
(7)

6.8 Function definition CROT

Arguments sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Ki1, Keq, S1, S2, S3, S4, S5, S6, S7, P1, P2, P3, P4, P5, P6, P7, I1

Mathematical Expression

$$\frac{sf \cdot V \cdot \left(\frac{S1}{Kms1} - \frac{P1}{Kms1 \cdot Keq}\right)}{1 + \frac{S1}{Kms1} + \frac{P1}{Kmp1} + \frac{S2}{Kms2} + \frac{P2}{Kmp2} + \frac{S3}{Kms3} + \frac{P3}{Kmp3} + \frac{S4}{Kms4} + \frac{P4}{Kmp4} + \frac{S5}{Kms5} + \frac{P5}{Kmp5} + \frac{86}{Kms6} + \frac{P6}{Kmp6} + \frac{S7}{Kms7} + \frac{P7}{Kmp7}}$$

6.9 Function definition MSCHAD

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

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

6.10 Function definition MCKATA

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

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

6.11 Function definition MCKATB

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

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

6.12 Function definition MTP

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

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

6.13 Function definition RES

Arguments Ks, S, K1

Mathematical Expression

$$Ks \cdot (S - K1) \tag{13}$$

7 Rules

This is an overview of two rules.

7.1 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{C14AcylCoAMAT} \right] + \left[ \text{C16HydroxyacylCoAMAT} \right] + \left[ \text{C14EnoylCoAMAT} \right] + \left[ \text{C14EnoylCoAMAT} \right] + \left[ \text{C12HydroxyacylCoAMAT} \right] + \left[ \text{C12AcylCoAMAT} \right] + \left[ \text{C12EnoylCoAMAT} \right] + \left[ \text{C12HydroxyacylCoAMAT} \right] + \left[ \text{C10EnoylCoAMAT} \right] + \left[ \text{C10EnoylCoAMAT} \right] + \left[ \text{C10HydroxyacylCoAMAT} \right] + \left[ \text{C10KetoacylCoAMAT} \right] + \left[ \text{C8AcylCoAMAT} \right] + \left[ \text{C8EnoylCoAMAT} \right] + \left[ \text{C8HydroxyacylCoAMAT} \right] + \left[ \text{C8KetoacylCoAMAT} \right] + \left[ \text{C6EnoylCoAMAT} \right] + \left[ \text{C6HydroxyacylCoAMAT} \right] + \left[ \text{C4HydroxyacylCoAMAT} \right] + \left[ \text{C4AcylCoAMAT} \right] + \left[ \text{C4EnoylCoAMAT} \right] + \left[ \text{C4HydroxyacylCoAMAT} \right] + \left[ \text{C4AcetoacylCoAMAT} \right] + \left
```

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

7.2 Rule C16AcylCoACYT

Rule C16AcylCoACYT is an assignment rule for species C16AcylCoACYT:

$$C16AcylCoACYT = 26.8 \cdot 2.71828182845905^{-0.18 \cdot t}$$
 (15)

8 Reactions

This model contains 59 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

			an reactions		
No	Id	Name	Reaction Equation	SBO	
1	vcpt1C16		C16AcylCoACYT, CarCYT,	CoACYT, MalCoACYT, C16Acy	ICoACYT, CarCYT,
2	vcactC16		C16AcylCarCYT CarMAT, Car	CYT, C16AcylCarCYT, CarMAT	, C16AcylCarMAT,
2			CarMAT. Car	CYT, C14AcylCarCYT, CarMAT	, C14AcylCarMAT,
3	vcactC14		C14AcylCalC11	CYT, C12AcylCarCYT, CarMAT	
4	vcactC12		C12AcvlCarCYT ======	CYT, C10AcylCarCYT, CarMAT	
5	vcactC10		CTOACYTCATCTT -		
6	vcactC8		('X \ cvl('or('V')'	CYT, C8AcylCarCYT, CarMAT, C	
7	vcactC6		C6AcylCarCYT CarMAT, CarC	CYT, C6AcylCarCYT, CarMAT, C	C6AcylCarMAT, Car
8	vcactC4		C4AcylCarCYT CarMAT, CarC	CYT, C4AcylCarCYT, CarMAT, C	C4AcylCarMAT, Car
9	vcpt2C16			MAT, C12AcylCarMAT, C10Acyl	CarMAT, C8AcylCa
-	_		C16AcvlCarl	MAT, C12AcylCarMAT, C10Acyl	CarMAT, C8AcylCa
10	vcpt2C14		C14AcylCarMAT C16AcylCarM	MAT, C14AcylCarMAT, C10Acyl	CarMAT, C8AcylCa
11	vcpt2C12		C12AcylCarMAT	MAT, C14AcylCarMAT, C12Acyl	-
12	vcpt2C10		CIOACYICarwiAi	AT, C14AcylCarMAT, C12AcylC	
13	vcpt2C8		C8AcylCarMAT =======		
14	vcpt2C6		C6AcylCarMAT C16AcylCarM	AT, C14AcylCarMAT, C12AcylC	arMAT, C10AcylCa

N⁰	Id	Name	Reaction Equation	SBO
15	vcpt2C4		C4AcylCarMAT ————————————————————————————————————	AT, C14AcylCarMAT, C12AcylCarMAT, C10AcylCar
	-		C1(A = 1C = AMAT C14AcylCoA	MAT, C12AcylCoAMAT, FADtMAT, C14EnoylCo
16	vvlcadC16			
1.7	7 1044		C14A IC AMAT C16AcylCoA	MAT, C12AcylCoAMAT, FADtMAT, C16EnoylCo
17	vvlcadC14		FADHMAT	
10				MAT, C14AcylCoAMAT, FADtMAT, C16EnoylCo
18	vvlcadC12		EADUMAT	
10			C14AcylCoA	MAT, C12AcylCoAMAT, C10AcylCoAMAT, C8Ac
19	vlcadC16		EADIIMAT	
•			C16AcylCoA	MAT, C12AcylCoAMAT, C10AcylCoAMAT, C8Ac
20	vlcadC14		FADHMAT	
•			C16AcylCoA	MAT, C14AcylCoAMAT, C10AcylCoAMAT, C8Ac
21	vlcadC12		EADIMAT	
22			C16AcylCoA	MAT, C14AcylCoAMAT, C12AcylCoAMAT, C8Ac
22	vlcadC10		ЕУРПИЛТ	
•			C16AcylCoAM	MAT, C14AcylCoAMAT, C12AcylCoAMAT, C10Ac
23	vlcadC8		C8AcylCoAMAT 	
2.4			C10AcylCoA	MAT, C8AcylCoAMAT, C6AcylCoAMAT, C4Acyl
24	vmcadC12		EADIDAAT	
			C12AcylCoA	MAT, C8AcylCoAMAT, C6AcylCoAMAT, C4Acyl
25	vmcadC10		C10AcylCoAMAT ————————————————————————————————————	

N₀	Id	Name	Reaction Equation	SBO
26			CSA cylCoAMAT —	12AcylCoAMAT, C10AcylCoAMAT, C6AcylCoAMAT, C4AcylC
20	Vincacio		EADIMAT	
2.7	vmcadC6		$C_{\text{AcylCoAMAT}} = C_{\text{AcylCoAMAT}}$	12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, C4AcylC
21	Vincadoo		EADIMAT	
28	vmcadC4		$C4$ AcvlCoAMAT \rightleftharpoons	12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, C6AcylC
	Vmodes 2		EADIMAT	
29	vscadC6		$C6AcvlCoAMAT \rightleftharpoons$	4AcylCoAMAT, FADtMAT, C4EnoylCoAMAT, C6AcylCoAMAT
			FADHMAT	
30	vscadC4		C4AcylCoAMAT =	6AcylCoAMAT, FADtMAT, C6EnoylCoAMAT, C4AcylCoAMAT
			EADUMAT	
31	vcrotC16		C16EnoylCoAMAT	C14EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C
32	vcrot.C14			C16EnovlCoAMAT, C12EnovlCoAMAT, C10EnovlCoAMAT, C
			•	C16EnovlCoAMAT, C14EnovlCoAMAT, C10EnovlCoAMAT, C
			•	C16EnovlCoAMAT, C14EnovlCoAMAT, C12EnovlCoAMAT, C
34	vcrotC10		C10EnoylCoAMAT	C16EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C1
35	vcrotC8		C8EnoylCoAMAT =	C16EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C1
36	vcrotC6		C6EnoylCoAMAT =	
37	vcrotC4			C16EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C1
			C16HvdroxvacylCo	AMAT C14HydroxyacylCoAMAT, C12HydroxyacylCoAMAT, C
50	VIIISCIIAAGIC		NADHMAT	
39	vmschadC14		C14HydroxyacylCoA	AMAT C16HydroxyacylCoAMAT, C12HydroxyacylCoAMAT, C
			NADHMAT	
	26 27 28 29 30 31 32 33 34 35 36 37 38	27 vmcadC6 28 vmcadC4 29 vscadC6 30 vscadC4 31 vcrotC16 32 vcrotC14 33 vcrotC12 34 vcrotC10 35 vcrotC8 36 vcrotC6 37 vcrotC4 38 vmschadC16	26 vmcadC8 27 vmcadC6 28 vmcadC4 29 vscadC6 30 vscadC4 31 vcrotC16 32 vcrotC14 33 vcrotC12 34 vcrotC10 35 vcrotC8 36 vcrotC6 37 vcrotC4 38 vmschadC16	26 vmcadC8 C8AcylCoAMAT = FADHMAT 27 vmcadC6 C6AcylCoAMAT = FADHMAT 28 vmcadC4 C4AcylCoAMAT = FADHMAT 29 vscadC6 C6AcylCoAMAT = FADHMAT 30 vscadC4 C4AcylCoAMAT = FADHMAT 31 vcrotC16 C16EnoylCoAMAT 32 vcrotC14 C14EnoylCoAMAT 33 vcrotC12 C12EnoylCoAMAT 34 vcrotC10 C10EnoylCoAMAT 35 vcrotC8 C8EnoylCoAMAT 36 vcrotC6 C6EnoylCoAMAT 37 vcrotC4 C4EnoylCoAMAT 38 vmschadC16 C16HydroxyacylCo. NADHMAT 39 vmschadC14 C14HydroxyacylCo.

Nº	Id	Name	Reaction Equation	SBO
40	vmschadC12		C12HydroxyacylCoAMA	C16HydroxyacylCoAMAT, C14HydroxyacylCoAMAT, C
10	VIIIDOIIQQ012		ΝΔΟΗΜΔΤ	
41			C10HydroyyyaaylCa AMA	C16HydroxyacylCoAMAT, C14HydroxyacylCoAMAT, C
41	vmschadC10		NIADIIMAT	
				C16HydroxyacylCoAMAT, C14HydroxyacylCoAMAT, C1
42	vmschadC8		C8HydroxyacylCoAMAI NADHMAT	\ \
			NADHMAI	C16HydroxyacylCoAMAT, C14HydroxyacylCoAMAT, C1
43	vmschadC6			C16HydroxyacylCoAMAT, C14HydroxyacylCoAMAT, C1
			NADHMAT	C1(III) decreased C2 AMAT C14II decreased C2 AMAT C1
44	vmschadC4		C4HydroxyacylCoAMAT	C16HydroxyacylCoAMAT, C14HydroxyacylCoAMAT, C1
			NADHMAT	
45	vmckatC16		C C16KetoacvlCoAMAT =	C14KetoacylCoAMAT, C12KetoacylCoAMAT, C10KetoacylC
			A and ICa AMAT	
46	vmckatC14		C1/KetoncylCoAMAT —	216KetoacylCoAMAT, C12KetoacylCoAMAT, C10KetoacylC
70	VIIICKAUCIA		A antrolCa A M AT	
47	1		CION A IC AMATE	216KetoacylCoAMAT, C14KetoacylCoAMAT, C10KetoacylC
47	vmckatC12		C12KetoacylCoAMAT = AcetylCoAMAT	
				C16KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylC
48	vmckatC10		-	
			AcetylCoAMAT C1	6KetoacylCoAMAT_C14KetoacylCoAMAT_C12KetoacylCo
49	vmckatC8			6KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCo
			AcetylCoAMAT	(Veterrile AMAT C14Veterrile AMAT C12Veterrile
50	vmckatC6		C6KetoacylCoAMAT ←	6KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCo
			AcetylCoAMAT	

20	Nº Id	Name	Reaction Equation	SBO
	51 vmckatC4		C4AcetoacylCoAMAT	CoAMAT, C14KetoacylCoAMAT, C12KetoacylC
			C14EnovlCoAN	MAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C
	52 vmtpC16		C16EnoylCoAMAT - NA DUMAT	
			C16EnoylCoAM	MAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C
	53 vmtpC14			
			AcetylCoAMAT + NADHMAT	AAT C14En and Ca AMAT C10En and C1AMAT C
	54 vmtpC12		C12EnoylCoAMAT = C16EnoylCoAM	MAT, C14EnoylCoAMAT, C10EnoylCoAMAT, C
	•		AcetylCoAMAT + NADHMAT	
P	55 vmtpC10		C10EnoylCoAMAT C16EnoylCoAM	MAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C
rodu	55 vmtpC10		AcetylCoAMAT + NADHMAT	
исе			C16EnovlCoAM	AT, C14EnoylCoAMAT, C12EnoylCoAMAT, C1
d b	56 vmtpC8		C8EnoylCoAMAT =	
A			AcetylCoAMAT + NADHMAT	
3ML;	57 vacesink		$AcetylCoAMAT \xrightarrow{AcetylCoAMAT} \emptyset$	
Produced by SBML2LETEX	58 vfadhsink	Σ	$FADHMAT \xrightarrow{FADHMAT} \emptyset$	
×	59 vnadhsink	Σ	NADHMAT $\stackrel{\text{NADHMAT}}{\longleftarrow} \emptyset$	
		-		

8.1 Reaction vcpt1C16

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

Reaction equation

© C16AcylCoACYT, CarCYT, CoACYT, MalCoACYT, C16AcylCoACYT, CarCYT, C16AcylCarCYT, CoACYT
(16)

Modifiers

Table 6: Properties of each modifier.

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

Product

Table 7: Properties of each product.

Id	Name	SBO
C16AcylCarCYT		

Kinetic Law

Derived unit contains undeclared units

$$\begin{split} & CPT1\left(sf, V, Kms1, Kms2, Kmp1, Kmp2, Ki1, Keq, S1, S2, P1, P2, I1, n\right) \\ & = \frac{sf \cdot V \cdot \left(\frac{S1 \cdot S2}{Kms1 \cdot Kms2} - \frac{P1 \cdot P2}{Kms1 \cdot Kms2 \cdot Keq}\right)}{\left(1 + \frac{S1}{Kms1} + \frac{P1}{Kmp1} + \left(\frac{I1}{Ki1}\right)^{n}\right) \cdot \left(1 + \frac{S2}{Kms2} + \frac{P2}{Kmp2}\right)} \end{split} \tag{18}$$

Table 8: Properties of each parameter.

			1		
Id	Name	SBO	Value	Unit	Constant
Keqcpt1			0.450	dimensionless	
Kicpt1Mal	LCoACYT		9.100	μ mol·l ⁻¹	
Kmcpt1C16	6AcylCarCYT		136.000	μ mol·l ⁻¹	
Kmcpt1C16	SAcylCoACYT		13.800	μ mol·l ⁻¹	
Kmcpt1Ca	CCYT		125.000	μ mol·l ⁻¹	
Kmcpt1Co	ACYT		40.700	μ mol·l ⁻¹	
Vcpt1			0.012	$\mu \text{mol} \cdot l^{-1} \cdot (60 \text{ s})^{-1}$	
ncpt1			2.480	dimensionless	$\overline{\mathbf{Z}}$
sfcpt1C16	3		1.000	dimensionless	

8.2 Reaction vcactC16

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

Reaction equation

$$\frac{\text{CarMAT, CarCYT, C16AcylCarCYT, CarMAT, C16AcylCarMAT, CarCYT}}{(19)} C16AcylCarMAT$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
C16AcylCarCYT		

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
CarMAT		
CarCYT		
C16AcylCarCYT		
CarMAT		
C16AcylCarMAT		
CarCYT		

Product

Table 11: Properties of each product.

Id	Name	SBO
C16AcylCarMAT		

Kinetic Law

Derived unit contains undeclared units

$$\begin{split} &CACT\left(Vf, Vr, Kms1, Kms2, Kmp1, Kmp2, Kis1, Kip2, Keq, S1, S2, P1, P2\right) \\ &= \frac{Vf \cdot \left(S1 \cdot S2 - \frac{P1 \cdot P2}{Keq}\right)}{S1 \cdot S2 + Kms2 \cdot S1 + Kms1 \cdot S2 \cdot \left(1 + \frac{P2}{Kip2}\right) + \frac{Vf}{Vr \cdot Keq} \cdot \left(Kmp2 \cdot P1 \cdot \left(1 + \frac{S1}{Kis1}\right) + P2 \cdot \left(Kmp1 + P1\right)\right)} \end{split}$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KicactC1	6AcylCarCYT		56.0	$\mu mol \cdot l^{-1}$	
KmcactC1	6AcylCarCYT		15.0	μ mol·l ⁻¹	\square
KmcactC1	6AcylCarMAT		15.0	μ mol·l ⁻¹	

8.3 Reaction vcactC14

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

Reaction equation

$$C14AcylCarCYT \xleftarrow{CarMAT, CarCYT, C14AcylCarCYT, CarMAT, C14AcylCarMAT, CarCYT}_{(22)} C14AcylCarMAT$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
C14AcylCarCYT		

Modifiers

Table 14: Properties of each modifier.

Id	Name	SBO
CarMAT		
CarCYT		
C14AcylCarCYT		
CarMAT		
C14AcylCarMAT		
CarCYT		

Product

Table 15: Properties of each product.

Id	Name	SBO
C14AcylCarMAT		

Kinetic Law

Derived unit contains undeclared units

$$\begin{aligned} &CACT\left(Vf,Vr,Kms1,Kms2,Kmp1,Kmp2,Kis1,Kip2,Keq,S1,S2,P1,P2\right) & (24) \\ &= \frac{Vf \cdot \left(S1 \cdot S2 - \frac{P1 \cdot P2}{Keq}\right)}{S1 \cdot S2 + Kms2 \cdot S1 + Kms1 \cdot S2 \cdot \left(1 + \frac{P2}{Kip2}\right) + \frac{Vf}{Vr \cdot Keq} \cdot \left(Kmp2 \cdot P1 \cdot \left(1 + \frac{S1}{Kis1}\right) + P2 \cdot \left(Kmp1 + P1\right)\right)} \end{aligned}$$

Table 16: Properties of each parameter.

$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$						
KmcactC14AcylCarCYT 15.0 μ mol·l ⁻¹	Id	Name	SBO	Value	Unit	Constant
	KmcactC1	4AcylCarCYT			•	

8.4 Reaction vcactC12

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

Reaction equation

$$C12AcylCarCYT \xleftarrow{CarMAT, CarCYT, C12AcylCarCYT, CarMAT, C12AcylCarMAT, CarCYT}_{(25)} C12AcylCarMAT$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
C12AcylCarCYT		

Modifiers

Table 18: Properties of each modifier.

Id	Name	SBO
CarMAT		
CarCYT		

Id	Name	SBO
C12AcylCarCYT		
CarMAT		
C12AcylCarMAT		
CarCYT		

Product

Table 19: Properties of each product.

Id	Name	SBO
C12AcylCarMAT		

Kinetic Law

Derived unit contains undeclared units

$$\begin{aligned} &CACT\left(Vf,Vr,Kms1,Kms2,Kmp1,Kmp2,Kis1,Kip2,Keq,S1,S2,P1,P2\right) & (27) \\ &= \frac{Vf \cdot \left(S1 \cdot S2 - \frac{P1 \cdot P2}{Keq}\right)}{S1 \cdot S2 + Kms2 \cdot S1 + Kms1 \cdot S2 \cdot \left(1 + \frac{P2}{Kip2}\right) + \frac{Vf}{Vr \cdot Keq} \cdot \left(Kmp2 \cdot P1 \cdot \left(1 + \frac{S1}{Kis1}\right) + P2 \cdot \left(Kmp1 + P1\right)\right)} \end{aligned}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KmcactC12	2AcylCarCYT 2AcylCarCYT 2AcylCarMAT		56.0 15.0 15.0	$\begin{array}{c} \mu \text{mol} \cdot l^{-1} \\ \mu \text{mol} \cdot l^{-1} \\ \mu \text{mol} \cdot l^{-1} \end{array}$	1 1 1 1 1 1 1 1 1 1

8.5 Reaction vcactC10

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

Reaction equation

$$C10AcylCarCYT \xleftarrow{CarMAT, CarCYT, C10AcylCarCYT, CarMAT, C10AcylCarMAT, CarCYT}_{(28)} C10AcylCarMAT$$

Reactant

Table 21: Properties of each reactant.

Id Name SBO

C10AcylCarCYT

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
CarMAT		
CarCYT		
C10AcylCarCYT		
CarMAT		
C10AcylCarMAT		
CarCYT		

Product

Table 23: Properties of each product.

Id	Name	SBO
C10AcylCarMAT		

Kinetic Law

Derived unit contains undeclared units

$$\begin{split} &CACT\left(Vf,Vr,Kms1,Kms2,Kmp1,Kmp2,Kis1,Kip2,Keq,S1,S2,P1,P2\right) \\ &= \frac{Vf \cdot \left(S1 \cdot S2 - \frac{P1 \cdot P2}{Keq}\right)}{S1 \cdot S2 + Kms2 \cdot S1 + Kms1 \cdot S2 \cdot \left(1 + \frac{P2}{Kip2}\right) + \frac{Vf}{Vr \cdot Keq} \cdot \left(Kmp2 \cdot P1 \cdot \left(1 + \frac{S1}{Kis1}\right) + P2 \cdot \left(Kmp1 + P1\right)\right)} \end{split}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
	OAcylCarCYT		56.0 15.0	$\mu \text{mol} \cdot l^{-1}$ $\mu \text{mol} \cdot l^{-1}$	
	OAcylCarCYT OAcylCarMAT		15.0	μ mol·l ⁻¹	☑ ☑

8.6 Reaction vcactC8

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

Reaction equation

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
C8AcylCarCYT		

Modifiers

Table 26: Properties of each modifier.

Id	Name	SBO
CarMAT		
CarCYT		
C8AcylCarCYT		
CarMAT		
C8AcylCarMAT		
CarCYT		

Product

Table 27: Properties of each product.

•	Id	Name	
	C8AcylCarMAT		

Kinetic Law

Derived unit contains undeclared units

$$\begin{aligned} & CACT\left(Vf, Vr, Kms1, Kms2, Kmp1, Kmp2, Kis1, Kip2, Keq, S1, S2, P1, P2\right) & (33) \\ & = \frac{Vf \cdot \left(S1 \cdot S2 - \frac{P1 \cdot P2}{Keq}\right)}{S1 \cdot S2 + Kms2 \cdot S1 + Kms1 \cdot S2 \cdot \left(1 + \frac{P2}{Kip2}\right) + \frac{Vf}{Vr \cdot Keq} \cdot \left(Kmp2 \cdot P1 \cdot \left(1 + \frac{S1}{Kis1}\right) + P2 \cdot \left(Kmp1 + P1\right)\right)} \end{aligned}$$

Table 28: Properties of each parameter.

		*			
Id	Name	SBO	Value	Unit	Constant
KmcactC8/	AcylCarCYT AcylCarCYT AcylCarMAT		56.0 15.0 15.0	$ \mu \text{mol} \cdot l^{-1} \\ \mu \text{mol} \cdot l^{-1} \\ \mu \text{mol} \cdot l^{-1} $	Z
10400001	10, 100111111		15.0	paritor 1	V

8.7 Reaction vcactC6

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

Reaction equation

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
C6AcylCarCYT		

Modifiers

Table 30: Properties of each modifier.

Id	Name	SBO
CarMAT		
CarCYT		
C6AcylCarCYT		
CarMAT		
C6AcylCarMAT		
CarCYT		

Product

Table 31: Properties of each product.

Id	Name	SBO
C6AcylCarMAT		

Kinetic Law

Derived unit contains undeclared units

$$\begin{aligned} & CACT\left(Vf, Vr, Kms1, Kms2, Kmp1, Kmp2, Kis1, Kip2, Keq, S1, S2, P1, P2\right) & (36) \\ & = \frac{Vf \cdot \left(S1 \cdot S2 - \frac{P1 \cdot P2}{Keq}\right)}{S1 \cdot S2 + Kms2 \cdot S1 + Kms1 \cdot S2 \cdot \left(1 + \frac{P2}{Kip2}\right) + \frac{Vf}{Vr \cdot Keq} \cdot \left(Kmp2 \cdot P1 \cdot \left(1 + \frac{S1}{Kis1}\right) + P2 \cdot \left(Kmp1 + P1\right)\right)} \end{aligned}$$

Table 32: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KicactC6	AcylCarCYT		56.0	$\mu mol \cdot l^{-1}$	
KmcactC6	AcylCarCYT		15.0	μ mol·l ⁻¹	
KmcactC6	AcylCarMAT		15.0	μ mol·l ⁻¹	\square

8.8 Reaction vcactC4

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

Reaction equation

$$C4AcylCarCYT \xleftarrow{CarMAT, CarCYT, C4AcylCarCYT, CarMAT, C4AcylCarMAT, CarCYT} C4AcylCarMAT (37)$$

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
C4AcylCarCYT		

Modifiers

Table 34: Properties of each modifier.

Id	Name	SBO
CarMAT		
CarCYT		
C4AcylCarCYT		
CarMAT		
C4AcylCarMAT		
CarCYT		

Product

Table 35: Properties of each product.

Id	Name	SBO
C4AcvlCarMAT		

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$\begin{split} &CACT\left(Vf,Vr,Kms1,Kms2,Kmp1,Kmp2,Kis1,Kip2,Keq,S1,S2,P1,P2\right) \\ &= \frac{Vf \cdot \left(S1 \cdot S2 - \frac{P1 \cdot P2}{Keq}\right)}{S1 \cdot S2 + Kms2 \cdot S1 + Kms1 \cdot S2 \cdot \left(1 + \frac{P2}{Kip2}\right) + \frac{Vf}{Vr \cdot Keq} \cdot \left(Kmp2 \cdot P1 \cdot \left(1 + \frac{S1}{Kis1}\right) + P2 \cdot \left(Kmp1 + P1\right)\right)} \end{split}$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KmcactC4A	cylCarCYT cylCarCYT cylCarMAT		56.0 15.0 15.0	μ mol·l ⁻¹ μ mol·l ⁻¹ μ mol·l ⁻¹	

8.9 Reaction vcpt2C16

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

Reaction equation

Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
C16AcylCarMAT		

Modifiers

Table 38: Properties of each modifier.

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

Product

Table 39: Properties of each product.

Id	Name	SBO
C16AcylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

```
    v9 = CPT2 (sfcpt2C16, Vcpt2, Kmcpt2C16AcylCarMAT, Kmcpt2C14AcylCarMAT, Kmcpt2C12AcylCarMAT, Kmcpt2C10AcylCarMAT, Kmcpt2C8AcylCarMAT, Kmcpt2C6AcylCarMAT, Kmcpt2C6AcylCarMAT, Kmcpt2C4AcylCarMAT, Kmcpt2C16AcylCoAMAT, Kmcpt2C14AcylCoAMAT, Kmcpt2C12AcylCoAMAT, Kmcpt2C10AcylCoAMAT, Kmcpt2C8AcylCoAMAT, Kmcpt2C6AcylCoAMAT, Kmcpt2C6AcylCoAMAT, Kmcpt2C4AcylCoAMAT, Kmcpt2CarMAT, Keqcpt2, [C16AcylCarMAT], [C14AcylCarMAT], [C12AcylCarMAT], [C10AcylCarMAT], [C8AcylCarMAT], [C6AcylCarMAT], [C4AcylCarMAT], [C14AcylCoAMAT], [C14AcylCoAMAT], [C12AcylCoAMAT], [C10AcylCoAMAT], [C8AcylCoAMAT], [C6AcylCoAMAT], [C4AcylCoAMAT], [C4AcylCoAMAT
```

CPT2 (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Keq, S1, S2, S3, S4, S5, S6, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8)

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

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcpt2C16			0.85	dimensionless	\overline{Z}

8.10 Reaction vcpt2C14

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

Reaction equation

Reactant

Table 41: Properties of each reactant.

Id	Name	
C14AcylCarMAT		

Modifiers

Table 42: Properties of each modifier.

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

Product

Table 43: Properties of each product.

- Incirc ici i i coperiore	01 04011	pro unt .
Id	Name	SBO
C14AcylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

```
\begin{split} \nu_{10} &= \text{CPT2} \left( \text{sfcpt2C14}, \text{Vcpt2}, \text{Kmcpt2C14AcylCarMAT}, \text{Kmcpt2C16AcylCarMAT}, \\ &\quad \text{Kmcpt2C12AcylCarMAT}, \text{Kmcpt2C10AcylCarMAT}, \text{Kmcpt2C8AcylCarMAT}, \\ &\quad \text{Kmcpt2C6AcylCarMAT}, \text{Kmcpt2C4AcylCoAMAT}, \text{Kmcpt2C0AMAT}, \\ &\quad \text{Kmcpt2C14AcylCoAMAT}, \text{Kmcpt2C16AcylCoAMAT}, \text{Kmcpt2C12AcylCoAMAT}, \\ &\quad \text{Kmcpt2C10AcylCoAMAT}, \text{Kmcpt2C8AcylCoAMAT}, \text{Kmcpt2C6AcylCoAMAT}, \\ &\quad \text{Kmcpt2C4AcylCoAMAT}, \text{Kmcpt2CarMAT}, \text{Keqcpt2}, [\text{C14AcylCarMAT}], \\ &\quad \text{[C16AcylCarMAT]}, [\text{C12AcylCarMAT}], [\text{C10AcylCarMAT}], [\text{C8AcylCarMAT}], \\ &\quad \text{[C6AcylCarMAT]}, [\text{C4AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C8AcylCoAMAT}], \\ &\quad \text{[C16AcylCoAMAT]}, [\text{C12AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C3AcylCoAMAT}], \\ &\quad \text{[C6AcylCoAMAT]}, [\text{C4AcylCoAMAT}], [\text{C4AcylC
```

CPT2 (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Keq, S1, S2, S3, S4, S5, S6, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8)

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

Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcpt2C14			1.0	dimensionless	Ø

8.11 Reaction vcpt2C12

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

Reaction equation

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

(46)

Reactant

Table 45: Properties of each reactant.

Table 43. Troperties	or cacir	cactant.
Id	Name	SBO
C12AcylCarMAT		

Table 46: Properties of each modifier.

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

Id	Name	SBO
C10AcylCoAMAT		
C8AcylCoAMAT		
C6AcylCoAMAT		
C4AcylCoAMAT		
CarMAT		

Table 47: Properties of each product.

Id	Name	SBO
C12AcylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

```
\begin{split} \nu_{11} &= \text{CPT2} \left( \text{sfcpt2C12}, \text{Vcpt2}, \text{Kmcpt2C12AcylCarMAT}, \text{Kmcpt2C16AcylCarMAT}, \\ \text{Kmcpt2C14AcylCarMAT}, \text{Kmcpt2C10AcylCarMAT}, \text{Kmcpt2C8AcylCarMAT}, \\ \text{Kmcpt2C6AcylCarMAT}, \text{Kmcpt2C4AcylCarMAT}, \text{Kmcpt2CoAMAT}, \\ \text{Kmcpt2C12AcylCoAMAT}, \text{Kmcpt2C16AcylCoAMAT}, \text{Kmcpt2C14AcylCoAMAT}, \\ \text{Kmcpt2C10AcylCoAMAT}, \text{Kmcpt2C8AcylCoAMAT}, \text{Kmcpt2C6AcylCoAMAT}, \\ \text{Kmcpt2C4AcylCoAMAT}, \text{Kmcpt2CarMAT}, \text{Keqcpt2}, [\text{C12AcylCarMAT}], \\ \text{[C16AcylCarMAT]}, [\text{C14AcylCarMAT}], [\text{C10AcylCarMAT}], [\text{C8AcylCarMAT}], \\ \text{[C6AcylCarMAT]}, [\text{C4AcylCarMAT}], [\text{C10AcylCoAMAT}], [\text{C12AcylCoAMAT}], \\ \text{[C16AcylCoAMAT]}, [\text{C14AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C3CarMAT}], \\ \text{[C6AcylCoAMAT]}, [\text{C4AcylCoAMAT}], [\text{C4AcylCoAMAT}], [\text{C4AcylCoAMAT}], \\ \text{[C47)} \end{split}
```

CPT2 (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Keq, S1, S2, S3, S4, S5, S6, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8)

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

Table 48: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcpt2C12			0.95	dimensionless	

8.12 Reaction vcpt2C10

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

Reaction equation

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

Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
C10AcylCarMAT		

Table 50: Properties of each modifier.

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

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

Table 51: Properties of each product.

Id	Name	SBO
C10AcylCoAMAT		

Kinetic Law

```
v_{12} = \text{CPT2} \left( \text{sfcpt2C10}, \text{Vcpt2}, \text{Kmcpt2C10AcylCarMAT}, \text{Kmcpt2C16AcylCarMAT}, \text{Kmcpt2C14AcylCarMAT}, \text{Kmcpt2C12AcylCarMAT}, \text{Kmcpt2C6AcylCarMAT}, \text{Kmcpt2C6AcylCarMAT}, \text{Kmcpt2C6AcylCarMAT}, \text{Kmcpt2C0AMAT}, \text{Kmcpt2C10AcylCoAMAT}, \text{Kmcpt2C16AcylCoAMAT}, \text{Kmcpt2C14AcylCoAMAT}, \text{Kmcpt2C12AcylCoAMAT}, \text{Kmcpt2C6AcylCoAMAT}, \text{Kmcpt2C6AcylCoAMAT}, \text{Kmcpt2C6AcylCoAMAT}, \text{Kmcpt2C4AcylCoAMAT}, \text{Kmcpt2CarMAT}, \text{Keqcpt2}, \text{[C10AcylCarMAT]}, \text{[C16AcylCarMAT]}, \text{[C16AcylCarMAT]}, \text{[C14AcylCarMAT]}, \text{[C12AcylCarMAT]}, \text{[C10AcylCarMAT]}, \text{[C16AcylCoAMAT]}, \text{[C16AcylCoAMAT]}, \text{[C14AcylCoAMAT]}, \text{[C12AcylCoAMAT]}, \text{[C8AcylCoAMAT]}, \text{[C16AcylCoAMAT]}, \text{
```

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

Table 52: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcpt2C10			0.95	dimensionless	

8.13 Reaction vcpt2C8

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

Reaction equation

Reactant

Table 53: Properties of each reactant.

Id	Name	SBO
C8AcylCarMAT		

Table 54: Properties of each modifier.

Id	Name	SBO
C16AcylCarMAT		
C14AcylCarMAT		
C12AcylCarMAT		
C10AcylCarMAT		
C6AcylCarMAT		
C4AcylCarMAT		
CoAMAT		

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

Table 55: Properties of each product.

Id	Name	SBO
C8AcylCoAMAT		

Kinetic Law

 $v_{13} = \text{CPT2} \left(\text{sfcpt2C8}, \text{Vcpt2}, \text{Kmcpt2C8AcylCarMAT}, \text{Kmcpt2C16AcylCarMAT}, \\ \text{Kmcpt2C14AcylCarMAT}, \text{Kmcpt2C12AcylCarMAT}, \text{Kmcpt2C10AcylCarMAT}, \\ \text{Kmcpt2C6AcylCarMAT}, \text{Kmcpt2C4AcylCarMAT}, \text{Kmcpt2CoAMAT}, \\ \text{Kmcpt2C8AcylCoAMAT}, \text{Kmcpt2C16AcylCoAMAT}, \text{Kmcpt2C14AcylCoAMAT}, \\ \text{Kmcpt2C12AcylCoAMAT}, \text{Kmcpt2C10AcylCoAMAT}, \text{Kmcpt2C6AcylCoAMAT}, \\ \text{Kmcpt2C4AcylCoAMAT}, \text{Kmcpt2CarMAT}, \text{Keqcpt2}, [\text{C8AcylCarMAT}], \\ [\text{C16AcylCarMAT}], [\text{C14AcylCarMAT}], [\text{C12AcylCarMAT}], [\text{C10AcylCarMAT}], \\ [\text{C6AcylCarMAT}], [\text{C4AcylCarMAT}], [\text{C12AcylCoAMAT}], [\text{C10AcylCoAMAT}], \\ [\text{C16AcylCoAMAT}], [\text{C14AcylCoAMAT}], [\text{C12AcylCoAMAT}], [\text{C10AcylCoAMAT}], \\ [\text{C6AcylCoAMAT}], [\text{C4AcylCoAMAT}], [\text{C4AcylCoAMAT}], [\text{C33}) \\ (53)$

CPT2 (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Keq, S1, S2, S3, S4, S5, S6, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8)

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

Table 56: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcpt2C8			0.35	dimensionless	$ \mathcal{L} $

8.14 Reaction vcpt2C6

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

Reaction equation

Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
C6AcylCarMAT		

Modifiers

Table 58: Properties of each modifier.

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

Product

Table 59: Properties of each product.

Id	Name	SBO
C6AcylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

```
v_{14} = \text{CPT2} \left( \text{sfcpt2C6}, \text{Vcpt2}, \text{Kmcpt2C6AcylCarMAT}, \text{Kmcpt2C16AcylCarMAT}, \\ \text{Kmcpt2C14AcylCarMAT}, \text{Kmcpt2C12AcylCarMAT}, \text{Kmcpt2C10AcylCarMAT}, \\ \text{Kmcpt2C8AcylCarMAT}, \text{Kmcpt2C4AcylCarMAT}, \text{Kmcpt2CoAMAT}, \\ \text{Kmcpt2C6AcylCoAMAT}, \text{Kmcpt2C16AcylCoAMAT}, \text{Kmcpt2C14AcylCoAMAT}, \\ \text{Kmcpt2C12AcylCoAMAT}, \text{Kmcpt2C10AcylCoAMAT}, \text{Kmcpt2C8AcylCoAMAT}, \\ \text{Kmcpt2C4AcylCoAMAT}, \text{Kmcpt2CarMAT}, \text{Keqcpt2}, [\text{C6AcylCarMAT}], [\text{C16AcylCarMAT}], [\text{C14AcylCarMAT}], [\text{C12AcylCarMAT}], [\text{C10AcylCarMAT}], [\text{C8AcylCarMAT}], [\text{C4AcylCoAMAT}], [\text{C16AcylCoAMAT}], [\text{C14AcylCoAMAT}], [\text{C12AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C16AcylCoAMAT}], [\text{C16AcylCoAMAT}]
```

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

Table 60: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcpt2C6			0.15	dimensionless	

8.15 Reaction vcpt2C4

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

Reaction equation

(58)

Reactant

Table 61: Properties of each reactant.

Id	Name	SBO
C4AcylCarMAT		

Table 62: Properties of each modifier.

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

Table 63: Properties of each product.

•	Id	Name	
	C4AcylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

```
v_{15} = \text{CPT2} \left( \text{sfcpt2C4}, \text{Vcpt2}, \text{Kmcpt2C4AcylCarMAT}, \text{Kmcpt2C16AcylCarMAT}, \\ \text{Kmcpt2C14AcylCarMAT}, \text{Kmcpt2C12AcylCarMAT}, \text{Kmcpt2C10AcylCarMAT}, \\ \text{Kmcpt2C8AcylCarMAT}, \text{Kmcpt2C6AcylCarMAT}, \text{Kmcpt2CoAMAT}, \\ \text{Kmcpt2C4AcylCoAMAT}, \text{Kmcpt2C16AcylCoAMAT}, \text{Kmcpt2C14AcylCoAMAT}, \\ \text{Kmcpt2C12AcylCoAMAT}, \text{Kmcpt2C10AcylCoAMAT}, \text{Kmcpt2C8AcylCoAMAT}, \\ \text{Kmcpt2C6AcylCoAMAT}, \text{Kmcpt2CarMAT}, \text{Keqcpt2}, [\text{C4AcylCarMAT}], \\ [\text{C16AcylCarMAT}], [\text{C14AcylCarMAT}], [\text{C12AcylCarMAT}], [\text{C10AcylCarMAT}], \\ [\text{C8AcylCarMAT}], [\text{C6AcylCarMAT}], [\text{C16AcylCoAMAT}], [\text{C10AcylCoAMAT}], \\ [\text{C16AcylCoAMAT}], [\text{C14AcylCoAMAT}], [\text{C12AcylCoAMAT}], [\text{C10AcylCoAMAT}], \\ [\text{C8AcylCoAMAT}], [\text{C6AcylCoAMAT}], [\text{C16AcylCoAMAT}], [\text{C37MAT}]) \\ [\text{C8AcylCoAMAT}], [\text{C6AcylCoAMAT}], [\text{C37MAT}]) \\ [\text{C6AcylCoAMAT}], [\text{C37MAT}], [\text{C37MAT}], [\text{C37MAT}]) \\ [\text{C37MAT}], [\text{C37MAT}], [\text{C37MAT}], [\text{C37MAT}], [\text{C37MAT}], [\text{C37MAT}]) \\ [\text{C37MAT}], [\text{C37MAT}], [\text{C37MAT}], [\text{C37MAT}], [\text{C37MAT}], [\text{C37MAT}]) \\ [\text{C37MAT}], [\text{C37MAT}], [\text{C37MAT}], [\text{C37MAT}], [\text{C37MAT}], [\text{C37MAT}], [\text{C37MAT}]) \\ [\text{C37MAT}], [
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CPT2 (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Keq, S1, S2, S3, S4, S5, S6, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8)

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

Table 64: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcpt2C4			0.01	dimensionless	\square

8.16 Reaction vvlcadC16

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

Reaction equation

C16AcylCoAMAT, C12AcylCoAMAT, FADtMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C

(61)

Reactant

Table 65: Properties of each reactant.

Id	Name	SBO
C16AcylCoAMAT		

Modifiers

Table 66: Properties of each modifier.

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

Products

Table 67: Properties of each product.

Id	Name	SBO
C16EnoylCoAMAT		
FADHMAT		

Kinetic Law

Derived unit contains undeclared units

 $v_{16} = VLCAD (sfvlcadC16, Vvlcad, KmvlcadC16AcylCoAMAT, KmvlcadC14AcylCoAMAT, KmvlcadC12AcylCoAMAT, KmvlcadFAD, KmvlcadC16EnoylCoAMAT, KmvlcadC14EnoylCoAMAT, KmvlcadC12EnoylCoAMAT, KmvlcadFADH, Keqvlcad, [C16AcylCoAMAT], [C14AcylCoAMAT], [C12AcylCoAMAT], [FADtMAT], [C16EnoylCoAMAT], [C14EnoylCoAMAT], [C12EnoylCoAMAT], [FADHMAT]) <math display="block">(62)$

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

$$P4) = \frac{sf \cdot V \cdot \left(\frac{S1 \cdot (S4 - P4)}{Kms1 \cdot Kms4} - \frac{P1 \cdot P4}{Kms1 \cdot Kms4 \cdot Keq}\right)}{\left(1 + \frac{S1}{Kms1} + \frac{P1}{Kmp1} + \frac{S2}{Kms2} + \frac{P2}{Kmp2} + \frac{S3}{Kms3} + \frac{P3}{Kmp3}\right) \cdot \left(1 + \frac{S4 - P4}{Kms4} + \frac{P4}{Kmp4}\right)}$$
(63)

Table 68: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfvlcadC16			1.0	dimensionless	Ø

8.17 Reaction vvlcadC14

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

Reaction equation

Reactant

Table 69: Properties of each reactant.

Id	Name	SBO
C14AcylCoAMAT		

Table 70: Properties of each modifier.

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

Table 71: Properties of each product.

Id	Name	SBO
C14EnoylCoAMAT FADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$\label{eq:v17} \begin{split} \nu_{17} &= \text{VLCAD} \left(\text{sfvlcadC14}, \text{Vvlcad}, \text{KmvlcadC14AcylCoAMAT}, \text{KmvlcadC16AcylCoAMAT}, \\ & \text{KmvlcadC12AcylCoAMAT}, \text{KmvlcadFAD}, \text{KmvlcadC14EnoylCoAMAT}, \\ & \text{KmvlcadC16EnoylCoAMAT}, \text{KmvlcadC12EnoylCoAMAT}, \text{KmvlcadFADH}, \text{Keqvlcad}, \\ & \text{[C14AcylCoAMAT]}, \text{[C16AcylCoAMAT]}, \text{[C12AcylCoAMAT]}, \text{[FADtMAT]}, \\ & \text{[C14EnoylCoAMAT]}, \text{[C16EnoylCoAMAT]}, \text{[C12EnoylCoAMAT]}, \text{[FADHMAT]}) \end{split}$$

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

$$P4) = \frac{sf \cdot V \cdot \left(\frac{S1 \cdot (S4 - P4)}{Kms1 \cdot Kms4} - \frac{P1 \cdot P4}{Kms1 \cdot Kms4 \cdot Keq}\right)}{\left(1 + \frac{S1}{Kms1} + \frac{P1}{Kmp1} + \frac{S2}{Kms2} + \frac{P2}{Kmp2} + \frac{S3}{Kms3} + \frac{P3}{Kmp3}\right) \cdot \left(1 + \frac{S4 - P4}{Kms4} + \frac{P4}{Kmp4}\right)}$$
(66)

Table 72: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfvlcadC14			0.42	dimensionless	

8.18 Reaction vvlcadC12

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

Reaction equation

C12AcylCoAMAT, C14AcylCoAMAT, FADtMAT, C16EnoylCoAMAT, C14EnoylCoAMAT, C
(67)

Reactant

Table 73: Properties of each reactant.

Id	Name	SBO
C12AcylCoAMAT		

Table 74: Properties of each modifier.

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

Table 75: Properties of each product

Tuble 75: Troperties	or each p	oroudet.
Id	Name	SBO
C12EnoylCoAMAT FADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$\label{eq:v18} \begin{split} \nu_{18} &= \text{VLCAD} \left(\text{sfvlcadC12}, \text{Vvlcad}, \text{KmvlcadC12AcylCoAMAT}, \text{KmvlcadC16AcylCoAMAT}, \\ &\quad \text{KmvlcadC14AcylCoAMAT}, \text{KmvlcadFAD}, \text{KmvlcadC12EnoylCoAMAT}, \\ &\quad \text{KmvlcadC16EnoylCoAMAT}, \text{KmvlcadC14EnoylCoAMAT}, \text{KmvlcadFADH}, \text{Keqvlcad}, \\ &\quad \text{[C12AcylCoAMAT]}, \text{[C16AcylCoAMAT]}, \text{[C14AcylCoAMAT]}, \text{[FADtMAT]}, \\ &\quad \text{[C12EnoylCoAMAT]}, \text{[C16EnoylCoAMAT]}, \text{[C14EnoylCoAMAT]}, \text{[FADHMAT]}) \end{split}$$

VLCAD (sf, V, Kms1, Kms2, Kms3, Kms4, Kmp1, Kmp2, Kmp3, Kmp4, Keq, S1, S2, S3, S4, P1, P2, P3.

$$P4) = \frac{sf \cdot V \cdot \left(\frac{S1 \cdot (S4 - P4)}{Kms1 \cdot Kms4} - \frac{P1 \cdot P4}{Kms1 \cdot Kms4 \cdot Keq}\right)}{\left(1 + \frac{S1}{Kms1} + \frac{P1}{Kmp1} + \frac{S2}{Kms2} + \frac{P2}{Kmp2} + \frac{S3}{Kms3} + \frac{P3}{Kmp3}\right) \cdot \left(1 + \frac{S4 - P4}{Kms4} + \frac{P4}{Kmp4}\right)}$$
(69)

Table 76: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfvlcadC12			0.11	dimensionless	

8.19 Reaction vlcadC16

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

Reaction equation

C16AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, FADtMAT, C14

Reactant

Table 77: Properties of each reactant.

Id	Name	SBO
C16AcylCoAMAT		

Modifiers

Table 78: Properties of each modifier.

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

Products

Table 79: Properties of each product.

Id	Name	SBO
C16EnoylCoAMAT		
FADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$\label{eq:v19} \begin{split} \nu_{19} &= LCAD \left(sflcadC16, Vlcad, KmlcadC16AcylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC10AcylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC12EnoylCoAMAT, KmlcadC10EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, Keqlcad, [C16AcylCoAMAT], [C14AcylCoAMAT], [C12AcylCoAMAT], [C10AcylCoAMAT], [C8AcylCoAMAT], [FADtMAT], [C16EnoylCoAMAT], [C14EnoylCoAMAT], [C12EnoylCoAMAT], [C10EnoylCoAMAT], [C8EnoylCoAMAT], [C171) \\ \end{split}$$

LCAD (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Keq, S1, S2, S3, S4, S5, S6, P1, P2, P3, P4, P5, P6) (72)

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

Table 80: Properties of each parameter.

Id	Name	SBO	Value		Constant
sflcadC16			0.9	dimensionless	\overline{Z}

8.20 Reaction vlcadC14

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

Reaction equation

C14AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, FADtMAT, C16

(73)

Reactant

Table 81: Properties of each reactant.

Id	Name	SBO
C14AcylCoAMAT		

Modifiers

Table 82: Properties of each modifier.

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

Products

Table 83: Properties of each product.

Id	Name	SBO
C14EnoylCoAMAT FADHMAT		

Kinetic Law

 $v_{20} = LCAD \left(sflcadC14, Vlcad, KmlcadC14AcylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC10AcylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC12EnoylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC12EnoylCoAMAT, KmlcadC10EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, Keqlcad, [C14AcylCoAMAT], [C16AcylCoAMAT], [C12AcylCoAMAT], [C10AcylCoAMAT], [C8AcylCoAMAT], [FADtMAT], [C14EnoylCoAMAT], [C16EnoylCoAMAT], [C12EnoylCoAMAT], [C10EnoylCoAMAT], [C8EnoylCoAMAT], [C174) [C174] [C$

LCAD (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Keq, S1, S2, S3, S4, S5, S6, P1, P2, P3, P4, P5, P6) (75)

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

Table 84: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sflcadC14			1.0	dimensionless	

8.21 Reaction vlcadC12

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

Reaction equation

Reactant

Table 86: Properties of each modifier.

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

Table 87: Properties of each product.

Id	Name	SBO
C12EnoylCoAMAT		
FADHMAT		

Kinetic Law

 $v_{21} = LCAD \left(sflcadC12, Vlcad, KmlcadC12AcylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC10AcylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC12EnoylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC10EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, Keqlcad, [C12AcylCoAMAT], [C16AcylCoAMAT], [C14AcylCoAMAT], [C10AcylCoAMAT], [C8AcylCoAMAT], [FADtMAT], [C14EnoylCoAMAT], [C16EnoylCoAMAT], [C14EnoylCoAMAT], [C10EnoylCoAMAT], [C8DtMAT], [C77) [C77) [C77] [C77]$

LCAD (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Keq, S1, S2, S3, S4, S5, S6, P1, P2, P3, P4, P5, P6) (78)

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

Table 88: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sflcadC12			0.9	dimensionless	

8.22 Reaction vlcadC10

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

Reaction equation

C10AcylCoAMAT, C14AcylCoAMAT, C12AcylCoAMAT, C8AcylCoAMAT, FADtMAT, C16
(79)

Reactant

Table 90: Properties of each modifier.

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

Table 91: Properties of each product.

Name	SBO
	Name

Kinetic Law

 $v_{22} = LCAD \left(sflcadC10, Vlcad, KmlcadC10AcylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC8AcylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC10EnoylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC12EnoylCoAMAT, KmlcadC8EnoylCoAMAT, KmlcadFADH, Keqlcad, [C10AcylCoAMAT], [C16AcylCoAMAT], [C14AcylCoAMAT], [C12AcylCoAMAT], [C8AcylCoAMAT], [FADtMAT], [C10EnoylCoAMAT], [C16EnoylCoAMAT], [C14EnoylCoAMAT], [C12EnoylCoAMAT], [C8EnoylCoAMAT], [C8DHMAT]) (80)$

LCAD (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Keq, S1, S2, S3, S4, S5, S6, P1, P2, P3, P4, P5, P6) (81)

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

Table 92: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sflcadC10			0.75	dimensionless	

8.23 Reaction vlcadC8

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

Reaction equation

Reactant

Table 93: Properties of each reactant.

Id	Name	SBO
C8AcylCoAMAT		

Table 94: Properties of each modifier.

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

Table 95: Properties of each product.

Id	Name	SBO
C8EnoylCoAMAT FADHMAT		

Kinetic Law

 $v_{23} = LCAD (sflcadC8, Vlcad, KmlcadC8AcylCoAMAT, KmlcadC16AcylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC12AcylCoAMAT, KmlcadC10AcylCoAMAT, KmlcadC14AcylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC16EnoylCoAMAT, KmlcadC14EnoylCoAMAT, KmlcadC12EnoylCoAMAT, KmlcadC10EnoylCoAMAT, KmlcadFADH, Keqlcad, [C8AcylCoAMAT], [C16AcylCoAMAT], [C14AcylCoAMAT], [C12AcylCoAMAT], [C10AcylCoAMAT], [FADtMAT], [C8EnoylCoAMAT], [C16EnoylCoAMAT], [C16EnoylCoAMAT], [C16EnoylCoAMAT], [C10EnoylCoAMAT], [C10EnoylCoAMAT], [C33) [C10EnoylCoAMAT], [C33) [C33] [C33]$

LCAD (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Keq, S1, S2, S3, S4, S5, S6, P1, P2, P3, P4, P5, P6) (84)

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

Table 96: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sflcadC8			0.4	dimensionless	

8.24 Reaction vmcadC12

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

Reaction equation

C12AcylCoAMAT, C8AcylCoAMAT, C6AcylCoAMAT, C4AcylCoAMAT, FADtMAT, C10Er

Reactant

Table 98: Properties of each modifier.

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

Table 99: Properties of each product.

Name	SBO
	Name

Kinetic Law

$$\begin{split} \nu_{24} &= \text{MCAD} \left(\text{sfmcadC12}, \text{Vmcad}, \text{KmmcadC12AcylCoAMAT}, \text{KmmcadC10AcylCoAMAT}, \\ &\quad \text{KmmcadC8AcylCoAMAT}, \text{KmmcadC6AcylCoAMAT}, \text{KmmcadC4AcylCoAMAT}, \\ &\quad \text{KmmcadFAD}, \text{KmmcadC12EnoylCoAMAT}, \text{KmmcadC10EnoylCoAMAT}, \\ &\quad \text{KmmcadC8EnoylCoAMAT}, \text{KmmcadC6EnoylCoAMAT}, \text{KmmcadC4EnoylCoAMAT}, \\ &\quad \text{KmmcadFADH}, \text{Keqmcad}, [\text{C12AcylCoAMAT}], [\text{C10AcylCoAMAT}], \\ &\quad \text{[C8AcylCoAMAT]}, [\text{C6AcylCoAMAT}], [\text{C4AcylCoAMAT}], [\text{FADtMAT}], \\ &\quad \text{[C12EnoylCoAMAT]}, [\text{C10EnoylCoAMAT}], [\text{C8EnoylCoAMAT}], [\text{C6EnoylCoAMAT}], \\ &\quad \text{[C4EnoylCoAMAT]}, [\text{FADHMAT}]) \\ &\quad \text{(86)} \end{split}$$

MCAD (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Keq, S1, S2, S3, S4, S5, S6, P1, P2, P3, P4, P5, P6) (87)

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

Table 100: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmcadC12			0.38	dimensionless	

8.25 Reaction vmcadC10

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

Reaction equation

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

Reactant

Table 101: Properties of each reactant.

Id	Name	SBO
C10AcylCoAMAT		

Table 102: Properties of each modifier.

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

Table 103: Properties of each product.

Id	Name	SBO
C10EnoylCoAMAT		
FADHMAT		

Kinetic Law

$$\begin{split} \nu_{25} &= \text{MCAD} \left(\text{sfmcadC10}, \text{Vmcad}, \text{KmmcadC10AcylCoAMAT}, \text{KmmcadC12AcylCoAMAT}, \\ &\quad \text{KmmcadC8AcylCoAMAT}, \text{KmmcadC6AcylCoAMAT}, \text{KmmcadC4AcylCoAMAT}, \\ &\quad \text{KmmcadFAD}, \text{KmmcadC10EnoylCoAMAT}, \text{KmmcadC12EnoylCoAMAT}, \\ &\quad \text{KmmcadC8EnoylCoAMAT}, \text{KmmcadC6EnoylCoAMAT}, \text{KmmcadC4EnoylCoAMAT}, \\ &\quad \text{KmmcadFADH}, \text{Keqmcad}, [\text{C10AcylCoAMAT}], [\text{C12AcylCoAMAT}], [\text{C3AcylCoAMAT}], [\text{C4AcylCoAMAT}], [\text{C4AcylCoAMAT}], [\text{C4DenoylCoAMAT}], [\text{C10EnoylCoAMAT}], [\text{C12EnoylCoAMAT}], [\text{C3EnoylCoAMAT}], [\text{C4EnoylCoAMAT}], [\text{C4EnoylCoAMAT}$$

MCAD (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Keq, S1, S2, S3, S4, S5, S6, P1, P2, P3, P4, P5, P6) (90)

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

Table 104: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmcadC10			0.8	dimensionless	

8.26 Reaction vmcadC8

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

Reaction equation

Reactant

Table 105: Properties of each reactant.

Id	Name	SBO
C8AcylCoAMAT		

Table 106: Properties of each modifier.

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

Table 107: Properties of each product.

Id	Name	SBO
C8EnoylCoAMAT FADHMAT		

Kinetic Law

 $v_{26} = MCAD (sfmcadC8, Vmcad, KmmcadC8AcylCoAMAT, KmmcadC12AcylCoAMAT, KmmcadC10AcylCoAMAT, KmmcadC6AcylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadC10EnoylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC10EnoylCoAMAT, KmmcadC6EnoylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadC4EnoylCoAMAT], [C12AcylCoAMAT], [C10AcylCoAMAT], [C6AcylCoAMAT], [C4AcylCoAMAT], [FADtMAT], [C8EnoylCoAMAT], [C12EnoylCoAMAT], [C10EnoylCoAMAT], [C6EnoylCoAMAT], [C4EnoylCoAMAT], [FADtMAT]) (92)$

MCAD (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Keq, S1, S2, S3, S4, S5, S6, P1, P2, P3, P4, P5, P6) (93)

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

Table 108: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmcadC8			0.87	dimensionless	

8.27 Reaction vmcadC6

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

Reaction equation

Reactant

Table 109: Properties of each reactant.

Id	Name	SBO
C6AcylCoAMAT		

Table 110: Properties of each modifier.

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

Table 111: Properties of each product.

Name	SBO
	Name

Kinetic Law

 $v_{27} = MCAD \, (sfmcadC6, Vmcad, KmmcadC6AcylCoAMAT, KmmcadC12AcylCoAMAT, KmmcadC10AcylCoAMAT, KmmcadC8AcylCoAMAT, KmmcadC4AcylCoAMAT, KmmcadC10EnoylCoAMAT, KmmcadC6EnoylCoAMAT, KmmcadC12EnoylCoAMAT, KmmcadC10EnoylCoAMAT, KmmcadC8EnoylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadC4EnoylCoAMAT, KmmcadFADH, Keqmcad, [C6AcylCoAMAT], [C12AcylCoAMAT], [C10AcylCoAMAT], [C8AcylCoAMAT], [C4AcylCoAMAT], [FADtMAT], [C6EnoylCoAMAT], [C12EnoylCoAMAT], [C10EnoylCoAMAT], [C8EnoylCoAMAT], [C4EnoylCoAMAT], [C4EnoylCo$

MCAD (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Keq, S1, S2, S3, S4, S5, S6, P1, P2, P3, P4, P5, P6) (96)

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

Table 112: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmcadC6			1.0	dimensionless	

8.28 Reaction vmcadC4

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

Reaction equation

Reactant

Table 113: Properties of each reactant.

Id	Name	SBO
C4AcylCoAMAT		

Table 114: Properties of each modifier.

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

Table 115: Properties of each product.

Id	Name	SBO
C4EnoylCoAMAT		
FADHMAT		

Kinetic Law

$$\begin{split} v_{28} &= \text{MCAD} \left(\text{sfmcadC4}, \text{Vmcad}, \text{KmmcadC4AcylCoAMAT}, \text{KmmcadC12AcylCoAMAT}, \\ & \text{KmmcadC10AcylCoAMAT}, \text{KmmcadC8AcylCoAMAT}, \text{KmmcadC6AcylCoAMAT}, \\ & \text{KmmcadFAD}, \text{KmmcadC4EnoylCoAMAT}, \text{KmmcadC12EnoylCoAMAT}, \\ & \text{KmmcadC10EnoylCoAMAT}, \text{KmmcadC8EnoylCoAMAT}, \text{KmmcadC6EnoylCoAMAT}, \\ & \text{KmmcadFADH}, \text{Keqmcad}, [\text{C4AcylCoAMAT}], [\text{C12AcylCoAMAT}], \\ & [\text{C10AcylCoAMAT}], [\text{C8AcylCoAMAT}], [\text{C6AcylCoAMAT}], [\text{FADtMAT}], \\ & [\text{C4EnoylCoAMAT}], [\text{C12EnoylCoAMAT}], [\text{C10EnoylCoAMAT}], [\text{C8EnoylCoAMAT}], \\ & [\text{C6EnoylCoAMAT}], [\text{FADHMAT}]) \\ & (98) \end{split}$$

MCAD (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Keq, S1, S2, S3, S4, S5, S6, P1, P2, P3, P4, P5, P6) (99)

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

Table 116: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmcadC4			0.12	dimensionless	

8.29 Reaction vscadC6

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

Reaction equation

Reactant

Table 117: Properties of each reactant.

Id	Name	SBO
C6AcylCoAMAT		

Table 118: Properties of each modifier.

Id	Name	SBO
C4AcylCoAMAT		
FADtMAT		
C4EnoylCoAMAT		
C6AcylCoAMAT		
C4AcylCoAMAT		
FADtMAT		
C6EnoylCoAMAT		
C4EnoylCoAMAT		
FADHMAT		

Products

Table 119: Properties of each product.

Id	Name	SBO
C6EnoylCoAMAT		
FADHMAT		

Kinetic Law

Derived unit contains undeclared units

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

$$= \frac{\text{sf} \cdot \text{V} \cdot \left(\frac{\text{S1} \cdot (\text{S3} - \text{P3})}{\text{Kms1} \cdot \text{Kms3}} - \frac{\text{P1} \cdot \text{P3}}{\text{Kms1} \cdot \text{Kms3} \cdot \text{Keq}}\right)}{\left(1 + \frac{\text{S1}}{\text{Kms1}} + \frac{\text{P1}}{\text{Kmp1}} + \frac{\text{S2}}{\text{Kms2}} + \frac{\text{P2}}{\text{Kmp2}}\right) \cdot \left(1 + \frac{\text{S3} - \text{P3}}{\text{Kms3}} + \frac{\text{P3}}{\text{Kmp3}}\right)}$$
(102)

Table 120: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfscadC6			0.3	dimensionless	

8.30 Reaction vscadC4

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

Reaction equation

C4AcylCoAMAT, FADtMAT, C6EnoylCoAMAT, C4AcylCoAMAT, C6AcylCoAMAT, FADtM
(103)

Reactant

Table 121: Properties of each reactant.

Id	Name	SBO
C4AcylCoAMAT		

Modifiers

Table 122: Properties of each modifier.

Id	Name	SBO
C6AcylCoAMAT		
FADtMAT		
C6EnoylCoAMAT		
C4AcylCoAMAT		
C6AcylCoAMAT		
FADtMAT		
C4EnoylCoAMAT		
C6EnoylCoAMAT		
FADHMAT		

Products

Table 123: Properties of each product.

Id	Name	SBO
C4EnoylCoAMAT FADHMAT		

Kinetic Law

Derived unit contains undeclared units

 $v_{30} = SCAD$ (sfscadC4, Vscad, KmscadC4AcylCoAMAT, KmscadC6AcylCoAMAT, KmscadFAD, KmscadC4EnoylCoAMAT, KmscadC6EnoylCoAMAT, KmscadFADH, Keqscad, [C4AcylCoAMAT], [C6AcylCoAMAT], [FADtMAT], [C4EnoylCoAMAT], [C6EnoylCoAMAT], [FADHMAT]) (104)

$$= \frac{\text{sf} \cdot \text{V} \cdot \left(\frac{\text{S1} \cdot (\text{S3} - \text{P3})}{\text{Kms1} \cdot \text{Kms3}} - \frac{\text{P1} \cdot \text{P3}}{\text{Kms1} \cdot \text{Kms3} \cdot \text{Keq}}\right)}{\left(1 + \frac{\text{S1}}{\text{Kms1}} + \frac{\text{P1}}{\text{Kmp1}} + \frac{\text{S2}}{\text{Kms2}} + \frac{\text{P2}}{\text{Kmp2}}\right) \cdot \left(1 + \frac{\text{S3} - \text{P3}}{\text{Kms3}} + \frac{\text{P3}}{\text{Kmp3}}\right)}$$
(105)

Table 124: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfscadC4			1.0	dimensionless	

8.31 Reaction vcrotC16

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

Reaction equation

Reactant

Table 125: Properties of each reactant.

Id	Name	SBO
C16EnoylCoAMAT		

Table 126: Properties of each modifier.

Table 126: Properties of e	ach mod	ifier.
Id	Name	SBO
C14EnoylCoAMAT		
C12EnoylCoAMAT		
C10EnoylCoAMAT		
C8EnoylCoAMAT		
C6EnoylCoAMAT		
C4EnoylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
${\tt C8HydroxyacylCoAMAT}$		
${\tt C6HydroxyacylCoAMAT}$		
${\tt C4HydroxyacylCoAMAT}$		
${\tt C4AcetoacylCoAMAT}$		
C16EnoylCoAMAT		
C14EnoylCoAMAT		
C12EnoylCoAMAT		
C10EnoylCoAMAT		
C8EnoylCoAMAT		
C6EnoylCoAMAT		
C4EnoylCoAMAT		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
C4HydroxyacylCoAMAT		
C4AcetoacylCoAMAT		

Product

Table 127: Properties of each product.

Id Name SBC		
C16HydroxyacylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

v31 = CROT (sfcrotC16, Vcrot, KmcrotC16EnoylCoAMAT, KmcrotC14EnoylCoAMAT, KmcrotC12EnoylCoAMAT, KmcrotC10EnoylCoAMAT, KmcrotC8EnoylCoAMAT, KmcrotC4EnoylCoAMAT, KmcrotC4EnoylCoAMAT, KmcrotC16HydroxyacylCoAMAT, KmcrotC14HydroxyacylCoAMAT, KmcrotC12HydroxyacylCoAMAT, KmcrotC10HydroxyacylCoAMAT, KmcrotC8HydroxyacylCoAMAT, KmcrotC6HydroxyacylCoAMAT, KmcrotC6HydroxyacylCoAMAT, KmcrotC4HydroxyacylCoAMAT, KicrotC4AcetoacylCoA, Keqcrot, [C16EnoylCoAMAT], [C14EnoylCoAMAT], [C12EnoylCoAMAT], [C10EnoylCoAMAT], [C8EnoylCoAMAT], [C6EnoylCoAMAT], [C4EnoylCoAMAT], [C16HydroxyacylCoAMAT], [C14HydroxyacylCoAMAT], [C12HydroxyacylCoAMAT], [C4HydroxyacylCoAMAT], [C6HydroxyacylCoAMAT], [C4HydroxyacylCoAMAT], [C4AcetoacylCoAMAT])

CROT (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Ki1, Keq, S1, S2, S3, S4, S5, S6, S7, P1, P2, P3, P4, P5, P6, P7, I1)

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

Table 128: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcrotC16			0.13	dimensionless	

8.32 Reaction vcrotC14

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

Reaction equation

Reactant

Table 129: Properties of each reactant.

Id	Name	SBO
C14EnoylCoAMAT		

Id Name	SBO
---------	-----

Modifiers

Table 130: Properties of each modifier.

Id	Name	SBO
C16EnoylCoAMAT		
C12EnoylCoAMAT		
C10EnoylCoAMAT		
C8EnoylCoAMAT		
C6EnoylCoAMAT		
C4EnoylCoAMAT		
C16HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
${\tt C8HydroxyacylCoAMAT}$		
C6HydroxyacylCoAMAT		
${\tt C4HydroxyacylCoAMAT}$		
C4AcetoacylCoAMAT		
C14EnoylCoAMAT		
C16EnoylCoAMAT		
C12EnoylCoAMAT		
C10EnoylCoAMAT		
C8EnoylCoAMAT		
C6EnoylCoAMAT		
C4EnoylCoAMAT		
C14HydroxyacylCoAMAT		
C16HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
${\tt C6HydroxyacylCoAMAT}$		
${\tt C4HydroxyacylCoAMAT}$		
C4AcetoacylCoAMAT		

Product

Table 131: Properties of each product.

Id	Name	SBO
C14HydroxyacylCoAMAT		

|--|

Kinetic Law

Derived unit contains undeclared units

```
v<sub>32</sub> = CROT (sfcrotC14, Vcrot, KmcrotC14EnoylCoAMAT, KmcrotC16EnoylCoAMAT, KmcrotC12EnoylCoAMAT, KmcrotC10EnoylCoAMAT, KmcrotC8EnoylCoAMAT, KmcrotC4EnoylCoAMAT, KmcrotC4EnoylCoAMAT, KmcrotC14HydroxyacylCoAMAT, KmcrotC16HydroxyacylCoAMAT, KmcrotC12HydroxyacylCoAMAT, KmcrotC10HydroxyacylCoAMAT, KmcrotC8HydroxyacylCoAMAT, KmcrotC6HydroxyacylCoAMAT, KmcrotC4HydroxyacylCoAMAT, KicrotC4AcetoacylCoA, Keqcrot, [C14EnoylCoAMAT], [C16EnoylCoAMAT], [C12EnoylCoAMAT], [C10EnoylCoAMAT], [C8EnoylCoAMAT], [C6EnoylCoAMAT], [C14HydroxyacylCoAMAT], [C16HydroxyacylCoAMAT], [C19HydroxyacylCoAMAT], [C4HydroxyacylCoAMAT], [C4Hydrox
```

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

Table 132: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcrotC14			0.2	dimensionless	Ø

8.33 Reaction vcrotC12

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

Reaction equation

Reactant

Table 133: Properties of each reactant.

Id	Name	
C12EnoylCoAMAT		

Table 134: Properties of each modifier.

Id	Name	SBO
C16EnoylCoAMAT		
C14EnoylCoAMAT		
C10EnoylCoAMAT		
C8EnoylCoAMAT		
C6EnoylCoAMAT		
C4EnoylCoAMAT		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
${\tt C4HydroxyacylCoAMAT}$		
C4AcetoacylCoAMAT		
C12EnoylCoAMAT		
C16EnoylCoAMAT		
C14EnoylCoAMAT		
C10EnoylCoAMAT		
C8EnoylCoAMAT		
C6EnoylCoAMAT		
C4EnoylCoAMAT		
C12HydroxyacylCoAMAT		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
C4HydroxyacylCoAMAT		
C4AcetoacylCoAMAT		

Product

Table 135: Properties of each product.

Id	Name	
C12HydroxyacylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

```
    v<sub>33</sub> = CROT (sfcrotC12, Vcrot, KmcrotC12EnoylCoAMAT, KmcrotC16EnoylCoAMAT, KmcrotC14EnoylCoAMAT, KmcrotC10EnoylCoAMAT, KmcrotC8EnoylCoAMAT, KmcrotC4EnoylCoAMAT, KmcrotC4EnoylCoAMAT, KmcrotC12HydroxyacylCoAMAT, KmcrotC16HydroxyacylCoAMAT, KmcrotC14HydroxyacylCoAMAT, KmcrotC10HydroxyacylCoAMAT, KmcrotC8HydroxyacylCoAMAT, KmcrotC6HydroxyacylCoAMAT, KmcrotC6HydroxyacylCoAMAT, KmcrotC4HydroxyacylCoAMAT, KicrotC4AcetoacylCoA, Keqcrot, [C12EnoylCoAMAT], [C16EnoylCoAMAT], [C14EnoylCoAMAT], [C10EnoylCoAMAT], [C8EnoylCoAMAT], [C6EnoylCoAMAT], [C4EnoylCoAMAT], [C12HydroxyacylCoAMAT], [C16HydroxyacylCoAMAT], [C14HydroxyacylCoAMAT], [C10HydroxyacylCoAMAT], [C8HydroxyacylCoAMAT], [C6HydroxyacylCoAMAT], [C4AcetoacylCoAMAT], [C4HydroxyacylCoAMAT], [C4AcetoacylCoAMAT])
```

CROT (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Ki1, Keq, S1, S2, S3, S4, S5, S6, S7, P1, P2, P3, P4, P5, P6, P7, I1)

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

Table 136: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcrotC12			0.25	dimensionless	

8.34 Reaction vcrotC10

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

Reaction equation

C10EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C8EnoylCoAMAT, C6EnoylCoAMAT, C6E

(115)

Reactant

Table 137: Properties of each reactant.

Id Name SBO

C10EnoylCoAMAT

Table 138: Properties of each modifier.

Id	Name	SBO
C16EnoylCoAMAT		
C14EnoylCoAMAT		
C12EnoylCoAMAT		
C8EnoylCoAMAT		
C6EnoylCoAMAT		
C4EnoylCoAMAT		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
${\tt C8HydroxyacylCoAMAT}$		
${\tt C6HydroxyacylCoAMAT}$		
${\tt C4HydroxyacylCoAMAT}$		
${\tt C4AcetoacylCoAMAT}$		
C10EnoylCoAMAT		
C16EnoylCoAMAT		
C14EnoylCoAMAT		
C12EnoylCoAMAT		
C8EnoylCoAMAT		
C6EnoylCoAMAT		
C4EnoylCoAMAT		
${\tt C10HydroxyacylCoAMAT}$		
C16HydroxyacylCoAMAT		
${\tt C14HydroxyacylCoAMAT}$		
C12HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		

Id	Name	SBO
C6HydroxyacylCoAMAT		
${\tt C4HydroxyacylCoAMAT}$		
C4AcetoacylCoAMAT		

Product

Table 139: Properties of each product.

Id	Name	SBO
C10HydroxyacylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

V34 = CROT (sfcrotC10, Vcrot, KmcrotC10EnoylCoAMAT, KmcrotC16EnoylCoAMAT, KmcrotC14EnoylCoAMAT, KmcrotC12EnoylCoAMAT, KmcrotC8EnoylCoAMAT, KmcrotC4EnoylCoAMAT, KmcrotC10HydroxyacylCoAMAT, KmcrotC16HydroxyacylCoAMAT, KmcrotC16HydroxyacylCoAMAT, KmcrotC12HydroxyacylCoAMAT, KmcrotC14HydroxyacylCoAMAT, KmcrotC6HydroxyacylCoAMAT, KmcrotC8HydroxyacylCoAMAT, KmcrotC6HydroxyacylCoAMAT, KmcrotC4HydroxyacylCoAMAT, KicrotC4AcetoacylCoA, Keqcrot, [C10EnoylCoAMAT], [C16EnoylCoAMAT], [C14EnoylCoAMAT], [C12EnoylCoAMAT], [C8EnoylCoAMAT], [C6EnoylCoAMAT], [C4EnoylCoAMAT], [C10HydroxyacylCoAMAT], [C16HydroxyacylCoAMAT], [C14HydroxyacylCoAMAT], [C12HydroxyacylCoAMAT], [C8HydroxyacylCoAMAT], [C6HydroxyacylCoAMAT], [C4AcetoacylCoAMAT], [C4HydroxyacylCoAMAT], [C4AcetoacylCoAMAT])

CROT (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Ki1, Keq, S1, S2, S3, S4, S5, S6, S7, P1, P2, P3, P4, P5, P6, P7, I1)

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

Table 140: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcrotC10			0.33	dimensionless	

8.35 Reaction vcrotC8

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

Reaction equation

C8EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C6EnoylCoAMAT, C118)

Reactant

Table 141: Properties of each reactant.

Id	Name	SBO
C8EnoylCoAMAT		

Table 142: Properties of each modifier.

Id	Name	SBO
C16EnoylCoAMAT		
C14EnoylCoAMAT		
C12EnoylCoAMAT		
C10EnoylCoAMAT		
C6EnoylCoAMAT		
C4EnoylCoAMAT		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
C4HydroxyacylCoAMAT		
C4AcetoacylCoAMAT		
C8EnoylCoAMAT		
C16EnoylCoAMAT		

Id	Name	SBO
C14EnoylCoAMAT		
C12EnoylCoAMAT		
C10EnoylCoAMAT		
C6EnoylCoAMAT		
C4EnoylCoAMAT		
C8HydroxyacylCoAMAT		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
C4HydroxyacylCoAMAT		
C4AcetoacylCoAMAT		

Product

Table 143: Properties of each product.

1	1	
Id	Name	SBO
C8HydroxyacylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

```
\begin{split} \nu_{35} &= \text{CROT} \left( \text{sfcrotC8}, \text{Vcrot}, \text{KmcrotC8EnoylCoAMAT}, \text{KmcrotC16EnoylCoAMAT}, \\ & \text{KmcrotC14EnoylCoAMAT}, \text{KmcrotC12EnoylCoAMAT}, \text{KmcrotC4EnoylCoAMAT}, \\ & \text{KmcrotC6EnoylCoAMAT}, \text{KmcrotC4EnoylCoAMAT}, \\ & \text{KmcrotC8HydroxyacylCoAMAT}, \text{KmcrotC16HydroxyacylCoAMAT}, \\ & \text{KmcrotC14HydroxyacylCoAMAT}, \text{KmcrotC12HydroxyacylCoAMAT}, \\ & \text{KmcrotC10HydroxyacylCoAMAT}, \text{KmcrotC6HydroxyacylCoAMAT}, \\ & \text{KmcrotC4HydroxyacylCoAMAT}, \text{KicrotC4AcetoacylCoA}, \text{Keqcrot}, \\ & [\text{C8EnoylCoAMAT}], [\text{C16EnoylCoAMAT}], [\text{C14EnoylCoAMAT}], [\text{C12EnoylCoAMAT}], \\ & \text{[C10EnoylCoAMAT]}, [\text{C6EnoylCoAMAT}], [\text{C4EnoylCoAMAT}], \\ & [\text{C12HydroxyacylCoAMAT}], [\text{C10HydroxyacylCoAMAT}], [\text{C6HydroxyacylCoAMAT}], \\ & \text{[C4HydroxyacylCoAMAT]}, [\text{C4AcetoacylCoAMAT}], \\ & \text{[C4HydroxyacylCoAMAT]}, [\text{C4AcetoacylCoAMAT}], \\ & \text{[C4HydroxyacylCoAMAT]}, [\text{C4AcetoacylCoAMAT}], \\ & \text{[C4HydroxyacylCoAMAT]}, [\text{C4AcetoacylCoAMAT}], \\ & \text{[C119)} \\ \end{pmatrix} \end{split}
```

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

Table 144: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcrotC8			0.58	dimensionless	

8.36 Reaction vcrotC6

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

Reaction equation

Reactant

Table 145: Properties of each reactant.

Id	Name	SBO
C6EnoylCoAMAT		

Table 146: Properties of each modifier.

Id	Name	SBO
C16EnoylCoAMAT		
C14EnoylCoAMAT		
C12EnoylCoAMAT		
C10EnoylCoAMAT		
C8EnoylCoAMAT		
C4EnoylCoAMAT		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		

Id	Name	SBO
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C4HydroxyacylCoAMAT		
C4AcetoacylCoAMAT		
C6EnoylCoAMAT		
C16EnoylCoAMAT		
C14EnoylCoAMAT		
C12EnoylCoAMAT		
C10EnoylCoAMAT		
C8EnoylCoAMAT		
C4EnoylCoAMAT		
C6HydroxyacylCoAMAT		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
${\tt C4HydroxyacylCoAMAT}$		
C4AcetoacylCoAMAT		

Product

Table 147: Properties of each product.

Table 147. I Toperties of each product.			
Id	Name	SBO	
C6HydroxyacylCoAMAT			

Kinetic Law

Derived unit contains undeclared units

$$\label{eq:v36} \begin{split} \nu_{36} &= \text{CROT}\,(\text{sfcrotC6}, \text{Vcrot}, \text{KmcrotC6EnoylCoAMAT}, \text{KmcrotC16EnoylCoAMAT}, \\ &\quad \text{KmcrotC14EnoylCoAMAT}, \text{KmcrotC10EnoylCoAMAT}, \\ &\quad \text{KmcrotC8EnoylCoAMAT}, \text{KmcrotC4EnoylCoAMAT}, \\ &\quad \text{KmcrotC6HydroxyacylCoAMAT}, \text{KmcrotC16HydroxyacylCoAMAT}, \\ &\quad \text{KmcrotC14HydroxyacylCoAMAT}, \text{KmcrotC12HydroxyacylCoAMAT}, \\ &\quad \text{KmcrotC10HydroxyacylCoAMAT}, \text{KmcrotC8HydroxyacylCoAMAT}, \\ &\quad \text{KmcrotC4HydroxyacylCoAMAT}, \text{KicrotC4AcetoacylCoA}, \text{Keqcrot}, \\ &\quad \text{[C6EnoylCoAMAT]}, \text{[C16EnoylCoAMAT]}, \text{[C14EnoylCoAMAT]}, \text{[C12EnoylCoAMAT]}, \\ &\quad \text{[C10EnoylCoAMAT]}, \text{[C8EnoylCoAMAT]}, \text{[C4EnoylCoAMAT]}, \\ &\quad \text{[C12HydroxyacylCoAMAT]}, \text{[C10HydroxyacylCoAMAT]}, \text{[C3HydroxyacylCoAMAT]}, \\ &\quad \text{[C4HydroxyacylCoAMAT]}, \text{[C4AcetoacylCoAMAT]}, \\ &\quad \text{[C4HydroxyacylCoAMAT]}, \text{[C4AcetoacylCoAMAT]}, \\ &\quad \text{[C4HydroxyacylCoAMAT]}, \text{[C4AcetoacylCoAMAT]}, \\ &\quad \text{[C422)} \end{split}$$

CROT (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Ki1, Keq, S1, S2, S3, S4, S5, S6, S7, P1, P2, P3, P4, P5, P6, P7, I1)

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

Table 148: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcrotC6			0.83	dimensionless	$lue{2}$

8.37 Reaction vcrotC4

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

Reaction equation

Reactant

Table 149: Properties of each reactant.

Id	Name	SBO
C4EnoylCoAMAT		

Id Name SBC

Modifiers

Table 150: Properties of each modifier.

Id	Name	SBO
C16EnoylCoAMAT		
C14EnoylCoAMAT		
C12EnoylCoAMAT		
C10EnoylCoAMAT		
C8EnoylCoAMAT		
C6EnoylCoAMAT		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
C4AcetoacylCoAMAT		
C4EnoylCoAMAT		
C16EnoylCoAMAT		
C14EnoylCoAMAT		
C12EnoylCoAMAT		
C10EnoylCoAMAT		
C8EnoylCoAMAT		
C6EnoylCoAMAT		
C4HydroxyacylCoAMAT		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
C4AcetoacylCoAMAT		

Product

Table 151: Properties of each product.

	1	
Id	Name	SBO
C4HydroxyacylCoA	MAT	

Id	Name	SBO
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Kinetic Law

Derived unit contains undeclared units

v₃₇ = CROT (sfcrotC4, Vcrot, KmcrotC4EnoylCoAMAT, KmcrotC16EnoylCoAMAT, KmcrotC14EnoylCoAMAT, KmcrotC12EnoylCoAMAT, KmcrotC10EnoylCoAMAT, KmcrotC14EnoylCoAMAT, KmcrotC6EnoylCoAMAT, KmcrotC6EnoylCoAMAT, KmcrotC16HydroxyacylCoAMAT, KmcrotC16HydroxyacylCoAMAT, KmcrotC12HydroxyacylCoAMAT, KmcrotC12HydroxyacylCoAMAT, KmcrotC10HydroxyacylCoAMAT, KmcrotC8HydroxyacylCoAMAT, KmcrotC6HydroxyacylCoAMAT, KicrotC4AcetoacylCoA, Keqcrot, [C4EnoylCoAMAT], [C16EnoylCoAMAT], [C14EnoylCoAMAT], [C12EnoylCoAMAT], [C10EnoylCoAMAT], [C4HydroxyacylCoAMAT], [C16HydroxyacylCoAMAT], [C14HydroxyacylCoAMAT], [C12HydroxyacylCoAMAT], [C6HydroxyacylCoAMAT], [C6HydroxyacylCoAMAT], [C4AcetoacylCoAMAT])

CROT (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Ki1, Keq, S1, S2, S3, S4, S5, S6, S7, P1, P2, P3, P4, P5, P6, P7, I1)

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

Table 152: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcrotC4			1.0	dimensionless	\overline{Z}

8.38 Reaction vmschadC16

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

Reaction equation

Reactant

Table 153: Properties of each reactant.

rable 133. I roperties of each reactant.		
Id	Name	SBO
C16HydroxyacylCoAMAT		

Table 154: Properties of each modifier.

Id	Name	SBO
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
${\tt C6HydroxyacylCoAMAT}$		
$\mathtt{C4HydroxyacylCoAMAT}$		
NADtMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
${\tt C6KetoacylCoAMAT}$		
${\tt C4AcetoacylCoAMAT}$		
C16HydroxyacylCoAMAT		
${\tt C14HydroxyacylCoAMAT}$		
C12HydroxyacylCoAMAT		
${\tt C10HydroxyacylCoAMAT}$		
${\tt C8HydroxyacylCoAMAT}$		
${\tt C6HydroxyacylCoAMAT}$		
${\tt C4HydroxyacylCoAMAT}$		
NADtMAT		
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
${\tt C4AcetoacylCoAMAT}$		
NADHMAT		

Products

Table 155: Properties of each product.

Id	Name	SBO
C16KetoacylCoAMAT NADHMAT		

Kinetic Law

Derived unit contains undeclared units

```
v<sub>38</sub> = MSCHAD (sfmschadC16, Vmschad, KmmschadC16HydroxyacylCoAMAT, KmmschadC14HydroxyacylCoAMAT, KmmschadC12HydroxyacylCoAMAT,
```

KmmschadC10HydroxyacylCoAMAT, KmmschadC8HydroxyacylCoAMAT,

Kmmschad C6 Hydroxyacyl CoAMAT, Kmmschad C4 Hydroxyacyl CoAMAT,

KmmschadNADMAT, KmmschadC16KetoacylCoAMAT,

KmmschadC14KetoacylCoAMAT, KmmschadC12KetoacylCoAMAT,

Kmmschad C10 Ketoacyl CoAMAT, Kmmschad C8 Ketoacyl CoAMAT,

KmmschadC6KetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT,

KmmschadNADHMAT, Keqmschad, [C16HydroxyacylCoAMAT],

[C14 Hydroxyacyl CoAMAT], [C12 Hydroxyacyl CoAMAT], [C10 Hydroxyacyl

[C8HydroxyacylCoAMAT], [C6HydroxyacylCoAMAT], [C4HydroxyacylCoAMAT],

[NADtMAT], [C16KetoacylCoAMAT], [C14KetoacylCoAMAT],

[C12KetoacylCoAMAT], [C10KetoacylCoAMAT], [C8KetoacylCoAMAT],

[C6KetoacylCoAMAT], [C4AcetoacylCoAMAT], [NADHMAT])

(128)

MSCHAD (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Keq, S1, S2, S3, S4, S5, S6, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8)

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

Table 156: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmschadO	216		0.6	dimensionless	

8.39 Reaction vmschadC14

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

Reaction equation

C14HydroxyacylCoAMAT, C12HydroxyacylCoAMAT, C10HydroxyacylCoAMAT, C8
(130)

Reactant

Table 157: Properties of each reactant.

Id Name SBO

C14HydroxyacylCoAMAT

Table 158: Properties of each modifier.

Id	Name	SBO
C16HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
C4HydroxyacylCoAMAT		
NADtMAT		
C16KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
C4AcetoacylCoAMAT		
C14HydroxyacylCoAMAT		
C16HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
C4HydroxyacylCoAMAT		
NADtMAT		

Id	Name	SBO
C14KetoacylCoAMAT		
C16KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
C4AcetoacylCoAMAT		
NADHMAT		

Products

Table 159: Properties of each product.

Id	Name	SBO
C14KetoacylCoAMAT NADHMAT		

Kinetic Law

Derived unit contains undeclared units

```
w<sub>39</sub> = MSCHAD (sfmschadC14, Vmschad, KmmschadC14HydroxyacylCoAMAT, KmmschadC16HydroxyacylCoAMAT, KmmschadC12HydroxyacylCoAMAT, KmmschadC8HydroxyacylCoAMAT, KmmschadC8HydroxyacylCoAMAT, KmmschadC6HydroxyacylCoAMAT, KmmschadC4HydroxyacylCoAMAT, KmmschadC14KetoacylCoAMAT, KmmschadC14KetoacylCoAMAT, KmmschadC12KetoacylCoAMAT, KmmschadC16KetoacylCoAMAT, KmmschadC12KetoacylCoAMAT, KmmschadC8KetoacylCoAMAT, KmmschadC8KetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT], [C16HydroxyacylCoAMAT], [C12HydroxyacylCoAMAT], [C10HydroxyacylCoAMAT], [C8HydroxyacylCoAMAT], [C14KetoacylCoAMAT], [C14KetoacylCoAMAT], [C16KetoacylCoAMAT], [C12KetoacylCoAMAT], [C10KetoacylCoAMAT], [C8KetoacylCoAMAT], [C6KetoacylCoAMAT], [C4AcetoacylCoAMAT], [NADHMAT])
```

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

Table 160: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmschadC14	4		0.5	dimensionless	

8.40 Reaction vmschadC12

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

Reaction equation

Reactant

Table 161: Properties of each reactant

Table 101. Hoperties of each reactant.		
Id	Name	SBO
C12HydroxyacylCoAMAT		

Table 162: Properties of each modifier.

Id	Name	SBO
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
C4HydroxyacylCoAMAT		
NADtMAT		

T.1	N.T.	CDC
Id	Name	SBO
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
C4AcetoacylCoAMAT		
C12HydroxyacylCoAMAT		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
C4HydroxyacylCoAMAT		
NADtMAT		
C12KetoacylCoAMAT		
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
C4AcetoacylCoAMAT		
NADHMAT		

Products

Table 163: Properties of each product.

Id	Name	SBO
C12KetoacylCoAMAT NADHMAT		

Kinetic Law

Derived unit contains undeclared units

```
    v40 = MSCHAD (sfmschadC12, Vmschad, KmmschadC12HydroxyacylCoAMAT, KmmschadC16HydroxyacylCoAMAT, KmmschadC14HydroxyacylCoAMAT, KmmschadC8HydroxyacylCoAMAT, KmmschadC8HydroxyacylCoAMAT, KmmschadC4HydroxyacylCoAMAT, KmmschadC4HydroxyacylCoAMAT, KmmschadC12KetoacylCoAMAT, KmmschadC12KetoacylCoAMAT, KmmschadC12KetoacylCoAMAT, KmmschadC14KetoacylCoAMAT, KmmschadC8KetoacylCoAMAT, KmmschadC8KetoacylCoAMAT, KmmschadC8KetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT, KmmschadC4AcetoacylCoAMAT], [C16HydroxyacylCoAMAT], [C16HydroxyacylCoAMAT], [C16HydroxyacylCoAMAT], [C16HydroxyacylCoAMAT], [C10HydroxyacylCoAMAT], [C8HydroxyacylCoAMAT], [C12KetoacylCoAMAT], [C16KetoacylCoAMAT], [C16KetoacylCoAMAT], [C16KetoacylCoAMAT], [C16KetoacylCoAMAT], [C6KetoacylCoAMAT], [C4AcetoacylCoAMAT], [NADHMAT])
```

MSCHAD (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Keq, S1, S2, S3, S4, S5, S6, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8)

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

Table 164: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmschadC	12		0.43	dimensionless	

8.41 Reaction vmschadC10

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

Reaction equation

Reactant

Table 165: Properties of each reactant.

Id	Name	
C10HydroxyacylCoAMAT		

Modifiers

Table 166: Properties of each modifier.

Id	Name	SBO
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
${\tt C4HydroxyacylCoAMAT}$		
NADtMAT		
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
${\tt C4AcetoacylCoAMAT}$		
${\tt C10HydroxyacylCoAMAT}$		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
${\tt C8HydroxyacylCoAMAT}$		
${\tt C6HydroxyacylCoAMAT}$		
$\mathtt{C4HydroxyacylCoAMAT}$		
NADtMAT		
C10KetoacylCoAMAT		
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
${\tt C4AcetoacylCoAMAT}$		
NADHMAT		

Products

Table 167: Properties of each product.		
Id	Name	SBO
C10KetoacylCoAMAT NADHMAT		

Kinetic Law

Derived unit contains undeclared units

```
v_{41} = \mathsf{MSCHAD}(\mathsf{sfmschadC10}, \mathsf{Vmschad}, \mathsf{KmmschadC10HydroxyacylCoAMAT}, \\ \mathsf{KmmschadC16HydroxyacylCoAMAT}, \mathsf{KmmschadC14HydroxyacylCoAMAT}, \\ \mathsf{KmmschadC12HydroxyacylCoAMAT}, \mathsf{KmmschadC8HydroxyacylCoAMAT}, \\ \mathsf{KmmschadC6HydroxyacylCoAMAT}, \mathsf{KmmschadC4HydroxyacylCoAMAT}, \\ \mathsf{KmmschadC10KetoacylCoAMAT}, \mathsf{KmmschadC10KetoacylCoAMAT}, \\ \mathsf{KmmschadC16KetoacylCoAMAT}, \mathsf{KmmschadC14KetoacylCoAMAT}, \\ \mathsf{KmmschadC12KetoacylCoAMAT}, \mathsf{KmmschadC8KetoacylCoAMAT}, \\ \mathsf{KmmschadC6KetoacylCoAMAT}, \mathsf{KmmschadC4AcetoacylCoAMAT}, \\ \mathsf{KmmschadNADHMAT}, \mathsf{Keqmschad}, [C10HydroxyacylCoAMAT], \\ [C16HydroxyacylCoAMAT], [C14HydroxyacylCoAMAT], [C12HydroxyacylCoAMAT], \\ [C8HydroxyacylCoAMAT], [C6HydroxyacylCoAMAT], [C4HydroxyacylCoAMAT], \\ [NADtMAT], [C10KetoacylCoAMAT], [C16KetoacylCoAMAT], \\ [C14KetoacylCoAMAT], [C12KetoacylCoAMAT], [C8KetoacylCoAMAT], \\ [C6KetoacylCoAMAT], [C4AcetoacylCoAMAT], [NADHMAT]) \\ (137)
```

MSCHAD (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Keq, S1, S2, S3, S4, S5, S6, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8)

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

Table 168: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmschadC1	0		0.64	dimensionless	Ø

8.42 Reaction vmschadC8

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

Reaction equation

C8HydroxyacylCoAMAT, C14HydroxyacylCoAMAT, C12HydroxyacylCoAMAT, C16HydroxyacylCoAMAT, C

Reactant

Table 169: Properties of each reactant.		
Id	Name	SBO
C8HydroxyacylCoAMAT		

Table 170: Properties of each modifier.

Id	Name	SBO
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
C4HydroxyacylCoAMAT		
NADtMAT		
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C6KetoacylCoAMAT		
C4AcetoacylCoAMAT		
C8HydroxyacylCoAMAT		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
${\tt C6HydroxyacylCoAMAT}$		
C4HydroxyacylCoAMAT		
NADtMAT		

Id	Name	SBO
C8KetoacylCoAMAT		
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C6KetoacylCoAMAT		
${\tt C4AcetoacylCoAMAT}$		
NADHMAT		

Products

Table 171: Properties of each product.

Id	Name	SBO
C8KetoacylCoAMAT NADHMAT		

Kinetic Law

Derived unit contains undeclared units

```
v_{42} = \text{MSCHAD} (\text{sfmschadC8}, \text{Vmschad}, \text{KmmschadC8HydroxyacylCoAMAT}, \\ \text{KmmschadC16HydroxyacylCoAMAT}, \text{KmmschadC14HydroxyacylCoAMAT}, \\ \text{KmmschadC12HydroxyacylCoAMAT}, \text{KmmschadC10HydroxyacylCoAMAT}, \\ \text{KmmschadC6HydroxyacylCoAMAT}, \text{KmmschadC4HydroxyacylCoAMAT}, \\ \text{KmmschadC6HydroxyacylCoAMAT}, \text{KmmschadC8KetoacylCoAMAT}, \\ \text{KmmschadC16KetoacylCoAMAT}, \text{KmmschadC14KetoacylCoAMAT}, \\ \text{KmmschadC12KetoacylCoAMAT}, \text{KmmschadC10KetoacylCoAMAT}, \\ \text{KmmschadC6KetoacylCoAMAT}, \text{KmmschadC4AcetoacylCoAMAT}, \\ \text{KmmschadNADHMAT}, \text{Keqmschad}, [\text{C8HydroxyacylCoAMAT}], [\text{C16HydroxyacylCoAMAT}], [\text{C16HydroxyacylCoAMAT}], [\text{C19HydroxyacylCoAMAT}], [\text{C10HydroxyacylCoAMAT}], [\text{C19HydroxyacylCoAMAT}], [\text{C4HydroxyacylCoAMAT}], [\text{C14KetoacylCoAMAT}], [\text{C12KetoacylCoAMAT}], [\text{C10KetoacylCoAMAT}], [\text{C6KetoacylCoAMAT}], [\text{C4HydATAT}], [\text{C14KetoacylCoAMAT}], [\text{C14KetoacylCoAMAT}], [\text{C14HydATAT}]) \\ \text{[C12KetoacylCoAMAT]}, [\text{C10KetoacylCoAMAT}], [\text{C6KetoacylCoAMAT}], [\text{C14NDHMAT}]) \\ \text{[C14OHydAT]}, [\text{C14NDHMAT}], [
```

MSCHAD (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Keq, S1, S2, S3, S4, S5, S6, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8)

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

Table 172: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmschadC8			0.89	dimensionless	Ø

8.43 Reaction vmschadC6

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

Reaction equation

Reactant

Table 173: Properties of each reactant.

Id Name SBO

C6HydroxyacylCoAMAT

Table 174: Properties of each modifier.

Id	Name	SBO
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C4HydroxyacylCoAMAT		
NADtMAT		

Id	Name	SBO
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
C4AcetoacylCoAMAT		
C6HydroxyacylCoAMAT		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C4HydroxyacylCoAMAT		
NADtMAT		
C6KetoacylCoAMAT		
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
C4AcetoacylCoAMAT		
NADHMAT		

Products

Table 175: Properties of each product.

Id	Name	SBO
C6KetoacylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

```
v_{43} = \mathsf{MSCHAD}(\mathsf{sfmschadC6}, \mathsf{Vmschad}, \mathsf{KmmschadC6HydroxyacylCoAMAT}, \\ \mathsf{KmmschadC16HydroxyacylCoAMAT}, \mathsf{KmmschadC14HydroxyacylCoAMAT}, \\ \mathsf{KmmschadC12HydroxyacylCoAMAT}, \mathsf{KmmschadC10HydroxyacylCoAMAT}, \\ \mathsf{KmmschadC8HydroxyacylCoAMAT}, \mathsf{KmmschadC4HydroxyacylCoAMAT}, \\ \mathsf{KmmschadC8HydroxyacylCoAMAT}, \mathsf{KmmschadC6KetoacylCoAMAT}, \\ \mathsf{KmmschadC16KetoacylCoAMAT}, \mathsf{KmmschadC14KetoacylCoAMAT}, \\ \mathsf{KmmschadC12KetoacylCoAMAT}, \mathsf{KmmschadC10KetoacylCoAMAT}, \\ \mathsf{KmmschadC8KetoacylCoAMAT}, \mathsf{KmmschadC4AcetoacylCoAMAT}, \\ \mathsf{KmmschadNADHMAT}, \mathsf{Keqmschad}, [\mathsf{C6HydroxyacylCoAMAT}], \\ [\mathsf{C16HydroxyacylCoAMAT}], [\mathsf{C14HydroxyacylCoAMAT}], [\mathsf{C12HydroxyacylCoAMAT}], \\ [\mathsf{C10HydroxyacylCoAMAT}], [\mathsf{C8HydroxyacylCoAMAT}], [\mathsf{C4HydroxyacylCoAMAT}], \\ [\mathsf{C10KetoacylCoAMAT}], [\mathsf{C16KetoacylCoAMAT}], [\mathsf{C14KetoacylCoAMAT}], \\ [\mathsf{C12KetoacylCoAMAT}], [\mathsf{C10KetoacylCoAMAT}], [\mathsf{C8KetoacylCoAMAT}], \\ [\mathsf{C4AcetoacylCoAMAT}], [\mathsf{NADHMAT}]) \\ [\mathsf{C4AcetoacylCoAMAT}], [\mathsf{C4AcetoacylCoAMAT}], [\mathsf{NADHMAT}]) \\ [\mathsf{C4AcetoacylCoAMAT}], [\mathsf{C4
```

MSCHAD (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Keq, S1, S2, S3, S4, S5, S6, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8)

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

Table 176: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmschadC6			1.0	dimensionless	

8.44 Reaction vmschadC4

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

Reaction equation

Reactant

Table 177: Properties of each reactant.	Table 177:	Properties	of each	reactant.
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Table 177: Properties of each reactant.			
Id	Name	SBO	
C4HydroxyacylCoAMAT			

Modifiers

Table 178: Properties of each modifier.

Id	Name	SBO
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
NADtMAT		
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
C4HydroxyacylCoAMAT		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
${\tt C6HydroxyacylCoAMAT}$		
NADtMAT		
C4AcetoacylCoAMAT		
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
NADHMAT		

Products

Table 179: Properties	of each pr	oduct.
Id	Name	SBO
C4AcetoacylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

```
v_{44} = \mathsf{MSCHAD}(\mathsf{sfmschadC4}, \mathsf{Vmschad}, \mathsf{KmmschadC4HydroxyacylCoAMAT}, \\ \mathsf{KmmschadC16HydroxyacylCoAMAT}, \mathsf{KmmschadC14HydroxyacylCoAMAT}, \\ \mathsf{KmmschadC12HydroxyacylCoAMAT}, \mathsf{KmmschadC10HydroxyacylCoAMAT}, \\ \mathsf{KmmschadC8HydroxyacylCoAMAT}, \mathsf{KmmschadC6HydroxyacylCoAMAT}, \\ \mathsf{KmmschadC8HydroxyacylCoAMAT}, \mathsf{KmmschadC4AcetoacylCoAMAT}, \\ \mathsf{KmmschadC16KetoacylCoAMAT}, \mathsf{KmmschadC14KetoacylCoAMAT}, \\ \mathsf{KmmschadC12KetoacylCoAMAT}, \mathsf{KmmschadC10KetoacylCoAMAT}, \\ \mathsf{KmmschadC8KetoacylCoAMAT}, \mathsf{KmmschadC6KetoacylCoAMAT}, \\ \mathsf{KmmschadC8KetoacylCoAMAT}, \mathsf{Keqmschad}, [C4HydroxyacylCoAMAT], \\ [C16HydroxyacylCoAMAT], [C14HydroxyacylCoAMAT], [C12HydroxyacylCoAMAT], \\ [C10HydroxyacylCoAMAT], [C8HydroxyacylCoAMAT], [C6HydroxyacylCoAMAT], \\ [NADtMAT], [C4AcetoacylCoAMAT], [C16KetoacylCoAMAT], \\ [C14KetoacylCoAMAT], [C12KetoacylCoAMAT], [C10KetoacylCoAMAT], \\ [C8KetoacylCoAMAT], [C6KetoacylCoAMAT], [NADHMAT]) \\ (146)
```

MSCHAD (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Keq, S1, S2, S3, S4, S5, S6, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8)

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

Table 180: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmschadC4			0.67	dimensionless	\square

8.45 Reaction vmckatC16

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

Reaction equation

C16KetoacylCoAMAT, C12KetoacylCoAMAT, C10KetoacylCoAMAT, C8KetoacylCoAMAT (148)

Reactant

Table 181: Properties of each reactant.

Id Name SBO

C16KetoacylCoAMAT

Table 182: Properties of each modifier.

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

Id	Name	SBO
C14AcylCoAMAT		
C16AcylCoAMAT		
C12AcylCoAMAT		
C10AcylCoAMAT		
C8AcylCoAMAT		
C6AcylCoAMAT		
C4AcylCoAMAT		
AcetylCoAMAT		

Products

Table 183: Properties of each product.

Id	Name	SBO
C14AcylCoAMAT AcetylCoAMAT		
HOOGYTOOMINI		

Kinetic Law

Derived unit contains undeclared units

```
v_{45} = \text{MCKATA} \left( \text{sfmckatC16}, \text{Vmckat}, \text{KmmckatC16KetoacylCoAMAT}, \\ \text{KmmckatC14KetoacylCoAMAT}, \text{KmmckatC12KetoacylCoAMAT}, \\ \text{KmmckatC10KetoacylCoAMAT}, \text{KmmckatC8KetoacylCoAMAT}, \\ \text{KmmckatC6KetoacylCoAMAT}, \text{KmmckatC4AcetoacylCoAMAT}, \text{KmmckatC0AMAT}, \\ \text{KmmckatC14AcylCoAMAT}, \text{KmmckatC16AcylCoAMAT}, \\ \text{KmmckatC12AcylCoAMAT}, \text{KmmckatC10AcylCoAMAT}, \text{KmmckatC8AcylCoAMAT}, \\ \text{KmmckatC6AcylCoAMAT}, \text{KmmckatC4AcylCoAMAT}, \text{KmmckatAcetylCoAMAT}, \\ \text{Keqmckat}, [\text{C16KetoacylCoAMAT}], [\text{C14KetoacylCoAMAT}], [\text{C12KetoacylCoAMAT}], \\ [\text{C10KetoacylCoAMAT}], [\text{C8KetoacylCoAMAT}], [\text{C6KetoacylCoAMAT}], \\ [\text{C4AcetoacylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C8AcylCoAMAT}], [\text{C6AcylCoAMAT}], \\ [\text{C12AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C8AcylCoAMAT}], [\text{C6AcylCoAMAT}], \\ [\text{C4AcylCoAMAT}], [\text{AcetylCoAMAT}], \\ [\text{C4AcylCoAMAT}], [\text{AcetylCoAMAT}], \\ [\text{C4AcylCoAMAT}], [\text{C6AcylCoAMAT}], \\ [\text{C4AcylCoAMAT}], \\ [\text
```

MCKATA (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Keq, S1, S2, S3, S4, S5, S6, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8)

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

Table 184: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmckatC16			0.0	dimensionless	\square

8.46 Reaction vmckatC14

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

Reaction equation

C14KetoacylCoAMAT, C12KetoacylCoAMAT, C10KetoacylCoAMAT, C8KetoacylCoAM (151)

Reactant

Table 185: Properties of each reactant.

Id Name SBO

C14KetoacylCoAMAT

Table 186: Properties of each modifier.

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

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

Products

Table 187: Properties of each product.

Id	Name	SBO
C12AcylCoAMAT		
AcetylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

```
v_{46} = \text{MCKATA} \left( \text{sfmckatC14}, \text{Vmckat}, \text{KmmckatC14KetoacylCoAMAT}, \\ \text{KmmckatC16KetoacylCoAMAT}, \text{KmmckatC12KetoacylCoAMAT}, \\ \text{KmmckatC10KetoacylCoAMAT}, \text{KmmckatC8KetoacylCoAMAT}, \\ \text{KmmckatC6KetoacylCoAMAT}, \text{KmmckatC4AcetoacylCoAMAT}, \\ \text{KmmckatC12AcylCoAMAT}, \text{KmmckatC16AcylCoAMAT}, \\ \text{KmmckatC14AcylCoAMAT}, \text{KmmckatC10AcylCoAMAT}, \\ \text{KmmckatC6AcylCoAMAT}, \text{KmmckatC4AcylCoAMAT}, \\ \text{KmmckatC6AcylCoAMAT}, \text{KmmckatC4AcylCoAMAT}, \\ \text{Keqmckat}, [\text{C14KetoacylCoAMAT}], [\text{C16KetoacylCoAMAT}], [\text{C12KetoacylCoAMAT}], \\ [\text{C10KetoacylCoAMAT}], [\text{C8KetoacylCoAMAT}], [\text{C6KetoacylCoAMAT}], \\ [\text{C4AcetoacylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C12AcylCoAMAT}], [\text{C6AcylCoAMAT}], \\ [\text{C14AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C8AcylCoAMAT}], [\text{C6AcylCoAMAT}], \\ [\text{C4AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C4AcylCoAMAT}], [\text{C6AcylCoAMAT}], \\ [\text{C4AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C10AcylCoAMAT}], \\ [\text{C4AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C10AcylCoAMAT}], \\ [\text{C4AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C10AcylCoAMAT}], \\ [\text{C4AcylCoAMAT}], \\ [\text{C4AcylCoAMAT}
```

MCKATA (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Keq, S1, S2, S3, S4, S5, S6, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8)

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

Table 188: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmckatC14			0.2	dimensionless	

8.47 Reaction vmckatC12

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

Reaction equation

Reactant

Table 190: Properties of each modifier.

Id	Name	SBO
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
C4AcetoacylCoAMAT		
CoAMAT		

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

Products

Table 191: Properties of each product.

Id	Name	SBO
C10AcylCoAMAT		
AcetylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

v₄₇ = MCKATA (sfmckatC12, Vmckat, KmmckatC12KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC6KetoacylCoAMAT, KmmckatC4AcetoacylCoAMAT, KmmckatC0AMAT, KmmckatC10AcylCoAMAT, KmmckatC16AcylCoAMAT, KmmckatC14AcylCoAMAT, KmmckatC12AcylCoAMAT, KmmckatC8AcylCoAMAT, KmmckatC6AcylCoAMAT, KmmckatC4AcylCoAMAT, KmmckatAcetylCoAMAT, Keqmckat, [C12KetoacylCoAMAT], [C16KetoacylCoAMAT], [C14KetoacylCoAMAT], [C10KetoacylCoAMAT], [C8KetoacylCoAMAT], [C6KetoacylCoAMAT], [C4AcetoacylCoAMAT], [C0AMAT], [C10AcylCoAMAT], [C16AcylCoAMAT], [C16AcylCoAMA

[C4AcetoacylCoAMAT], [CoAMAT], [C10AcylCoAMAT], [C16AcylCoAMAT], [C14AcylCoAMAT], [C12AcylCoAMAT], [C8AcylCoAMAT], [C6AcylCoAMAT], [C4AcylCoAMAT], [AcetylCoAMAT])

(155)

MCKATA (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Keq, S1, S2, S3, S4, S5, S6, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8)

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

Table 192: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmckatC12			0.38	dimensionless	

8.48 Reaction vmckatC10

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

Reaction equation

C10KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCoAMAT, C8KetoacylCoAM (157)

Reactant

Table 193: Properties of each reactant.

Id	Name	SBO
C10KetoacylCoAMAT		

Modifiers

Table 194: Properties of each modifier.

Id	Name	SBO
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
${\tt C4AcetoacylCoAMAT}$		
CoAMAT		
C16AcylCoAMAT		
C14AcylCoAMAT		
C12AcylCoAMAT		
C10AcylCoAMAT		
C6AcylCoAMAT		
C4AcylCoAMAT		
C10KetoacylCoAMAT		
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
${\tt C4AcetoacylCoAMAT}$		
CoAMAT		
C8AcylCoAMAT		
C16AcylCoAMAT		
C14AcylCoAMAT		
C12AcylCoAMAT		
C10AcylCoAMAT		
C6AcylCoAMAT		
C4AcylCoAMAT		
AcetylCoAMAT		

Products

Table 195: Properties of each product.

Id	Name	SBO
C8AcylCoAMAT AcetylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

```
v48 = MCKATA (sfmckatC10, Vmckat, KmmckatC10KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT, KmmckatC12KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC6KetoacylCoAMAT, KmmckatC4AcetoacylCoAMAT, KmmckatCoAMAT, KmmckatC8AcylCoAMAT, KmmckatC16AcylCoAMAT, KmmckatC14AcylCoAMAT, KmmckatC12AcylCoAMAT, KmmckatC10AcylCoAMAT, KmmckatC6AcylCoAMAT, KmmckatC4AcylCoAMAT, KmmckatAcetylCoAMAT, Keqmckat, [C10KetoacylCoAMAT], [C16KetoacylCoAMAT], [C14KetoacylCoAMAT], [C12KetoacylCoAMAT], [C8KetoacylCoAMAT], [C6KetoacylCoAMAT], [C14AcylCoAMAT], [C12AcylCoAMAT], [C10AcylCoAMAT], [C16AcylCoAMAT], [C14AcylCoAMAT], [C12AcylCoAMAT], [C10AcylCoAMAT], [C6AcylCoAMAT], [C4AcylCoAMAT], [AcetylCoAMAT], [C4AcylCoAMAT], [AcetylCoAMAT], [C4AcylCoAMAT], [AcetylCoAMAT])
```

MCKATA (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Keq, S1, S2, S3, S4, S5, S6, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8)

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

Table 196: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmckatC10			0.65	dimensionless	

8.49 Reaction vmckatC8

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

Reaction equation

C8KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCoAMAT, C10KetoacylCoAMAT

(160)

Reactant

Table 197: Properties of each reactant.

Id Name SBO

C8KetoacylCoAMAT

Table 198: Properties of each modifier.

Id	Name	SBO
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C6KetoacylCoAMAT		
${\tt C4AcetoacylCoAMAT}$		
CoAMAT		
C16AcylCoAMAT		
C14AcylCoAMAT		
C12AcylCoAMAT		
C10AcylCoAMAT		
C8AcylCoAMAT		
C4AcylCoAMAT		
C8KetoacylCoAMAT		
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C6KetoacylCoAMAT		
${\tt C4AcetoacylCoAMAT}$		
CoAMAT		
C6AcylCoAMAT		
C16AcylCoAMAT		
C14AcylCoAMAT		
C12AcylCoAMAT		

Id	Name	SBO
C10AcylCoAMAT		
C8AcylCoAMAT		
C4AcylCoAMAT		
AcetylCoAMAT		

Products

Table 199: Properties of each product.

Id	Name	SBO
C6AcylCoAMAT AcetylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

```
v_{49} = \text{MCKATA} \left( \text{sfmckatC8}, \text{Vmckat}, \text{KmmckatC8KetoacylCoAMAT}, \\ \text{KmmckatC16KetoacylCoAMAT}, \text{KmmckatC14KetoacylCoAMAT}, \\ \text{KmmckatC12KetoacylCoAMAT}, \text{KmmckatC10KetoacylCoAMAT}, \\ \text{KmmckatC6KetoacylCoAMAT}, \text{KmmckatC4AcetoacylCoAMAT}, \text{KmmckatCoAMAT}, \\ \text{KmmckatC6AcylCoAMAT}, \text{KmmckatC16AcylCoAMAT}, \text{KmmckatC14AcylCoAMAT}, \\ \text{KmmckatC12AcylCoAMAT}, \text{KmmckatC10AcylCoAMAT}, \text{KmmckatC8AcylCoAMAT}, \\ \text{KmmckatC4AcylCoAMAT}, \text{KmmckatAcetylCoAMAT}, \text{Keqmckat}, \\ \left[ \text{C8KetoacylCoAMAT} \right], \left[ \text{C16KetoacylCoAMAT} \right], \left[ \text{C14KetoacylCoAMAT} \right], \\ \left[ \text{C12KetoacylCoAMAT} \right], \left[ \text{C10KetoacylCoAMAT} \right], \left[ \text{C16AcylCoAMAT} \right], \\ \left[ \text{C4AcetoacylCoAMAT} \right], \left[ \text{C10AcylCoAMAT} \right], \left[ \text{C8AcylCoAMAT} \right], \\ \left[ \text{C14AcylCoAMAT} \right], \left[ \text{C12AcylCoAMAT} \right], \left[ \text{C10AcylCoAMAT} \right], \left[ \text{C8AcylCoAMAT} \right], \\ \left[ \text{C4AcylCoAMAT} \right], \left[ \text{C4AcylCoAMAT}
```

MCKATA (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Keq, S1, S2, S3, S4, S5, S6, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8)

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

Table 200: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmckatC8			0.81	dimensionless	

8.50 Reaction vmckatC6

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

Reaction equation

C6KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCoAMAT, C10KetoacylCoAMAT (163)

Reactant

Table 201: Properties of each reactant.

Id	Name	SBO
C6KetoacylCoAMAT		

Table 202: Properties of each modifier.

Id	Name	SBO
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
${\tt C4AcetoacylCoAMAT}$		
CoAMAT		
C4AcylCoAMAT		
C16AcylCoAMAT		
C14AcylCoAMAT		
C12AcylCoAMAT		
C10AcylCoAMAT		
C8AcylCoAMAT		
C6AcylCoAMAT		
AcetylCoAMAT		

Products

Table 203: Properties of each product.

Id	Name	SBO
C4AcylCoAMAT		
${\tt AcetylCoAMAT}$		

Kinetic Law

Derived unit contains undeclared units

```
v_{50} = \text{MCKATA} (sfmckatC6, Vmckat, KmmckatC6KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT, KmmckatC12KetoacylCoAMAT, KmmckatC10KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC4AcetoacylCoAMAT, KmmckatC0AMAT, KmmckatC4AcylCoAMAT, KmmckatC16AcylCoAMAT, KmmckatC14AcylCoAMAT, KmmckatC12AcylCoAMAT, KmmckatC10AcylCoAMAT, KmmckatC8AcylCoAMAT, KmmckatC8AcylCoAMAT, KmmckatC6AcylCoAMAT, KmmckatAcetylCoAMAT, Keqmckat, [C6KetoacylCoAMAT], [C16KetoacylCoAMAT], [C14KetoacylCoAMAT], [C12KetoacylCoAMAT], [C10KetoacylCoAMAT], [C8KetoacylCoAMAT], [C14AcylCoAMAT], [C14AcylCoAMAT], [C14AcylCoAMAT], [C12AcylCoAMAT], [C10AcylCoAMAT], [C8AcylCoAMAT], [C6AcylCoAMAT], [C6AcylCoAMAT],
```

MCKATA (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Keq, S1, S2, S3, S4, S5, S6, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8)

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

Table 204: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmckatC6			1.0	dimensionless	Ø

8.51 Reaction vmckatC4

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

Reaction equation

Reactant

Table 206: Properties of each modifier.

Id	Name	SBO
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
CoAMAT		

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

Product

Table 207: Properties of each product.

Id	Name	SBO
AcetylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

 $v_{51} = MCKATB$ (sfmckatC4, Vmckat, KmmckatC4AcetoacylCoAMAT,

KmmckatC16KetoacylCoAMAT, KmmckatC14KetoacylCoAMAT, KmmckatC12KetoacylCoAMAT, KmmckatC10KetoacylCoAMAT, KmmckatC8KetoacylCoAMAT, KmmckatC6KetoacylCoAMAT, KmmckatC0AMAT, KmmckatC4AcylCoAMAT, KmmckatC16AcylCoAMAT, KmmckatC14AcylCoAMAT, KmmckatC12AcylCoAMAT, KmmckatC10AcylCoAMAT, KmmckatC8AcylCoAMAT, KmmckatC6AcylCoAMAT, KmmckatAcetylCoAMAT, Keqmckat, [C4AcetoacylCoAMAT], [C16KetoacylCoAMAT], [C14KetoacylCoAMAT], [C12KetoacylCoAMAT], [C10KetoacylCoAMAT], [C8KetoacylCoAMAT], [C6KetoacylCoAMAT], [C4AcylCoAMAT], [C16AcylCoAMAT], [C14AcylCoAMAT], [C12AcylCoAMAT], [C10AcylCoAMAT], [C8AcylCoAMAT], [C16AcylCoAMAT], [C16A

MCKATB (sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms6, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Keq, S1, S2, S3, S4, S5, S6, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8)

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

Table 208: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmckatC4			0.49	dimensionless	

8.52 Reaction vmtpC16

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

Reaction equation

Reactant

Table 209: Properties of each reactant.

Id Name SBO

Modifiers

Table 210: Properties of each modifier.

Id	Name	SBO
C14EnoylCoAMAT		
C12EnoylCoAMAT		
C10EnoylCoAMAT		
C8EnoylCoAMAT		
NADtMAT		
CoAMAT		
C16AcylCoAMAT		
C12AcylCoAMAT		
C10AcylCoAMAT		
C8AcylCoAMAT		
C6AcylCoAMAT		
${\tt C4AcetoacylCoAMAT}$		
C16EnoylCoAMAT		
C14EnoylCoAMAT		
C12EnoylCoAMAT		
C10EnoylCoAMAT		
C8EnoylCoAMAT		
NADtMAT		
CoAMAT		
C14AcylCoAMAT		
C16AcylCoAMAT		
C12AcylCoAMAT		
C10AcylCoAMAT		
C8AcylCoAMAT		
C6AcylCoAMAT		
NADHMAT		
AcetylCoAMAT		
C4AcetoacylCoAMAT		

Products

Table 211: Properties of each product.

Id	Name	SBO
C14AcylCoAMAT		

Id	Name	SBO
AcetylCoAMAT NADHMAT		

Kinetic Law

Derived unit contains undeclared units

```
\begin{split} \nu_{52} &= \text{MTP} (\text{sfmtpC16}, \text{Vmtp}, \text{KmmtpC16EnoylCoAMAT}, \text{KmmtpC14EnoylCoAMAT}, \\ &\quad \text{KmmtpC12EnoylCoAMAT}, \text{KmmtpC10EnoylCoAMAT}, \text{KmmtpC8EnoylCoAMAT}, \\ &\quad \text{KmmtpNADMAT}, \text{KmmtpCoAMAT}, \text{KmmtpC14AcylCoAMAT}, \\ &\quad \text{KmmtpC16AcylCoAMAT}, \text{KmmtpC12AcylCoAMAT}, \text{KmmtpC10AcylCoAMAT}, \\ &\quad \text{KmmtpC8AcylCoAMAT}, \text{KmmtpC6AcylCoAMAT}, \text{KmmtpNADHMAT}, \\ &\quad \text{KmmtpAcetylCoAMAT}, \text{KicrotC4AcetoacylCoA}, \text{Keqmtp}, [\text{C16EnoylCoAMAT}], \\ &\quad [\text{C14EnoylCoAMAT}], [\text{C12EnoylCoAMAT}], [\text{C10EnoylCoAMAT}], [\text{C8EnoylCoAMAT}], \\ &\quad [\text{NADtMAT}], [\text{C0AMAT}], [\text{C14AcylCoAMAT}], [\text{C16AcylCoAMAT}], \\ &\quad [\text{C12AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C8AcylCoAMAT}], [\text{C4AcetoacylCoAMAT}]) \\ &\quad (170) \end{split}
```

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

Table 212: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmtpC16			1.0	dimensionless	\checkmark

8.53 Reaction vmtpC14

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

Reaction equation

Reactant

Table 213: Properties of each reactant.

Id	Name	
C14EnoylCoAMAT		

Table 214: Properties of each modifier.

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

Products

Table 215: Properties of each product.

		1
Id	Name	SBO
C12AcylCoAMAT		
AcetylCoAMAT		
NADHMAT		

Kinetic Law

Derived unit contains undeclared units

```
\label{eq:v53} \begin{split} v_{53} &= \text{MTP} (\text{sfmtpC14}, \text{Vmtp}, \text{KmmtpC14EnoylCoAMAT}, \text{KmmtpC16EnoylCoAMAT}, \\ & \text{KmmtpC12EnoylCoAMAT}, \text{KmmtpC10EnoylCoAMAT}, \text{KmmtpC8EnoylCoAMAT}, \\ & \text{KmmtpNADMAT}, \text{KmmtpCoAMAT}, \text{KmmtpC12AcylCoAMAT}, \\ & \text{KmmtpC16AcylCoAMAT}, \text{KmmtpC14AcylCoAMAT}, \text{KmmtpC10AcylCoAMAT}, \\ & \text{KmmtpC8AcylCoAMAT}, \text{KmmtpC6AcylCoAMAT}, \text{KmmtpNADHMAT}, \\ & \text{KmmtpAcetylCoAMAT}, \text{KicrotC4AcetoacylCoA}, \text{Keqmtp}, [\text{C14EnoylCoAMAT}], \\ & [\text{C16EnoylCoAMAT}], [\text{C12EnoylCoAMAT}], [\text{C10EnoylCoAMAT}], [\text{C8EnoylCoAMAT}], \\ & [\text{NADtMAT}], [\text{C0AMAT}], [\text{C12AcylCoAMAT}], [\text{C16AcylCoAMAT}], \\ & [\text{NADHMAT}], [\text{AcetylCoAMAT}], [\text{C4AcetoacylCoAMAT}]) \\ & [\text{NADHMAT}], [\text{AcetylCoAMAT}], [\text{C4AcetoacylCoAMAT}]) \\ & (173) \end{split}
```

MTP(sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Ki1, Keq, S1, S2, S3, S4, S5, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8, I1)

$$= \frac{sf \cdot V \cdot \left(\frac{s1 \cdot (s7 - P7) \cdot s8}{Kms1 \cdot Kms7 \cdot Kms8} - \frac{P1 \cdot P7 \cdot P8}{Kms1 \cdot Kms7 \cdot Kms8 \cdot Keq}\right)}{\left(1 + \frac{s1}{Kms1} + \frac{P1}{Kmp1} + \frac{s2}{Kms2} + \frac{P2}{Kmp2} + \frac{s3}{Kms3} + \frac{P3}{Kmp3} + \frac{s4}{Kms4} + \frac{P4}{Kmp4} + \frac{s5}{Kms5} + \frac{P5}{Kmp5} + \frac{P6}{Kmp6} + \frac{I1}{Ki1}\right) \cdot \left(1 + \frac{s7 - P7}{Kms7}\right)}$$

Table 216: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmtpC14			0.9	dimensionless	

8.54 Reaction vmtpC12

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

Reaction equation

C12EnoylCoAMAT, C14EnoylCoAMAT, C10EnoylCoAMAT, C8EnoylCoAMAT, NADtMAT

(175)

Reactant

Table 217: Properties of each reactant.

Id	Name	SBO
C12EnoylCoAMAT		

Table 218: Properties of each modifier.

Id	Name	SBO
C16EnoylCoAMAT		
C14EnoylCoAMAT		
C10EnoylCoAMAT		
C8EnoylCoAMAT		
NADtMAT		
CoAMAT		
C16AcylCoAMAT		
C14AcylCoAMAT		
C12AcylCoAMAT		
C8AcylCoAMAT		
C6AcylCoAMAT		
${\tt C4AcetoacylCoAMAT}$		
C12EnoylCoAMAT		
C16EnoylCoAMAT		
C14EnoylCoAMAT		
C10EnoylCoAMAT		
C8EnoylCoAMAT		
NADtMAT		
CoAMAT		
C10AcylCoAMAT		
C16AcylCoAMAT		
C14AcylCoAMAT		
C12AcylCoAMAT		
C8AcylCoAMAT		
C6AcylCoAMAT		

Id	Name	SBO
NADHMAT		
AcetylCoAMAT		
C4AcetoacylCoAMAT		

Products

Table 219: Properties of each product.

Id	Name	SBO
C10AcylCoAMAT		
AcetylCoAMAT		
NADHMAT		

Kinetic Law

Derived unit contains undeclared units

```
v_{54} = \text{MTP} (\text{sfmtpC12}, \text{Vmtp}, \text{KmmtpC12EnoylCoAMAT}, \text{KmmtpC16EnoylCoAMAT}, \\ \text{KmmtpC14EnoylCoAMAT}, \text{KmmtpC10EnoylCoAMAT}, \text{KmmtpC8EnoylCoAMAT}, \\ \text{KmmtpNADMAT}, \text{KmmtpCoAMAT}, \text{KmmtpC10AcylCoAMAT}, \\ \text{KmmtpC16AcylCoAMAT}, \text{KmmtpC14AcylCoAMAT}, \text{KmmtpC12AcylCoAMAT}, \\ \text{KmmtpC8AcylCoAMAT}, \text{KmmtpC6AcylCoAMAT}, \text{KmmtpNADHMAT}, \\ \text{KmmtpAcetylCoAMAT}, \text{KicrotC4AcetoacylCoA}, \text{Keqmtp}, [\text{C12EnoylCoAMAT}], \\ [\text{C16EnoylCoAMAT}], [\text{C14EnoylCoAMAT}], [\text{C10EnoylCoAMAT}], [\text{C8EnoylCoAMAT}], \\ [\text{NADtMAT}], [\text{C0AMAT}], [\text{C10AcylCoAMAT}], [\text{C16AcylCoAMAT}], \\ [\text{NADHMAT}], [\text{C12AcylCoAMAT}], [\text{C8AcylCoAMAT}], [\text{C6AcylCoAMAT}], \\ [\text{NADHMAT}], [\text{AcetylCoAMAT}], [\text{C4AcetoacylCoAMAT}]) \\ (176)
```

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

Table 220: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmtpC12			0.81	dimensionless	

8.55 Reaction vmtpC10

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

Reaction equation

C10EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C8EnoylCoAMAT, NADtMAT

Reactant

Table 221: Properties of each reactant.

Id	Name	SBO
C10EnoylCoAMAT		

Table 222: Properties of each modifier.

Id	Name	SBO
C16EnoylCoAMAT		
C14EnoylCoAMAT		
C12EnoylCoAMAT		
C8EnoylCoAMAT		
NADtMAT		
CoAMAT		
C16AcylCoAMAT		
C14AcylCoAMAT		
C12AcylCoAMAT		
C10AcylCoAMAT		
C6AcylCoAMAT		
${\tt C4AcetoacylCoAMAT}$		
C10EnoylCoAMAT		
C16EnoylCoAMAT		
C14EnoylCoAMAT		

Id	Name	SBO
C12EnoylCoAMAT		
C8EnoylCoAMAT		
NADtMAT		
CoAMAT		
C8AcylCoAMAT		
C16AcylCoAMAT		
C14AcylCoAMAT		
C12AcylCoAMAT		
C10AcylCoAMAT		
C6AcylCoAMAT		
NADHMAT		
AcetylCoAMAT		
${\tt C4AcetoacylCoAMAT}$		

Products

Table 223: Properties of each product.

Id	Name	SBO
C8AcylCoAMAT		
${\tt AcetylCoAMAT}$		
NADHMAT		

Kinetic Law

Derived unit contains undeclared units

```
\label{eq:v55} \begin{split} v_{55} &= \text{MTP} (\text{sfmtpC10}, \text{Vmtp}, \text{KmmtpC10EnoylCoAMAT}, \text{KmmtpC16EnoylCoAMAT}, \\ & \text{KmmtpC14EnoylCoAMAT}, \text{KmmtpC12EnoylCoAMAT}, \text{KmmtpC8AcylCoAMAT}, \\ & \text{KmmtpNADMAT}, \text{KmmtpCoAMAT}, \text{KmmtpC8AcylCoAMAT}, \\ & \text{KmmtpC16AcylCoAMAT}, \text{KmmtpC14AcylCoAMAT}, \text{KmmtpC12AcylCoAMAT}, \\ & \text{KmmtpC10AcylCoAMAT}, \text{KmmtpC6AcylCoAMAT}, \text{KmmtpNADHMAT}, \\ & \text{KmmtpAcetylCoAMAT}, \text{KicrotC4AcetoacylCoA}, \text{Keqmtp}, [\text{C10EnoylCoAMAT}], \\ & [\text{C16EnoylCoAMAT}], [\text{C14EnoylCoAMAT}], [\text{C12EnoylCoAMAT}], [\text{C8EnoylCoAMAT}], \\ & [\text{NADtMAT}], [\text{CoAMAT}], [\text{C8AcylCoAMAT}], [\text{C16AcylCoAMAT}], [\text{C14AcylCoAMAT}], \\ & [\text{C12AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C6AcylCoAMAT}], [\text{C4AcetoacylCoAMAT}]) \\ & [\text{AcetylCoAMAT}], [\text{C4AcetoacylCoAMAT}] ) \end{split}
```

$$MTP(sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms7, Kms8, \\ Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Ki1, \\ Keq, S1, S2, S3, S4, S5, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8, I1)$$

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

Table 224: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmtpC10			0.73	dimensionless	

8.56 Reaction vmtpC8

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

Reaction equation

Reactant

Table 225: Properties of each reactant.

Id	Name	SBO
C8EnoylCoAMAT		

Table 226: Properties of each modifier.

L		
Id	Name	SBO
C16EnoylCoAMAT		
C14EnoylCoAMAT		
C12EnoylCoAMAT		
C10EnoylCoAMAT		
NADtMAT		
CoAMAT		
C16AcylCoAMAT		

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

Products

Table 227: Properties of each product.

Id	Name	SBO
C6AcylCoAMAT		
${ t AcetylCoAMAT}$		
NADHMAT		

Kinetic Law

Derived unit contains undeclared units

 $v_{56} = MTP (sfmtpC8, Vmtp, KmmtpC8EnoylCoAMAT, KmmtpC16EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC12EnoylCoAMAT, KmmtpC10EnoylCoAMAT, KmmtpC14EnoylCoAMAT, KmmtpC6AcylCoAMAT, KmmtpC16AcylCoAMAT, KmmtpC14AcylCoAMAT, KmmtpC12AcylCoAMAT, KmmtpC10AcylCoAMAT, KmmtpC8AcylCoAMAT, KmmtpNADHMAT, KmmtpAcetylCoAMAT, KicrotC4AcetoacylCoA, Keqmtp, [C8EnoylCoAMAT], [C16EnoylCoAMAT], [C14EnoylCoAMAT], [C12EnoylCoAMAT], [C10EnoylCoAMAT], [NADtMAT], [C0AMAT], [C6AcylCoAMAT], [C16AcylCoAMAT], [C14AcylCoAMAT], [C12AcylCoAMAT], [C4AcetoacylCoAMAT]) [C8AcylCoAMAT], [NADHMAT], [AcetylCoAMAT], [C4AcetoacylCoAMAT]) (182) [C16AcylCoAMAT], [C16AcylCoAMA$

MTP(sf, V, Kms1, Kms2, Kms3, Kms4, Kms5, Kms7, Kms8, Kmp1, Kmp2, Kmp3, Kmp4, Kmp5, Kmp6, Kmp7, Kmp8, Ki1, Keq, S1, S2, S3, S4, S5, S7, S8, P1, P2, P3, P4, P5, P6, P7, P8, I1)

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

Table 228: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmtpC8			0.34	dimensionless	$ \overline{\checkmark} $

8.57 Reaction vacesink

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

Reaction equation

$$AcetylCoAMAT \xrightarrow{AcetylCoAMAT} \emptyset$$
 (184)

Reactant

Table 229: Properties of each reactant.

Id	Name	SBO
AcetylCoAMAT		

Modifier

Table 230: Properties of each modifier.

Id	Name	SBO
AcetylCoAMAT		

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{57} = RES (Ksacesink, [AcetylCoAMAT], K1acesink)$$
 (185)

$$RES(Ks, S, K1) = Ks \cdot (S - K1)$$

$$(186)$$

Table 231: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K1acesink			30.0	$\mu mol \cdot l^{-1}$	
Ksacesink		ϵ	6.000000.0	$1 \cdot (60 \text{ s})^{-1}$	\checkmark

8.58 Reaction vfadhsink

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

Reaction equation

$$FADHMAT \xrightarrow{FADHMAT} \emptyset$$
 (187)

Reactant

Table 232: Properties of each reactant.

Id	Name	SBO
FADHMAT		

Table 233: Properties of each modifier.

Id	Name	SBO
FADHMAT		

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{58} = RES (Ksfadhsink, [FADHMAT], K1fadhsink)$$
 (188)

$$RES(Ks, S, K1) = Ks \cdot (S - K1)$$
(189)

Table 234: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K1fadhsink			0.46	$\mu mol \cdot l^{-1}$	\overline{Z}
Ksfadhsink			6000000.00	$1 \cdot (60 \mathrm{s})^{-1}$	\square

8.59 Reaction vnadhsink

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

Reaction equation

$$NADHMAT \xrightarrow{NADHMAT} \emptyset$$
 (190)

Reactant

Table 235: Properties of each reactant.

Id	Name	SBO
NADHMAT		

Table 236: Properties of each modifier.

Id	Name	SBO
NADHMAT		•

Id	Name	SBO

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{59} = RES (Ksnadhsink, [NADHMAT], K1nadhsink)$$
 (191)

$$RES(Ks, S, K1) = Ks \cdot (S - K1)$$
(192)

Table 237: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K1nadhsink			16.0	$\mu mol \cdot l^{-1}$	Ø
Ksnadhsink			6000000.0	$1 \cdot (60 \mathrm{s})^{-1}$	

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

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}16\mathrm{AcylCarCYT} = |v_1| - |v_2| \tag{193}$$

9.2 Species C16AcylCarMAT

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

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}16\mathrm{AcylCarMAT} = v_2 - v_9 \tag{194}$$

9.3 Species C16AcylCoAMAT

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

This species takes part in 54 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, vvlcadC16, vvlcadC14, vvlcadC14, vvlcadC12, vvlcadC12, vlcadC16, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC12, vlcadC10, vlcadC10, vlcadC10, vlcadC8, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC8, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC8, vmtpC8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}16\mathrm{AcylCoAMAT} = v_9 - v_{16} - v_{19} \tag{195}$$

9.4 Species C16EnoylCoAMAT

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

This species takes part in 40 reactions (as a reactant in vcrotC16, vmtpC16 and as a product in vvlcadC16, vlcadC16 and as a modifier in vvlcadC16, vvlcadC14, vvlcadC14, vvlcadC12, vvlcadC12, vlcadC12, vlcadC16, vlcadC14, vlcadC14, vlcadC12, vlcadC10, vlcadC10, vlcadC8, vcrotC16, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC8, vmtpC8).

$$\frac{d}{dt}C16EnoylCoAMAT = |v_{16}| + |v_{19}| - |v_{31}| - |v_{52}|$$
(196)

9.5 Species C16HydroxyacylCoAMAT

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

This species takes part in 28 reactions (as a reactant in vmschadC16 and as a product in vcrotC16 and as a modifier in vcrotC16, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC3, vcrotC8, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vmschadC16, vmschadC14, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC3, vmschadC6, vmschadC6, vmschadC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}16\mathrm{HydroxyacylCoAMAT} = |v_{31}| - |v_{38}| \tag{197}$$

9.6 Species C16KetoacylCoAMAT

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

This species takes part in 28 reactions (as a reactant in vmckatC16 and as a product in vmschadC16 and as a modifier in vmschadC16, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC3, vmschadC6, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmschadC4, vmckatC16, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC4, vmckatC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}16\mathrm{KetoacylCoAMAT} = v_{38} - v_{45} \tag{198}$$

9.7 Species 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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}14\mathrm{AcylCarCYT} = -v_3 \tag{199}$$

9.8 Species 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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}14\mathrm{AcylCarMAT} = |v_3| - |v_{10}| \tag{200}$$

9.9 Species C14AcylCoAMAT

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

This species takes part in 54 reactions (as a reactant in vvlcadC14, vlcadC14 and as a product in vcpt2C14, vmckatC16, 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, vlcadC16, vlcadC14, vlcadC12, vlcadC12, vlcadC10, vlcadC3, vlcadC8, vmckatC16, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC8, vmckatC6, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC8, vmtpC8).

$$\frac{d}{dt}C14AcylCoAMAT = |v_{10}| + |v_{45}| + |v_{52}| - |v_{17}| - |v_{20}|$$
(201)

9.10 Species C14EnoylCoAMAT

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

This species takes part in 40 reactions (as a reactant in vcrotC14, vmtpC14 and as a product in vvlcadC14, vlcadC14 and as a modifier in vvlcadC16, vvlcadC16, vvlcadC14, vvlcadC12, vvlcadC12, vvlcadC12, vlcadC16, vlcadC16, vlcadC16, vlcadC10, vlcadC10, vlcadC10, vlcadC8, vlcadC8, vcrotC16, vcrotC16, vcrotC14, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vmtpC16, vmtpC16, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC8, vmtpC8).

$$\frac{d}{dt}C14EnoylCoAMAT = |v_{17}| + |v_{20}| - |v_{32}| - |v_{53}|$$
 (202)

9.11 Species C14HydroxyacylCoAMAT

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

This species takes part in 28 reactions (as a reactant in vmschadC14 and as a product in vcrotC14 and as a modifier in vcrotC16, vcrotC16, vcrotC14, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC3, vcrotC8, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vmschadC16, vmschadC16, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC4).

$$\frac{d}{dt}C14HydroxyacylCoAMAT = v_{32} - v_{39}$$
 (203)

9.12 Species C14KetoacylCoAMAT

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

This species takes part in 28 reactions (as a reactant in vmckatC14 and as a product in vmschadC14 and as a modifier in vmschadC16, vmschadC16, vmschadC14, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC3, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmschadC4, vmckatC16, vmckatC14, vmckatC12, vmckatC12, vmckatC10, vmschadC6, vmsch

$$\frac{d}{dt}C14KetoacylCoAMAT = v_{39} - v_{46}$$
 (204)

9.13 Species C12AcylCarCYT

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}12\mathrm{AcylCarCYT} = -v_4 \tag{205}$$

9.14 Species 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, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}12\mathrm{A}\mathrm{c}\mathrm{y}\mathrm{l}\mathrm{C}\mathrm{a}\mathrm{r}\mathrm{M}\mathrm{A}\mathrm{T} = \boxed{v_4 - v_{11}} \tag{206}$$

9.15 Species C12AcylCoAMAT

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

This species takes part in 64 reactions (as a reactant in vvlcadC12, vlcadC12, vmcadC12 and as a product in vcpt2C12, vmckatC14, vmtpC14 and as a modifier in vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vvlcadC16, vvlcadC16, vvlcadC14, vvlcadC14, vvlcadC12, vlcadC16, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC12, vlcadC10, vlcadC10, vlcadC8, vmcadC8, vmcadC12, vmcadC10, vmcadC10, vmcadC10, vmcadC4, vmcadC4, vmcadC4, vmckatC16, vmckatC16, vmckatC14, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmtpC16, vmtpC16, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC8, vmtpC8).

$$\frac{d}{dt}C12AcylCoAMAT = v_{11} + v_{46} + v_{53} - v_{18} - v_{21} - v_{24}$$
 (207)

9.16 Species C12EnoylCoAMAT

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

This species takes part in 49 reactions (as a reactant in vcrotC12, vmtpC12 and as a product in vvlcadC12, vlcadC12, vmcadC12 and as a modifier in vvlcadC16, vvlcadC16, vvlcadC14, vvlcadC14, vvlcadC12, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC10, vlcadC10, vlcadC3, vmcadC8, vmcadC8, vmcadC6, vmcadC6, vmcadC4, vmcadC4, vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC12, vcrotC10, vcrotC3, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC10, vmtpC10, vmtpC8, vmtpC8).

$$\frac{d}{dt}C12EnoylCoAMAT = |v_{18} + |v_{21}| + |v_{24}| - |v_{33}| - |v_{54}|$$
(208)

9.17 Species C12HydroxyacylCoAMAT

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

This species takes part in 28 reactions (as a reactant in vmschadC12 and as a product in vcrotC12 and as a modifier in vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC12, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vmschadC16, vmschadC16, vmschadC14, vmschadC12, vmschadC10, vmschadC10, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}12\mathrm{HydroxyacylCoAMAT} = |v_{33}| - |v_{40}| \tag{209}$$

9.18 Species C12KetoacylCoAMAT

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

This species takes part in 28 reactions (as a reactant in vmckatC12 and as a product in vmschadC12 and as a modifier in vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC12, vmschadC10, vmschadC10, vmschadC3, vmschadC6, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmschadC4, vmckatC16, vmckatC16, vmckatC14, vmckatC12, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC4, vmckatC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}12\mathrm{KetoacylCoAMAT} = v_{40} - v_{47} \tag{210}$$

9.19 Species 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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}10\mathrm{AcylCarCYT} = -v_5 \tag{211}$$

9.20 Species 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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}10\mathrm{AcylCarMAT} = |v_5| - |v_{12}| \tag{212}$$

9.21 Species C10AcylCoAMAT

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

This species takes part in 58 reactions (as a reactant in vlcadC10, vmcadC10 and as a product in vcpt2C10, vmckatC12, vmtpC12 and as a modifier in vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC10, vlcadC8, vlcadC8, vmcadC12, vmcadC12, vmcadC10, vmcadC8, vmcadC6, vmcadC6, vmcadC4, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC12, vmckatC10, vmckatC10, vmckatC3, vmckatC8, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmtpC16, vmtpC16, vmtpC14, vmtpC12, vmtpC10, vmtpC10, vmtpC8, vmtpC8).

$$\frac{d}{dt}C10AcylCoAMAT = |v_{12}| + |v_{47}| + |v_{54}| - |v_{22}| - |v_{25}|$$
(213)

9.22 Species C10EnoylCoAMAT

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

This species takes part in 44 reactions (as a reactant in vcrotC10, vmtpC10 and as a product in vlcadC10, vmcadC10 and as a modifier in vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC10, vlcadC8, vmcadC12, vmcadC12, vmcadC10, vmcadC8, vmcadC8, vmcadC6, vmcadC6, vmcadC6, vmcadC4, vmcadC4, vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC10, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vmtpC16, vmtpC16, vmtpC16, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC8, vmtpC8).

$$\frac{d}{dt}C10EnoylCoAMAT = v_{22} + v_{25} - v_{34} - v_{55}$$
 (214)

9.23 Species C10HydroxyacylCoAMAT

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

This species takes part in 28 reactions (as a reactant in vmschadC10 and as a product in vcrotC10 and as a modifier in vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC10, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC10, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}10\mathrm{HydroxyacylCoAMAT} = v_{34} - v_{41} \tag{215}$$

9.24 Species C10KetoacylCoAMAT

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

This species takes part in 28 reactions (as a reactant in vmckatC10 and as a product in vmschadC10 and as a modifier in vmschadC16, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC10, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmschadC4, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC10, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC4, vmckatC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C}10\mathrm{KetoacylCoAMAT} = v_{41} - v_{48} \tag{216}$$

9.25 Species 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).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{C8AcylCarCYT} = -\nu_6 \tag{217}$$

9.26 Species 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).

$$\frac{d}{dt}C8AcylCarMAT = v_6 - v_{13}$$
 (218)

9.27 Species C8AcylCoAMAT

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

This species takes part in 58 reactions (as a reactant in vlcadC8, vmcadC8 and as a product in vcpt2C8, vmckatC10, vmtpC10 and as a modifier in vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC10, vlcadC10, vlcadC3, vmcadC12, vmcadC12, vmcadC10, vmcadC3, vmcadC6, vmcadC6, vmcadC4, vmcadC4, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC10, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmtpC16, vmtpC16, vmtpC16, vmtpC16, vmtpC12, vmtpC12, vmtpC10, vmtpC8, vmtpC8).

$$\frac{d}{dt}C8AcylCoAMAT = |v_{13}| + |v_{48}| + |v_{55}| - |v_{23}| - |v_{26}|$$
(219)

9.28 Species C8EnoylCoAMAT

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

This species takes part in 44 reactions (as a reactant in vcrotC8, vmtpC8 and as a product in vlcadC8, vmcadC8 and as a modifier in vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC10, vlcadC10, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC6, vmcadC6, vmcadC6, vmcadC4, vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC8, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC8).

$$\frac{d}{dt}C8EnoylCoAMAT = |v_{23}| + |v_{26}| - |v_{35}| - |v_{56}|$$
(220)

9.29 Species C8HydroxyacylCoAMAT

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

This species takes part in 28 reactions (as a reactant in vmschadC8 and as a product in vcrotC8 and as a modifier in vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC8, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vmschadC16, vmschadC16, vmschadC14, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC8, vmschadC6, vmschadC6, vmschadC4, vmschadC4).

$$\frac{\mathrm{d}}{\mathrm{d}t} \text{C8HydroxyacylCoAMAT} = v_{35} - v_{42} \tag{221}$$

9.30 Species C8KetoacylCoAMAT

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

This species takes part in 28 reactions (as a reactant in vmckatC8 and as a product in vmschadC8 and as a modifier in vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC10, vmschadC3, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmschadC4, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC12, vmckatC10, vmckatC10, vmckatC8, vmckatC6, vmckatC6, vmckatC4, vmckatC4).

$$\frac{d}{dt}C8KetoacylCoAMAT = v_{42} - v_{49}$$
 (222)

9.31 Species C6AcylCarCYT

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C6AcylCarCYT} = -v_7 \tag{223}$$

9.32 Species 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, vcpt2C8, vcpt2C6, vcpt2C4, vcpt2C4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C6AcylCarMAT} = v_7 - v_{14} \tag{224}$$

9.33 Species C6AcylCoAMAT

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

This species takes part in 52 reactions (as a reactant in vmcadC6, vscadC6 and as a product in vcpt2C6, vmckatC8, vmtpC8 and as a modifier in vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C4, vcpt2C4, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC8, vmcadC8, vmcadC6, vmcadC4, vmcadC4, vscadC6, vscadC4, vscadC4, vmckatC16, vmckatC16, vmckatC14, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC8, vmckatC6, vmckatC4, vmckatC4, vmtpC16, vmtpC16, vmtpC16, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC8).

$$\frac{d}{dt}C6AcylCoAMAT = |v_{14}| + |v_{49}| + |v_{56}| - |v_{27}| - |v_{29}|$$
(225)

9.34 Species C6EnoylCoAMAT

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

This species takes part in 28 reactions (as a reactant in vcrotC6 and as a product in vmcadC6, vscadC6 and as a modifier in vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC3, vmcadC8, vmcadC6, vmcadC4, vmcadC4, vscadC4, vscadC4, vscadC4, vcrotC16, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC3, vcrotC3, vcrotC4, vcrotC4).

$$\frac{d}{dt}C6EnoylCoAMAT = |v_{27}| + |v_{29}| - |v_{36}|$$
 (226)

9.35 Species C6HydroxyacylCoAMAT

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

This species takes part in 28 reactions (as a reactant in vmschadC6 and as a product in vcrotC6 and as a modifier in vcrotC16, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC8, vcrotC6, vcrotC4, vcrotC4, vmschadC16, vmschadC16, vmschadC16, vmschadC16, vcrotC4, vcrotC4, vcrotC4, vcrotC4, vmschadC16, vmschadC16, vcrotC4, vcrot

vmschadC14, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC3, vmschadC6, vmschadC4, vmschadC4).

$$\frac{d}{dt}C6HydroxyacylCoAMAT = v_{36} - v_{43}$$
 (227)

9.36 Species C6KetoacylCoAMAT

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

This species takes part in 28 reactions (as a reactant in vmckatC6 and as a product in vmschadC6 and as a modifier in vmschadC16, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC8, vmschadC8, vmschadC6, vmschadC4, vmschadC4, vmschadC4, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC10, vmckatC3, vmckatC8, vmschadC6, vmschadC4).

$$\frac{\mathrm{d}}{\mathrm{d}t} \text{C6KetoacylCoAMAT} = v_{43} - v_{50} \tag{228}$$

9.37 Species 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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C4AcylCarCYT} = -v_8 \tag{229}$$

9.38 Species 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).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{C4AcylCarMAT} = v_8 - v_{15} \tag{230}$$

9.39 Species C4AcylCoAMAT

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

This species takes part in 42 reactions (as a reactant in vmcadC4, vscadC4 and as a product in vcpt2C4, vmckatC6 and as a modifier in vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C4, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC8, vmcadC8, vmcadC6, vmcadC6, vmcadC6, vmcadC4, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC6, vmckatC4, vmckatC4).

$$\frac{d}{dt}C4AcylCoAMAT = |v_{15}| + |v_{50}| - |v_{28}| - |v_{30}|$$
(231)

9.40 Species C4EnoylCoAMAT

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

This species takes part in 28 reactions (as a reactant in vcrotC4 and as a product in vmcadC4, vscadC4 and as a modifier in vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC8, vmcadC6, vmcadC6, vmcadC6, vmcadC6, vscadC6, vscadC6, vscadC4, vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC6, vcrotC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C4EnoylCoAMAT} = |v_{28}| + |v_{30}| - |v_{37}| \tag{232}$$

9.41 Species C4HydroxyacylCoAMAT

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

This species takes part in 28 reactions (as a reactant in vmschadC4 and as a product in vcrotC4 and as a modifier in vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC8, vcrotC6, vcrotC6, vcrotC6, vcrotC4, vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC8, vmschadC6, vmschadC6, vmschadC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C4HydroxyacylCoAMAT} = |v_{37}| - |v_{44}| \tag{233}$$

9.42 Species C4AcetoacylCoAMAT

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

This species takes part in 52 reactions (as a reactant in vmckatC4 and as a product in vmschadC4 and as a modifier in vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC3, vcrotC8, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vmschadC16, vmschadC16, vmschadC14, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC3, vmschadC8, vmschadC6, vmschadC6, vmschadC4, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC3, vmckatC6, vmckatC6, vmckatC4, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC3, vmtpC8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C4AcetoacylCoAMAT} = v_{44} - v_{51} \tag{234}$$

9.43 Species AcetylCoAMAT

Initial concentration $30 \, \mu mol \cdot l^{-1}$

This species takes part in 26 reactions (as a reactant in vacesink and as a product in vmckatC16, vmckatC14, vmckatC12, vmckatC10, vmckatC8, vmckatC6, vmckatC4, vmtpC16, vmtpC14, vmtpC12, vmtpC10, vmtpC8 and as a modifier in vmckatC16, vmckatC14, vmckatC12, vmckatC10, vmckatC8, vmckatC6, vmckatC4, vmtpC16, vmtpC14, vmtpC12, vmtpC10, vmtpC8, vacesink).

$$\frac{d}{dt}AcetylCoAMAT = v_{45} + v_{46} + v_{47} + v_{48} + v_{49} + v_{50} + 2v_{51} + v_{52} + v_{53} + v_{54} + v_{55} + v_{56} - v_{57}$$
(235)

9.44 Species FADHMAT

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

This species takes part in 32 reactions (as a reactant in vfadhsink and as a product in vvlcadC16, vvlcadC14, vvlcadC12, vlcadC14, vlcadC12, vlcadC10, vlcadC3, vmcadC12, vmcadC10, vmcadC6, vmcadC6, vmcadC4, vscadC6, vscadC4 and as a modifier in vvlcadC16, vvlcadC14, vvlcadC12, vlcadC12, vlcadC12, vlcadC12, vlcadC12, vlcadC12, vlcadC12, vmcadC12, vmcadC10, vmcadC8, vmcadC6, vmcadC4, vscadC6, vscadC4, vfadhsink).

$$\frac{d}{dt}FADHMAT = v_{16} + v_{17} + v_{18} + v_{19} + v_{20} + v_{21} + v_{22} + v_{23} + v_{24} + v_{25} + v_{26} + v_{27} + v_{28} + v_{29} + v_{30} - v_{58}$$
(236)

9.45 Species NADHMAT

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

This species takes part in 26 reactions (as a reactant in vnadhsink and as a product in vmschadC16, vmschadC14, vmschadC12, vmschadC10, vmschadC8, vmschadC6, vmschadC4, vmtpC16, vmtpC14, vmtpC12, vmtpC10, vmtpC8 and as a modifier in vmschadC16, vmschadC14, vmschadC12, vmschadC10, vmschadC8, vmschadC6, vmschadC4, vmtpC16, vmtpC14, vmtpC12, vmtpC10, vmtpC8, vnadhsink).

$$\frac{d}{dt}NADHMAT = v_{38} + v_{39} + v_{40} + v_{41} + v_{42} + v_{43} + v_{44} + v_{52} + v_{53} + v_{54} + v_{55} + v_{56} - v_{59}$$
(237)

9.46 Species CoAMAT

Initial concentration 4970 µmol·1⁻¹

Involved in rule COAMAT

This species takes part in 38 reactions (as a modifier in vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C4, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC12, vmck

vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC10, vmtpC8, vmtpC8). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

9.47 Species C16AcylCoACYT

Initial concentration $26.8 \ \mu mol \cdot l^{-1}$

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.

9.48 Species CarCYT

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

This species takes part in 16 reactions (as a modifier in vcpt1C16, vcpt1C16, vcactC16, vcactC16, vcactC14, vcactC12, 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:

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

9.49 Species CoACYT

Initial concentration 140 µmol·1⁻¹

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:

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

9.50 Species MalCoACYT

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

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:

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

9.51 Species CarMAT

Initial concentration 950 μ mol·l⁻¹

This species takes part in 28 reactions (as a modifier in vcactC16, vcactC16, vcactC14, vcactC14, vcactC12, vcactC10, 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:

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

9.52 Species FADtMAT

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

This species takes part in 30 reactions (as a modifier in vvlcadC16, vvlcadC16, vvlcadC14, vvlcadC14, vvlcadC12, vvlcadC12, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC12, vlcadC10, vlcadC3, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC3, vmcadC6, vmcadC6, vmcadC4, vmcadC4, vscadC6, vscadC6, vscadC4, vscadC4), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

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

9.53 Species NADtMAT

Initial concentration 250 µmol·1⁻¹

This species takes part in 24 reactions (as a modifier in vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC3, vmschadC8, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC3, vm

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

9.54 Species CoAMATt

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CoAMATt} = 0\tag{244}$$

 $\mathfrak{BML2}^{AT}$ EX 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.

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