SBML Model Report

Model name: "vanEunen2013 - Network dynamics of fatty acid -oxidation (steady-state 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 Chelliah[1] and Kieran Smallbone[2] at January 15th 2014 at 10:54 a. m. and last time modified at March fourth 2014 at 11:24 a. m. Table 1 shows 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	1	initial assignments	0

Model Notes

vanEunen2013 - Network dynamics of fatty acid -oxidation (steady-state 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 steady-state 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: BIOMD0000000505 .

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

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 l

2.4 Unit uM

Name uM

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

2.5 Unit uM_per_min_per_mgProtein

Name uM per min per mgProtein

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

2.6 Unit l_per_min_per_mgProtein

Name l per min per mgProtein

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

2.7 Unit area

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

Definition m^2

2.8 Unit length

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

Definition m

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
VCYT			3	$2.2 \cdot 10^{-6}$	l	☑	
VMAT			3	$1.8 \cdot 10^{-6}$	l	☑	

3.1 Compartment VCYT

This is a three dimensional compartment with a constant size of $2.2 \cdot 10^{-6}$ 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 Condition
C16AcylCarCYT		VCYT	$\mu mol \cdot l^{-1}$	⊟	⊟
C16AcylCarMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C16AcylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C16EnoylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C16HydroxyacylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C16KetoacylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C14AcylCarCYT		VCYT	$\mu mol \cdot l^{-1}$	⊟	⊟
C14AcylCarMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C14AcylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C14EnoylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C14HydroxyacylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C14KetoacylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C12AcylCarCYT		VCYT	$\mu mol \cdot l^{-1}$	⊟	⊟
C12AcylCarMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C12AcylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C12EnoylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C12HydroxyacylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C12KetoacylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C10AcylCarCYT		VCYT	$\mu mol \cdot l^{-1}$	⊟	⊟
C10AcylCarMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C10AcylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
C10EnoylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C10HydroxyacylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C10KetoacylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C8AcylCarCYT		VCYT	$\mu mol \cdot l^{-1}$	⊟	⊟
C8AcylCarMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C8AcylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C8EnoylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C8HydroxyacylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C8KetoacylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C6AcylCarCYT		VCYT	$\mu mol \cdot l^{-1}$	⊟	⊟
C6AcylCarMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C6AcylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C6EnoylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C6HydroxyacylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C6KetoacylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C4AcylCarCYT		VCYT	$\mu mol \cdot l^{-1}$	⊟	⊟
C4AcylCarMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C4AcylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C4EnoylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C4HydroxyacylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
C4AcetoacylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
AcetylCoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
FADHMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
NADHMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	⊟
CoAMAT		VMAT	$\mu mol \cdot l^{-1}$	⊟	☑
C16AcylCoACYT		VCYT	$\mu mol \cdot l^{-1}$	☑	☑
CarCYT		VCYT	$\mu mol \cdot l^{-1}$	☑	☑

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
CoACYT		VCYT	$\mu mol \cdot l^{-1}$	☑	☑
MalCoACYT		VCYT	$\mu mol \cdot l^{-1}$	☑	☑
CarMAT		VMAT	$\mu mol \cdot l^{-1}$	☑	☑
FADtMAT		VMAT	$\mu mol \cdot l^{-1}$	☑	☑
NADtMAT		VMAT	$\mu mol \cdot l^{-1}$	☑	☑
CoAMATt		VMAT	$\mu mol \cdot l^{-1}$	☑	☑

5 Parameters

This model contains 140 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vfcact			0.420	$\mu mol \cdot l^{-1} \cdot (60\ s)^{-1}$	☑
Vrcact			0.420	$\mu mol \cdot l^{-1} \cdot (60\ s)^{-1}$	☑
KmcactCarMAT			130.000	$\mu mol \cdot l^{-1}$	☑
KmcactCarCYT			130.000	$\mu mol \cdot l^{-1}$	☑
KicactCarCYT			200.000	$\mu mol \cdot l^{-1}$	☑
Keqcact			1.000	dimensionless	☑
Vcpt2			0.391	$\mu mol \cdot l^{-1} \cdot (60\ s)^{-1}$	☑
Kmcpt2C16AcylCarMAT			51.000	$\mu mol \cdot l^{-1}$	☑
Kmcpt2C14AcylCarMAT			51.000	$\mu mol \cdot l^{-1}$	☑
Kmcpt2C12AcylCarMAT			51.000	$\mu mol \cdot l^{-1}$	☑
Kmcpt2C10AcylCarMAT			51.000	$\mu mol \cdot l^{-1}$	☑
Kmcpt2C8AcylCarMAT			51.000	$\mu mol \cdot l^{-1}$	☑
Kmcpt2C6AcylCarMAT			51.000	$\mu mol \cdot l^{-1}$	☑
Kmcpt2C4AcylCarMAT			51.000	$\mu mol \cdot l^{-1}$	☑
Kmcpt2CoAMAT			30.000	$\mu mol \cdot l^{-1}$	☑
Kmcpt2C16AcylCoAMAT			38.000	$\mu mol \cdot l^{-1}$	☑
Kmcpt2C14AcylCoAMAT			38.000	$\mu mol \cdot l^{-1}$	☑
Kmcpt2C12AcylCoAMAT			38.000	$\mu mol \cdot l^{-1}$	☑
Kmcpt2C10AcylCoAMAT			38.000	$\mu mol \cdot l^{-1}$	☑
Kmcpt2C8AcylCoAMAT			38.000	$\mu mol \cdot l^{-1}$	☑
Kmcpt2C6AcylCoAMAT			1000.000	$\mu mol \cdot l^{-1}$	☑
Kmcpt2C4AcylCoAMAT			1000000.000	$\mu mol \cdot l^{-1}$	☑
Kmcpt2CarMAT			350.000	$\mu mol \cdot l^{-1}$	☑
Keqcpt2			2.220	dimensionless	☑
Vvlcad			0.008	$\mu mol \cdot l^{-1} \cdot (60\ s)^{-1}$	☑
KmvlcadC16AcylCoAMAT			6.500	$\mu mol \cdot l^{-1}$	☑
KmvlcadC14AcylCoAMAT			4.000	$\mu mol \cdot l^{-1}$	☑
KmvlcadC12AcylCoAMAT			2.700	$\mu mol \cdot l^{-1}$	☑
KmvlcadFAD			0.120	$\mu mol \cdot l^{-1}$	☑
KmvlcadC16EnoylCoAMAT			1.080	$\mu mol \cdot l^{-1}$	☑
KmvlcadC14EnoylCoAMAT			1.080	$\mu mol \cdot l^{-1}$	☑
KmvlcadC12EnoylCoAMAT			1.080	$\mu mol \cdot l^{-1}$	☑
KmvlcadFADH			24.200	$\mu mol \cdot l^{-1}$	☑
Keqvlcad			6.000	dimensionless	☑
Vlcad			0.010	$\mu mol \cdot l^{-1} \cdot (60\ s)^{-1}$	☑
KmlcadC16AcylCoAMAT			2.500	$\mu mol \cdot l^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
KmlcadC14AcylCoAMAT			7.400	$\mu mol \cdot l^{-1}$	☑
KmlcadC12AcylCoAMAT			9.000	$\mu mol \cdot l^{-1}$	☑
KmlcadC10AcylCoAMAT			24.300	$\mu mol \cdot l^{-1}$	☑
KmlcadC8AcylCoAMAT			123.000	$\mu mol \cdot l^{-1}$	☑
KmlcadFAD			0.120	$\mu mol \cdot l^{-1}$	☑
KmlcadC16EnoylCoAMAT			1.080	$\mu mol \cdot l^{-1}$	☑
KmlcadC14EnoylCoAMAT			1.080	$\mu mol \cdot l^{-1}$	☑
KmlcadC12EnoylCoAMAT			1.080	$\mu mol \cdot l^{-1}$	☑
KmlcadC10EnoylCoAMAT			1.080	$\mu mol \cdot l^{-1}$	☑
KmlcadC8EnoylCoAMAT			1.080	$\mu mol \cdot l^{-1}$	☑
KmlcadFADH			24.200	$\mu mol \cdot l^{-1}$	☑
Keqlcad			6.000	dimensionless	☑
Vmcad			0.081	$\mu mol \cdot l^{-1} \cdot (60\ s)^{-1}$	☑
KmmcadC12AcylCoAMAT			5.700	$\mu mol \cdot l^{-1}$	☑
KmmcadC10AcylCoAMAT			5.400	$\mu mol \cdot l^{-1}$	☑
KmmcadC8AcylCoAMAT			4.000	$\mu mol \cdot l^{-1}$	☑
KmmcadC6AcylCoAMAT			9.400	$\mu mol \cdot l^{-1}$	☑
KmmcadC4AcylCoAMAT			135.000	$\mu mol \cdot l^{-1}$	☑
KmmcadFAD			0.120	$\mu mol \cdot l^{-1}$	☑
KmmcadC12EnoylCoAMAT			1.080	$\mu mol \cdot l^{-1}$	☑
KmmcadC10EnoylCoAMAT			1.080	$\mu mol \cdot l^{-1}$	☑
KmmcadC8EnoylCoAMAT			1.080	$\mu mol \cdot l^{-1}$	☑
KmmcadC6EnoylCoAMAT			1.080	$\mu mol \cdot l^{-1}$	☑
KmmcadC4EnoylCoAMAT			1.080	$\mu mol \cdot l^{-1}$	☑
KmmcadFADH			24.200	$\mu mol \cdot l^{-1}$	☑
Keqmcad			6.000	dimensionless	☑
Vscad			0.081	$\mu mol \cdot l^{-1} \cdot (60\ s)^{-1}$	☑
KmscadC6AcylCoAMAT			285.000	$\mu mol \cdot l^{-1}$	☑
KmscadC4AcylCoAMAT			10.700	$\mu mol \cdot l^{-1}$	☑
KmscadFAD			0.120	$\mu mol \cdot l^{-1}$	☑
KmscadC6EnoylCoAMAT			1.080	$\mu mol \cdot l^{-1}$	☑
KmscadC4EnoylCoAMAT			1.080	$\mu mol \cdot l^{-1}$	☑
KmscadFADH			24.200	$\mu mol \cdot l^{-1}$	☑
Keqscad			6.000	dimensionless	☑
Vcrot			3.600	$\mu mol \cdot l^{-1} \cdot (60\ s)^{-1}$	☑
KmcrotC16EnoylCoAMAT			150.000	$\mu mol \cdot l^{-1}$	☑
KmcrotC14EnoylCoAMAT			100.000	$\mu mol \cdot l^{-1}$	☑
KmcrotC12EnoylCoAMAT			25.000	$\mu mol \cdot l^{-1}$	☑
KmcrotC10EnoylCoAMAT			25.000	$\mu mol \cdot l^{-1}$	☑
KmcrotC8EnoylCoAMAT			25.000	$\mu mol \cdot l^{-1}$	☑
KmcrotC6EnoylCoAMAT			25.000	$\mu mol \cdot l^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
KmcrotC4EnoylCoAMAT			40.000	$\mu mol \cdot l^{-1}$	☑
KmcrotC16HydroxyacylCoAMAT			45.000	$\mu mol \cdot l^{-1}$	☑
KmcrotC14HydroxyacylCoAMAT			45.000	$\mu mol \cdot l^{-1}$	☑
KmcrotC12HydroxyacylCoAMAT			45.000	$\mu mol \cdot l^{-1}$	☑
KmcrotC10HydroxyacylCoAMAT			45.000	$\mu mol \cdot l^{-1}$	☑
KmcrotC8HydroxyacylCoAMAT			45.000	$\mu mol \cdot l^{-1}$	☑
KmcrotC6HydroxyacylCoAMAT			45.000	$\mu mol \cdot l^{-1}$	☑
KmcrotC4HydroxyacylCoAMAT			45.000	$\mu mol \cdot l^{-1}$	☑
KicrotC4AcetoacylCoA			1.600	$\mu mol \cdot l^{-1}$	☑
Keqcrot			3.130	dimensionless	☑
Vmschad			1.000	$\mu mol \cdot l^{-1} \cdot (60\ s)^{-1}$	☑
KmmschadC16HydroxyacylCoAMAT			1.500	$\mu mol \cdot l^{-1}$	☑
KmmschadC14HydroxyacylCoAMAT			1.800	$\mu mol \cdot l^{-1}$	☑
KmmschadC12HydroxyacylCoAMAT			3.700	$\mu mol \cdot l^{-1}$	☑
KmmschadC10HydroxyacylCoAMAT			8.800	$\mu mol \cdot l^{-1}$	☑
KmmschadC8HydroxyacylCoAMAT			16.300	$\mu mol \cdot l^{-1}$	☑
KmmschadC6HydroxyacylCoAMAT			28.600	$\mu mol \cdot l^{-1}$	☑
KmmschadC4HydroxyacylCoAMAT			69.900	$\mu mol \cdot l^{-1}$	☑
KmmschadNADMAT			58.500	$\mu mol \cdot l^{-1}$	☑
KmmschadC16KetoacylCoAMAT			1.400	$\mu mol \cdot l^{-1}$	☑
KmmschadC14KetoacylCoAMAT			1.400	$\mu mol \cdot l^{-1}$	☑
KmmschadC12KetoacylCoAMAT			1.600	$\mu mol \cdot l^{-1}$	☑
KmmschadC10KetoacylCoAMAT			2.300	$\mu mol \cdot l^{-1}$	☑
KmmschadC8KetoacylCoAMAT			4.100	$\mu mol \cdot l^{-1}$	☑
KmmschadC6KetoacylCoAMAT			5.800	$\mu mol \cdot l^{-1}$	☑
KmmschadC4AcetoacylCoAMAT			16.900	$\mu mol \cdot l^{-1}$	☑
KmmschadNADHMAT			5.400	$\mu mol \cdot l^{-1}$	☑
Keqmschad			$2.17 \cdot 10^{-4}$	dimensionless	☑
Vmckat			0.377	$\mu mol \cdot l^{-1} \cdot (60\ s)^{-1}$	☑
KmmckatC16KetoacylCoAMAT			1.100	$\mu mol \cdot l^{-1}$	☑
KmmckatC14KetoacylCoAMAT			1.200	$\mu mol \cdot l^{-1}$	☑
KmmckatC12KetoacylCoAMAT			1.300	$\mu mol \cdot l^{-1}$	☑
KmmckatC10KetoacylCoAMAT			2.100	$\mu mol \cdot l^{-1}$	☑
KmmckatC8KetoacylCoAMAT			3.200	$\mu mol \cdot l^{-1}$	☑
KmmckatC6KetoacylCoAMAT			6.700	$\mu mol \cdot l^{-1}$	☑
KmmckatC4AcetoacylCoAMAT			12.400	$\mu mol \cdot l^{-1}$	☑
KmmckatCoAMAT			26.600	$\mu mol \cdot l^{-1}$	☑
KmmckatC14AcylCoAMAT			13.830	$\mu mol \cdot l^{-1}$	☑
KmmckatC16AcylCoAMAT			13.830	$\mu mol \cdot l^{-1}$	☑
KmmckatC12AcylCoAMAT			13.830	$\mu mol \cdot l^{-1}$	☑
KmmckatC10AcylCoAMAT			13.830	$\mu mol \cdot l^{-1}$	☑
KmmckatC8AcylCoAMAT			13.830	$\mu mol \cdot l^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
KmmckatC6AcylCoAMAT			13.830	$\mu mol \cdot l^{-1}$	☑
KmmckatC4AcylCoAMAT			13.830	$\mu mol \cdot l^{-1}$	☑
KmmckatAcetylCoAMAT			30.000	$\mu mol \cdot l^{-1}$	☑
Keqmckat			1051.000	dimensionless	☑
Vmtp			2.840	$\mu mol \cdot l^{-1} \cdot (60\ s)^{-1}$	☑
KmmtpC16EnoylCoAMAT			25.000	$\mu mol \cdot l^{-1}$	☑
KmmtpC14EnoylCoAMAT			25.000	$\mu mol \cdot l^{-1}$	☑
KmmtpC12EnoylCoAMAT			25.000	$\mu mol \cdot l^{-1}$	☑
KmmtpC10EnoylCoAMAT			25.000	$\mu mol \cdot l^{-1}$	☑
KmmtpC8EnoylCoAMAT			25.000	$\mu mol \cdot l^{-1}$	☑
KmmtpNADMAT			60.000	$\mu mol \cdot l^{-1}$	☑
KmmtpCoAMAT			30.000	$\mu mol \cdot l^{-1}$	☑
KmmtpC14AcylCoAMAT			13.830	$\mu mol \cdot l^{-1}$	☑
KmmtpC16AcylCoAMAT			13.830	$\mu mol \cdot l^{-1}$	☑
KmmtpC12AcylCoAMAT			13.830	$\mu mol \cdot l^{-1}$	☑
KmmtpC10AcylCoAMAT			13.830	$\mu mol \cdot l^{-1}$	☑
KmmtpC8AcylCoAMAT			13.830	$\mu mol \cdot l^{-1}$	☑
KmmtpC6AcylCoAMAT			13.830	$\mu mol \cdot l^{-1}$	☑
KmmtpNADHMAT			50.000	$\mu mol \cdot l^{-1}$	☑
KmmtpAcetylCoAMAT			30.000	$\mu mol \cdot l^{-1}$	☑
Keqmtp			0.710	dimensionless	☑

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

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

6.2 Function definition CACT

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

Mathematical Expression

$$\frac{\mathrm{Vf}\cdot\left(\mathrm{S1}\cdot\mathrm{S2}-\frac{\mathrm{P1}\cdot\mathrm{P2}}{\mathrm{Keq}}\right)}{\mathrm{S1}\cdot\mathrm{S2}+\mathrm{Kms2}\cdot\mathrm{S1}+\mathrm{Kms1}\cdot\mathrm{S2}\cdot\left(1+\frac{\mathrm{P2}}{\mathrm{Kip2}}\right)+\frac{\mathrm{Vf}}{\mathrm{Vr}\cdot\mathrm{Keq}}\cdot\left(\mathrm{Kmp2}\cdot\mathrm{P1}\cdot\left(1+\frac{\mathrm{S1}}{\mathrm{Kis1}}\right)+\mathrm{P2}\cdot(\mathrm{Kmp1}+\mathrm{P1})\right)} \quad (2)$$

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

$$\frac{\mathrm{sf}\cdot\mathrm{V}\cdot\left(\frac{\mathrm{S1}\cdot\mathrm{S8}}{\mathrm{Kms1}\cdot\mathrm{Kms8}}-\frac{\mathrm{P1}\cdot\mathrm{P8}}{\mathrm{Kms1}\cdot\mathrm{Kms8}\cdot\mathrm{Keq}}\right)}{\left(1+\frac{\mathrm{S1}}{\mathrm{Kms1}}+\frac{\mathrm{P1}}{\mathrm{Kmp1}}+\frac{\mathrm{S2}}{\mathrm{Kms2}}+\frac{\mathrm{P2}}{\mathrm{Kmp2}}+\frac{\mathrm{S3}}{\mathrm{Kms3}}+\frac{\mathrm{P3}}{\mathrm{Kmp3}}+\frac{\mathrm{S4}}{\mathrm{Kms4}}+\frac{\mathrm{P4}}{\mathrm{Kmp4}}+\frac{\mathrm{S5}}{\mathrm{Kms5}}+\frac{\mathrm{P5}}{\mathrm{Kmp5}}+\frac{\mathrm{S6}}{\mathrm{Kms6}}+\frac{\mathrm{P6}}{\mathrm{Kmp6}}+\frac{\mathrm{S7}}{\mathrm{Kms7}}+\frac{\mathrm{P7}}{\mathrm{Kmp}} \quad (3)$$

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

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

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

$$\frac{\mathrm{sf}\cdot\mathrm{V}\cdot\left(\frac{\mathrm{S1}\cdot(\mathrm{S6}-\mathrm{P6})}{\mathrm{Kms1}\cdot\mathrm{Kms6}}-\frac{\mathrm{P1}\cdot\mathrm{P6}}{\mathrm{Kms1}\cdot\mathrm{Kms6}\cdot\mathrm{Keq}}\right)}{\left(1+\frac{\mathrm{S1}}{\mathrm{Kms1}}+\frac{\mathrm{P1}}{\mathrm{Kmp1}}+\frac{\mathrm{S2}}{\mathrm{Kms2}}+\frac{\mathrm{P2}}{\mathrm{Kmp2}}+\frac{\mathrm{S3}}{\mathrm{Kms3}}+\frac{\mathrm{P3}}{\mathrm{Kmp3}}+\frac{\mathrm{S4}}{\mathrm{Kms4}}+\frac{\mathrm{P4}}{\mathrm{Kmp4}}+\frac{\mathrm{S5}}{\mathrm{Kms5}}+\frac{\mathrm{P5}}{\mathrm{Kmp5}}\right)\cdot\left(1+\frac{\mathrm{S6}-\mathrm{P6}}{\mathrm{Kms6}}+\frac{\mathrm{P6}}{\mathrm{Kmp6}}\right)} \quad (5)$$

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

$$\frac{\mathrm{sf}\cdot \mathrm{V}\cdot \left(\frac{\mathrm{S1}\cdot(\mathrm{S6}-\mathrm{P6})}{\mathrm{Kms1}\cdot\mathrm{Kms6}}-\frac{\mathrm{P1}\cdot\mathrm{P6}}{\mathrm{Kms1}\cdot\mathrm{Kms6}\cdot\mathrm{Keq}}\right)}{\left(1+\frac{\mathrm{S1}}{\mathrm{Kms1}}+\frac{\mathrm{P1}}{\mathrm{Kmp1}}+\frac{\mathrm{S2}}{\mathrm{Kms2}}+\frac{\mathrm{P2}}{\mathrm{Kmp2}}+\frac{\mathrm{S3}}{\mathrm{Kms3}}+\frac{\mathrm{P3}}{\mathrm{Kmp3}}+\frac{\mathrm{S4}}{\mathrm{Kms4}}+\frac{\mathrm{P4}}{\mathrm{Kmp4}}+\frac{\mathrm{S5}}{\mathrm{Kms5}}+\frac{\mathrm{P5}}{\mathrm{Kmp5}}\right)\cdot\left(1+\frac{\mathrm{S6}-\mathrm{P6}}{\mathrm{Kms6}}+\frac{\mathrm{P6}}{\mathrm{Kmp6}}\right)} \tag{6}$$

6.7 Function definition SCAD

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

Mathematical Expression

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

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

$$\frac{\mathrm{sf}\cdot \mathrm{V}\cdot \left(\frac{\mathrm{S1}}{\mathrm{Kms1}}-\frac{\mathrm{P1}}{\mathrm{Kms1}\cdot\mathrm{Keq}}\right)}{1+\frac{\mathrm{S1}}{\mathrm{Kms1}}+\frac{\mathrm{P1}}{\mathrm{Kmp1}}+\frac{\mathrm{S2}}{\mathrm{Kms2}}+\frac{\mathrm{P2}}{\mathrm{Kmp2}}+\frac{\mathrm{S3}}{\mathrm{Kms3}}+\frac{\mathrm{P3}}{\mathrm{Kmp3}}+\frac{\mathrm{S4}}{\mathrm{Kms4}}+\frac{\mathrm{P4}}{\mathrm{Kmp4}}+\frac{\mathrm{S5}}{\mathrm{Kms5}}+\frac{\mathrm{P5}}{\mathrm{Kmp5}}+\frac{\mathrm{S6}}{\mathrm{Kms6}}+\frac{\mathrm{P6}}{\mathrm{Kmp6}}+\frac{\mathrm{S7}}{\mathrm{Kms7}}+\frac{\mathrm{P7}}{\mathrm{Kmp7}}} \tag{8}$$

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

$$\frac{\mathrm{sf}\cdot \mathrm{V}\cdot \left(\frac{\mathrm{S1}\cdot(\mathrm{S8}-\mathrm{P8})}{\mathrm{Kms1}\cdot\mathrm{Kms8}}-\frac{\mathrm{P1}\cdot\mathrm{P8}}{\mathrm{Kms1}\cdot\mathrm{Kms8}\cdot\mathrm{Keq}}\right)}{\left(1+\frac{\mathrm{S1}}{\mathrm{Kms1}}+\frac{\mathrm{P1}}{\mathrm{Kmp1}}+\frac{\mathrm{S2}}{\mathrm{Kms2}}+\frac{\mathrm{P2}}{\mathrm{Kmp2}}+\frac{\mathrm{S3}}{\mathrm{Kms3}}+\frac{\mathrm{P3}}{\mathrm{Kmp3}}+\frac{\mathrm{S4}}{\mathrm{Kms4}}+\frac{\mathrm{P4}}{\mathrm{Kmp4}}+\frac{\mathrm{S5}}{\mathrm{Kms5}}+\frac{\mathrm{P5}}{\mathrm{Kmp5}}+\frac{\mathrm{S6}}{\mathrm{Kms6}}+\frac{\mathrm{P6}}{\mathrm{Kmp6}}+\frac{\mathrm{S7}}{\mathrm{Kms7}}+\frac{\mathrm{P7}}{\mathrm{Kmp}} \tag{9}$$

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

$$\frac{\mathrm{sf}\cdot \mathrm{V}\cdot \left(\frac{\mathrm{S1}\cdot \mathrm{S8}}{\mathrm{Kms1}\cdot \mathrm{Kms8}}-\frac{\mathrm{P1}\cdot \mathrm{P8}}{\mathrm{Kms1}\cdot \mathrm{Kms8}\cdot \mathrm{Keq}}\right)}{\left(1+\frac{\mathrm{S1}}{\mathrm{Kms1}}+\frac{\mathrm{P1}}{\mathrm{Kmp1}}+\frac{\mathrm{S2}}{\mathrm{Kms2}}+\frac{\mathrm{P2}}{\mathrm{Kmp2}}+\frac{\mathrm{S3}}{\mathrm{Kms3}}+\frac{\mathrm{P3}}{\mathrm{Kmp3}}+\frac{\mathrm{S4}}{\mathrm{Kms4}}+\frac{\mathrm{P4}}{\mathrm{Kmp4}}+\frac{\mathrm{S5}}{\mathrm{Kms5}}+\frac{\mathrm{P5}}{\mathrm{Kmp5}}+\frac{\mathrm{S6}}{\mathrm{Kms6}}+\frac{\mathrm{P6}}{\mathrm{Kmp6}}+\frac{\mathrm{S7}}{\mathrm{Kms7}}+\frac{\mathrm{P7}}{\mathrm{Kmp7}}\right.} \tag{10}$$

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

$$\frac{\mathrm{sf}\cdot \mathrm{V}\cdot \left(\frac{\mathrm{S1}\cdot \mathrm{S8}}{\mathrm{Kms1}\cdot \mathrm{Kms8}}-\frac{\mathrm{P8}\cdot \mathrm{P8}}{\mathrm{Kms1}\cdot \mathrm{Kms8}\cdot \mathrm{Keq}}\right)}{\left(1+\frac{\mathrm{S1}}{\mathrm{Kms1}}+\frac{\mathrm{P1}}{\mathrm{Kmp1}}+\frac{\mathrm{S2}}{\mathrm{Kms2}}+\frac{\mathrm{P2}}{\mathrm{Kmp2}}+\frac{\mathrm{S3}}{\mathrm{Kms3}}+\frac{\mathrm{P3}}{\mathrm{Kmp3}}+\frac{\mathrm{S4}}{\mathrm{Kms4}}+\frac{\mathrm{P4}}{\mathrm{Kmp4}}+\frac{\mathrm{S5}}{\mathrm{Kms5}}+\frac{\mathrm{P5}}{\mathrm{Kmp5}}+\frac{\mathrm{S6}}{\mathrm{Kms6}}+\frac{\mathrm{P6}}{\mathrm{Kmp6}}+\frac{\mathrm{S7}}{\mathrm{Kms7}}+\frac{\mathrm{P7}}{\mathrm{Kmp7}}\right.} \tag{11}$$

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

$$\frac{\mathrm{sf}\cdot \mathrm{V}\cdot \left(\frac{\mathrm{S1}\cdot (\mathrm{S7}-\mathrm{P7})\cdot \mathrm{S8}}{\mathrm{Kms1}\cdot \mathrm{Kms7}\cdot \mathrm{Kms8}}-\frac{\mathrm{P1}\cdot \mathrm{P7}\cdot \mathrm{P8}}{\mathrm{Kms1}\cdot \mathrm{Kms7}\cdot \mathrm{Kms8}\cdot \mathrm{Keq}}\right)}{\left(1+\frac{\mathrm{S1}}{\mathrm{Kms1}}+\frac{\mathrm{P1}}{\mathrm{Kmp1}}+\frac{\mathrm{S2}}{\mathrm{Kms2}}+\frac{\mathrm{P2}}{\mathrm{Kmp2}}+\frac{\mathrm{S3}}{\mathrm{Kms3}}+\frac{\mathrm{P3}}{\mathrm{Kmp3}}+\frac{\mathrm{S4}}{\mathrm{Kms4}}+\frac{\mathrm{P4}}{\mathrm{Kmp4}}+\frac{\mathrm{S5}}{\mathrm{Kms5}}+\frac{\mathrm{P5}}{\mathrm{Kmp5}}+\frac{\mathrm{P6}}{\mathrm{Kmp6}}+\frac{\mathrm{I1}}{\mathrm{Ki1}}\right)\cdot \left(1+\frac{\mathrm{S7}-\mathrm{P7}}{\mathrm{Kms7}}+\right.} \tag{12}$$

6.13 Function definition RES

Arguments Ks, S, K1

Mathematical Expression

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

7 Rule

This is an overview of one rule.

7.1 Rule CoAMAT

Rule CoAMAT is an assignment rule for species CoAMAT:

$$\begin{aligned}\mathrm{CoAMAT} = [\mathrm{CoAMATt}] - ([\mathrm{C16AcylCoAMAT}] + [\mathrm{C16EnoylCoAMAT}] \\ + [\mathrm{C16HydroxyacylCoAMAT}] + [\mathrm{C16KetoacylCoAMAT}] + [\mathrm{C14AcylCoAMAT}] \\ + [\mathrm{C14EnoylCoAMAT}] + [\mathrm{C14HydroxyacylCoAMAT}] + [\mathrm{C14KetoacylCoAMAT}] \\ + [\mathrm{C12AcylCoAMAT}] + [\mathrm{C12EnoylCoAMAT}] + [\mathrm{C12HydroxyacylCoAMAT}] \\ + [\mathrm{C12KetoacylCoAMAT}] + [\mathrm{C10AcylCoAMAT}] + [\mathrm{C10EnoylCoAMAT}] \\ + [\mathrm{C10HydroxyacylCoAMAT}] + [\mathrm{C10KetoacylCoAMAT}] + [\mathrm{C8AcylCoAMAT}] \\ + [\mathrm{C8EnoylCoAMAT}] + [\mathrm{C8HydroxyacylCoAMAT}] + [\mathrm{C8KetoacylCoAMAT}] \\ + [\mathrm{C6AcylCoAMAT}] + [\mathrm{C6EnoylCoAMAT}] + [\mathrm{C6HydroxyacylCoAMAT}] \\ + [\mathrm{C6KetoacylCoAMAT}] + [\mathrm{C4AcylCoAMAT}] + [\mathrm{C4EnoylCoAMAT}] \\ + [\mathrm{C4HydroxyacylCoAMAT}] + [\mathrm{C4AcetoacylCoAMAT}] + [\mathrm{AcetylCoAMAT}])\end{aligned} \tag{14}$$

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

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

№	Id	Name	Reaction Equation	SBO
1	vcpt1C16		$\emptyset \xrightleftharpoons{\text{C16AcylCoACYT, CarCYT, CoACYT, MalCoACYT, C16AcylCoACYT, CarCYT,}} \emptyset$	
2	vcactC16		$\text{C16AcylCarCYT} \xrightleftharpoons{\text{CarMAT, CarCYT, C16AcylCarCYT, CarMAT, C16AcylCarMAT,}} \text{C16AcylCarMAT}$	
3	vcactC14		$\text{C14AcylCarCYT} \xrightleftharpoons{\text{CarMAT, CarCYT, C14AcylCarCYT, CarMAT, C14AcylCarMAT,}} \text{C14AcylCarMAT}$	
4	vcactC12		$\text{C12AcylCarCYT} \xrightleftharpoons{\text{CarMAT, CarCYT, C12AcylCarCYT, CarMAT, C12AcylCarMAT,}} \text{C12AcylCarMAT}$	
5	vcactC10		$\text{C10AcylCarCYT} \xrightleftharpoons{\text{CarMAT, CarCYT, C10AcylCarCYT, CarMAT, C10AcylCarMAT,}} \text{C10AcylCarMAT}$	
6	vcactC8		$\text{C8AcylCarCYT} \xrightleftharpoons{\text{CarMAT, CarCYT, C8AcylCarCYT, CarMAT, C8AcylCarMAT, Car}} \text{C8AcylCarMAT}$	
7	vcactC6		$\text{C6AcylCarCYT} \xrightleftharpoons{\text{CarMAT, CarCYT, C6AcylCarCYT, CarMAT, C6AcylCarMAT, Car}} \text{C6AcylCarMAT}$	
8	vcactC4		$\text{C4AcylCarCYT} \xrightleftharpoons{\text{CarMAT, CarCYT, C4AcylCarCYT, CarMAT, C4AcylCarMAT, Car}} \text{C4AcylCarMAT}$	
9	vcpt2C16		$\text{C16AcylCarMAT} \xrightleftharpoons{\text{C14AcylCarMAT, C12AcylCarMAT, C10AcylCarMAT, C8AcylCa}} \text{C16AcylCarMAT}$	
10	vcpt2C14		$\text{C14AcylCarMAT} \xrightleftharpoons{\text{C16AcylCarMAT, C12AcylCarMAT, C10AcylCarMAT, C8AcylCa}} \text{C14AcylCarMAT}$	
11	vcpt2C12		$\text{C12AcylCarMAT} \xrightleftharpoons{\text{C16AcylCarMAT, C14AcylCarMAT, C10AcylCarMAT, C8AcylCa}} \text{C12AcylCarMAT}$	
12	vcpt2C10		$\text{C10AcylCarMAT} \xrightleftharpoons{\text{C16AcylCarMAT, C14AcylCarMAT, C12AcylCarMAT, C8AcylCa}} \text{C10AcylCarMAT}$	
13	vcpt2C8		$\text{C8AcylCarMAT} \xrightleftharpoons{\text{C16AcylCarMAT, C14AcylCarMAT, C12AcylCarMAT, C10AcylCa}} \text{C8AcylCarMAT}$	
14	vcpt2C6		$\text{C6AcylCarMAT} \xrightleftharpoons{\text{C16AcylCarMAT, C14AcylCarMAT, C12AcylCarMAT, C10AcylCa}} \text{C6AcylCarMAT}$	

№	Id	Name	Reaction Equation	SBO
15	vcpt2C4		C4AcylCarMAT $\rightleftharpoons$ C16AcylCarMAT, C14AcylCarMAT, C12AcylCarMAT, C10AcylCa	
16	vvlcadC16		C16AcylCoAMAT + FADHMAT $\rightleftharpoons$ C14AcylCoAMAT, C12AcylCoAMAT, FADtMAT, C14EnoylCoA	
17	vvlcadC14		C14AcylCoAMAT + FADHMAT $\rightleftharpoons$ C16AcylCoAMAT, C12AcylCoAMAT, FADtMAT, C16EnoylCoA	
18	vvlcadC12		C12AcylCoAMAT + FADHMAT $\rightleftharpoons$ C16AcylCoAMAT, C14AcylCoAMAT, FADtMAT, C16EnoylCoA	
19	vlcadC16		C16AcylCoAMAT + FADHMAT $\rightleftharpoons$ C14AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT, C8Acy	
20	vlcadC14		C14AcylCoAMAT + FADHMAT $\rightleftharpoons$ C16AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT, C8Acy	
21	vlcadC12		C12AcylCoAMAT + FADHMAT $\rightleftharpoons$ C16AcylCoAMAT, C14AcylCoAMAT, C10AcylCoAMAT, C8Acy	
22	vlcadC10		C10AcylCoAMAT + FADHMAT $\rightleftharpoons$ C16AcylCoAMAT, C14AcylCoAMAT, C12AcylCoAMAT, C8Acy	
23	vlcadC8		C8AcylCoAMAT + FADHMAT $\rightleftharpoons$ C16AcylCoAMAT, C14AcylCoAMAT, C12AcylCoAMAT, C10Acy	
24	vmcadC12		C12AcylCoAMAT + FADHMAT $\rightleftharpoons$ C10AcylCoAMAT, C8AcylCoAMAT, C6AcylCoAMAT, C4AcylC	
25	vmcadC10		C10AcylCoAMAT + FADHMAT $\rightleftharpoons$ C12AcylCoAMAT, C8AcylCoAMAT, C6AcylCoAMAT, C4AcylC	

№	Id	Name	Reaction Equation	SBO
26	vmcadC8		C8AcylCoAMAT $\rightleftharpoons$ C12AcylCoAMAT, C10AcylCoAMAT, C6AcylCoAMAT, C4AcylC FADHMAT	
27	vmcadC6		C6AcylCoAMAT $\rightleftharpoons$ C12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, C4AcylC FADHMAT	
28	vmcadC4		C4AcylCoAMAT $\rightleftharpoons$ C12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, C6AcylC FADHMAT	
29	vscadC6		C6AcylCoAMAT $\rightleftharpoons$ C4AcylCoAMAT, FADtMAT, C4EnoylCoAMAT, C6AcylCoAMAT FADHMAT	
30	vscadC4		C4AcylCoAMAT $\rightleftharpoons$ C6AcylCoAMAT, FADtMAT, C6EnoylCoAMAT, C4AcylCoAMAT FADHMAT	
31	vcrotC16		C16EnoylCoAMAT $\rightleftharpoons$ C14EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C	
32	vcrotC14		C14EnoylCoAMAT $\rightleftharpoons$ C16EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C	
33	vcrotC12		C12EnoylCoAMAT $\rightleftharpoons$ C16EnoylCoAMAT, C14EnoylCoAMAT, C10EnoylCoAMAT, C	
34	vcrotC10		C10EnoylCoAMAT $\rightleftharpoons$ C16EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C	
35	vcrotC8		C8EnoylCoAMAT $\rightleftharpoons$ C16EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C1	
36	vcrotC6		C6EnoylCoAMAT $\rightleftharpoons$ C16EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C1	
37	vcrotC4		C4EnoylCoAMAT $\rightleftharpoons$ C16EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C1	
38	vmschadC16		C16HydroxyacylCoAMAT $\rightleftharpoons$ C14HydroxyacylCoAMAT, C12HydroxyacylCoAMAT, C NADHMAT	
39	vmschadC14		C14HydroxyacylCoAMAT $\rightleftharpoons$ C16HydroxyacylCoAMAT, C12HydroxyacylCoAMAT, C NADHMAT	

№	Id	Name	Reaction Equation	SBO
40	vmschadC12		C12HydroxyacylCoAMAT $\rightleftharpoons$ C16HydroxyacylCoAMAT, C14HydroxyacylCoAMAT, C NADHMAT	
41	vmschadC10		C10HydroxyacylCoAMAT $\rightleftharpoons$ C16HydroxyacylCoAMAT, C14HydroxyacylCoAMAT, C NADHMAT	
42	vmschadC8		C8HydroxyacylCoAMAT $\rightleftharpoons$ C16HydroxyacylCoAMAT, C14HydroxyacylCoAMAT, C1 NADHMAT	
43	vmschadC6		C6HydroxyacylCoAMAT $\rightleftharpoons$ C16HydroxyacylCoAMAT, C14HydroxyacylCoAMAT, C1 NADHMAT	
44	vmschadC4		C4HydroxyacylCoAMAT $\rightleftharpoons$ C16HydroxyacylCoAMAT, C14HydroxyacylCoAMAT, C1 NADHMAT	
45	vmckatC16		C16KetoacylCoAMAT $\rightleftharpoons$ C14KetoacylCoAMAT, C12KetoacylCoAMAT, C10KetoacylC AcetylCoAMAT	
46	vmckatC14		C14KetoacylCoAMAT $\rightleftharpoons$ C16KetoacylCoAMAT, C12KetoacylCoAMAT, C10KetoacylC AcetylCoAMAT	
47	vmckatC12		C12KetoacylCoAMAT $\rightleftharpoons$ C16KetoacylCoAMAT, C14KetoacylCoAMAT, C10KetoacylC AcetylCoAMAT	
48	vmckatC10		C10KetoacylCoAMAT $\rightleftharpoons$ C16KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylC AcetylCoAMAT	
49	vmckatC8		C8KetoacylCoAMAT $\rightleftharpoons$ C16KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCo AcetylCoAMAT	
50	vmckatC6		C6KetoacylCoAMAT $\rightleftharpoons$ C16KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCo AcetylCoAMAT	

№	Id	Name	Reaction Equation	SBO
51	vmckatC4		C4AcetoacylCoAMAT $\rightleftharpoons$ C16KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylC	
52	vmtpC16		C16EnoylCoAMAT $\rightleftharpoons$ C14EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C AcetylCoAMAT + NADHMAT	
53	vmtpC14		C14EnoylCoAMAT $\rightleftharpoons$ C16EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C AcetylCoAMAT + NADHMAT	
54	vmtpC12		C12EnoylCoAMAT $\rightleftharpoons$ C16EnoylCoAMAT, C14EnoylCoAMAT, C10EnoylCoAMAT, C AcetylCoAMAT + NADHMAT	
55	vmtpC10		C10EnoylCoAMAT $\rightleftharpoons$ C16EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C AcetylCoAMAT + NADHMAT	
56	vmtpC8		C8EnoylCoAMAT $\rightleftharpoons$ C16EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C1 AcetylCoAMAT + NADHMAT	
57	vacesink		AcetylCoAMAT $\rightleftharpoons$ AcetylCoAMAT, AcetylCoAMAT $\rightarrow \emptyset$	
58	vfadhsink		FADHMAT $\rightleftharpoons$ FADHMAT, FADHMAT $\rightarrow \emptyset$	
59	vnadhsink		NADHMAT $\rightleftharpoons$ NADHMAT, NADHMAT $\rightarrow \emptyset$	

8.1 Reaction vcpt1C16

This is a reversible reaction of no reactant forming one product influenced by 14 modifiers.

Reaction equation

$$\emptyset \xrightleftharpoons{\text{C16AcylCoACYT, CarCYT, CoACYT, MalCoACYT, C16AcylCoACYT, CarCYT, C16AcylCarCYT, CoACYT}} \quad (15)$$

Modifiers

Table 6: Properties of each modifier.

Id	Name	SBO
C16AcylCoACYT		
CarCYT		
CoACYT		
MalCoACYT		
C16AcylCoACYT		
CarCYT		
C16AcylCarCYT		
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

$$v_1 = \mathrm{CPT1}\,(\mathrm{sfcpt1C16}, \mathrm{Vcpt1}, \mathrm{Kmcpt1C16AcylCoACYT}, \mathrm{Kmcpt1CarCYT}, \mathrm{Kmcpt1C16AcylCarCYT}, \mathrm{Kmcpt1CoACYT}, \mathrm{Kicpt1MalCoACYT}, \mathrm{Keqcpt1}, [\mathrm{C16AcylCoACYT}], [\mathrm{CarCYT}], [\mathrm{C16AcylCarCYT}], [\mathrm{CoACYT}], [\mathrm{MalCoACYT}], \mathrm{ncpt1}) \tag{16}$$

$$\mathrm{CPT1}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Ki1}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}, \mathrm{I1}, \mathrm{n}) = \frac{\mathrm{sf} \cdot \mathrm{V} \cdot \left(\frac{\mathrm{S1} \cdot \mathrm{S2}}{\mathrm{Kms1} \cdot \mathrm{Kms2}} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Kms1} \cdot \mathrm{Kms2} \cdot \mathrm{Keq}}\right)}{\left(1 + \frac{\mathrm{S1}}{\mathrm{Kms1}} + \frac{\mathrm{P1}}{\mathrm{Kmp1}} + \left(\frac{\mathrm{I1}}{\mathrm{Ki1}}\right)^{\mathrm{n}}\right) \cdot \left(1 + \frac{\mathrm{S2}}{\mathrm{Kms2}} + \frac{\mathrm{P2}}{\mathrm{Kmp2}}\right)} \tag{17}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Keqcpt1			0.450	dimensionless	☑
Kicpt1MalCoACYT			9.100	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
Kmcpt1C16AcylCarCYT			136.000	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
Kmcpt1C16AcylCoACYT			13.800	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
Kmcpt1CarCYT			250.000	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
Kmcpt1CoACYT			40.700	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
Vcpt1			0.012	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
ncpt1			2.480	dimensionless	☑
sfcpt1C16			1.000	dimensionless	☑

8.2 Reaction vcactC16

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

Reaction equation

$$\mathrm{C16AcylCarCYT} \rightleftharpoons \mathrm{CarMAT}, \mathrm{CarCYT}, \mathrm{C16AcylCarCYT}, \mathrm{CarMAT}, \mathrm{C16AcylCarMAT}, \mathrm{CarCYT}, \mathrm{C16AcylCarCYT}, \tag{18}$$

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		
C16AcylCarCYT		
CarMAT		
C16AcylCarMAT		
CarCYT		

Product

Table 11: Properties of each product.

Id	Name	SBO
C16AcylCarMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{CACT}(\mathrm{Vfcact}, \mathrm{Vrcact}, \mathrm{KmcactC16AcylCarCYT}, \mathrm{KmcactCarMAT}, \mathrm{KmcactC16AcylCarMAT}, \mathrm{KmcactCarCYT}, \mathrm{KicactC16AcylCarCYT}, \mathrm{KicactCarCYT}, \mathrm{Keqcact}, [\mathrm{C16AcylCarCYT}], [\mathrm{CarMAT}], [\mathrm{C16AcylCarMAT}], [\mathrm{CarCYT}]) \tag{19}$$

$$\mathrm{CACT}(\mathrm{Vf}, \mathrm{Vr}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kis1}, \mathrm{Kip2}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}) \tag{20}$$

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

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KicactC16AcylCarCYT			56.0	$\mu mol \cdot l^{-1}$	☑
KmcactC16AcylCarCYT			15.0	$\mu mol \cdot l^{-1}$	☑
KmcactC16AcylCarMAT			15.0	$\mu mol \cdot l^{-1}$	☑

8.3 Reaction vcactC14

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

Reaction equation

$$\text{C14AcylCarCYT} \xrightleftharpoons{\text{CarMAT, CarCYT, C14AcylCarCYT, CarMAT, C14AcylCarMAT, CarCYT, C14AcylCarCYT,}} \tag{21}$$

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		
C14AcylCarCYT		
CarMAT		
C14AcylCarMAT		
CarCYT		

Product

Table 15: Properties of each product.

Id	Name	SBO
C14AcylCarMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{CACT}(\mathrm{Vfcact}, \mathrm{Vrcact}, \mathrm{KmcactC14AcylCarCYT}, \mathrm{KmcactCarMAT}, \mathrm{KmcactC14AcylCarMAT}, \mathrm{KmcactCarCYT}, \mathrm{KicactC14AcylCarCYT}, \mathrm{KicactCarCYT}, \mathrm{Keqcact}, [\mathrm{C14AcylCarCYT}], [\mathrm{CarMAT}], [\mathrm{C14AcylCarMAT}], [\mathrm{CarCYT}]) \tag{22}$$

$$\mathrm{CACT}(\mathrm{Vf}, \mathrm{Vr}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kis1}, \mathrm{Kip2}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}) \tag{23}$$
$$= \frac{\mathrm{Vf} \cdot \left(\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}\right)}{\mathrm{S1} \cdot \mathrm{S2} + \mathrm{Kms2} \cdot \mathrm{S1} + \mathrm{Kms1} \cdot \mathrm{S2} \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{Kip2}}\right) + \frac{\mathrm{Vf}}{\mathrm{Vr} \cdot \mathrm{Keq}} \cdot \left(\mathrm{Kmp2} \cdot \mathrm{P1} \cdot \left(1 + \frac{\mathrm{S1}}{\mathrm{Kis1}}\right) + \mathrm{P2} \cdot (\mathrm{Kmp1} + \mathrm{P1})\right)}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KicactC14AcylCarCYT			56.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
KmcactC14AcylCarCYT			15.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
KmcactC14AcylCarMAT			15.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑

8.4 Reaction vcactC12

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

Reaction equation

$$\mathrm{C12AcylCarCYT} \rightleftharpoons \mathrm{CarMAT}, \mathrm{CarCYT}, \mathrm{C12AcylCarCYT}, \mathrm{CarMAT}, \mathrm{C12AcylCarMAT}, \mathrm{CarCYT}, \mathrm{C12AcylCarCYT}, \tag{24}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
C12AcylCarCYT		

Modifiers

Table 18: Properties of each modifier.

Id	Name	SBO
CarMAT		
CarCYT		
C12AcylCarCYT		
CarMAT		
C12AcylCarMAT		
CarCYT		
C12AcylCarCYT		
CarMAT		
C12AcylCarMAT		
CarCYT		

Product

Table 19: Properties of each product.

Id	Name	SBO
C12AcylCarMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{CACT}(\mathrm{Vfcact}, \mathrm{Vrcact}, \mathrm{KmcactC12AcylCarCYT}, \mathrm{KmcactCarMAT}, \mathrm{KmcactC12AcylCarMAT}, \mathrm{KmcactCarCYT}, \mathrm{KicactC12AcylCarCYT}, \mathrm{KicactCarCYT}, \mathrm{Keqcact}, [\mathrm{C12AcylCarCYT}], [\mathrm{CarMAT}], [\mathrm{C12AcylCarMAT}], [\mathrm{CarCYT}]) \tag{25}$$

$$\mathrm{CACT}(\mathrm{Vf}, \mathrm{Vr}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kis1}, \mathrm{Kip2}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}) \tag{26}$$

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

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KicactC12AcylCarCYT			56.0	$\mu mol \cdot l^{-1}$	☑
KmcactC12AcylCarCYT			15.0	$\mu mol \cdot l^{-1}$	☑
KmcactC12AcylCarMAT			15.0	$\mu mol \cdot l^{-1}$	☑

8.5 Reaction vcactC10

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

Reaction equation

$$\text{C10AcylCarCYT} \xrightleftharpoons{\text{CarMAT, CarCYT, C10AcylCarCYT, CarMAT, C10AcylCarMAT, CarCYT, C10AcylCarCYT,}} \quad (27)$$

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		
C10AcylCarCYT		
CarMAT		
C10AcylCarMAT		
CarCYT		

Product

Table 23: Properties of each product.

Id	Name	SBO
C10AcylCarMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{CACT}(\mathrm{Vfcact}, \mathrm{Vrcact}, \mathrm{KmcactC10AcylCarCYT}, \mathrm{KmcactCarMAT}, \mathrm{KmcactC10AcylCarMAT}, \mathrm{KmcactCarCYT}, \mathrm{KicactC10AcylCarCYT}, \mathrm{KicactCarCYT}, \mathrm{Keqcact}, [\mathrm{C10AcylCarCYT}], [\mathrm{CarMAT}], [\mathrm{C10AcylCarMAT}], [\mathrm{CarCYT}]) \tag{28}$$

$$\mathrm{CACT}(\mathrm{Vf}, \mathrm{Vr}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kis1}, \mathrm{Kip2}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}) \tag{29}$$
$$= \frac{\mathrm{Vf} \cdot \left(\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}\right)}{\mathrm{S1} \cdot \mathrm{S2} + \mathrm{Kms2} \cdot \mathrm{S1} + \mathrm{Kms1} \cdot \mathrm{S2} \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{Kip2}}\right) + \frac{\mathrm{Vf}}{\mathrm{Vr} \cdot \mathrm{Keq}} \cdot \left(\mathrm{Kmp2} \cdot \mathrm{P1} \cdot \left(1 + \frac{\mathrm{S1}}{\mathrm{Kis1}}\right) + \mathrm{P2} \cdot (\mathrm{Kmp1} + \mathrm{P1})\right)}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KicactC10AcylCarCYT			56.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
KmcactC10AcylCarCYT			15.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
KmcactC10AcylCarMAT			15.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑

8.6 Reaction vcactC8

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

Reaction equation

$$\mathrm{C8AcylCarCYT} \rightleftharpoons \mathrm{CarMAT}, \mathrm{CarCYT}, \mathrm{C8AcylCarCYT}, \mathrm{CarMAT}, \mathrm{C8AcylCarMAT}, \mathrm{CarCYT}, \mathrm{C8AcylCarCYT}, \mathrm{CarM} \tag{30}$$

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		
C8AcylCarCYT		
CarMAT		
C8AcylCarMAT		
CarCYT		

Product

Table 27: Properties of each product.

Id	Name	SBO
C8AcylCarMAT		

Kinetic Law

Derived unit contains undeclared units

$$\begin{aligned} v_6 = \mathrm{CACT}(&\mathrm{Vfcact}, \mathrm{Vrcact}, \mathrm{KmcactC8AcylCarCYT}, \mathrm{KmcactCarMAT}, \\ &\mathrm{KmcactC8AcylCarMAT}, \mathrm{KmcactCarCYT}, \mathrm{KicactC8AcylCarCYT}, \mathrm{KicactCarCYT}, \\ &\mathrm{Keqcact}, [\mathrm{C8AcylCarCYT}], [\mathrm{CarMAT}], [\mathrm{C8AcylCarMAT}], [\mathrm{CarCYT}]) \end{aligned} \tag{31}$$

$$\mathrm{CACT}(\mathrm{Vf}, \mathrm{Vr}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kis1}, \mathrm{Kip2}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}) \tag{32}$$

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

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KicactC8AcylCarCYT			56.0	$\mu mol \cdot l^{-1}$	☑
KmcactC8AcylCarCYT			15.0	$\mu mol \cdot l^{-1}$	☑
KmcactC8AcylCarMAT			15.0	$\mu mol \cdot l^{-1}$	☑

8.7 Reaction vcactC6

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

Reaction equation

$$\text{C6AcylCarCYT} \xrightleftharpoons{\text{CarMAT, CarCYT, C6AcylCarCYT, CarMAT, C6AcylCarMAT, CarCYT, C6AcylCarCYT, CarM}} \tag{33}$$

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		
C6AcylCarCYT		
CarMAT		
C6AcylCarMAT		
CarCYT		

Product

Table 31: Properties of each product.

Id	Name	SBO
C6AcylCarMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{CACT}(\mathrm{Vfcact}, \mathrm{Vrcact}, \mathrm{KmcactC6AcylCarCYT}, \mathrm{KmcactCarMAT}, \mathrm{KmcactC6AcylCarMAT}, \mathrm{KmcactCarCYT}, \mathrm{KicactC6AcylCarCYT}, \mathrm{KicactCarCYT}, \mathrm{Keqcact}, [\mathrm{C6AcylCarCYT}], [\mathrm{CarMAT}], [\mathrm{C6AcylCarMAT}], [\mathrm{CarCYT}]) \quad (34)$$

$$\mathrm{CACT}(\mathrm{Vf}, \mathrm{Vr}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kis1}, \mathrm{Kip2}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}) \quad (35)$$
$$= \frac{\mathrm{Vf} \cdot \left(\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}\right)}{\mathrm{S1} \cdot \mathrm{S2} + \mathrm{Kms2} \cdot \mathrm{S1} + \mathrm{Kms1} \cdot \mathrm{S2} \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{Kip2}}\right) + \frac{\mathrm{Vf}}{\mathrm{Vr} \cdot \mathrm{Keq}} \cdot \left(\mathrm{Kmp2} \cdot \mathrm{P1} \cdot \left(1 + \frac{\mathrm{S1}}{\mathrm{Kis1}}\right) + \mathrm{P2} \cdot (\mathrm{Kmp1} + \mathrm{P1})\right)}$$

Table 32: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KicactC6AcylCarCYT			56.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
KmcactC6AcylCarCYT			15.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
KmcactC6AcylCarMAT			15.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑

8.8 Reaction vcactC4

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

Reaction equation

$$\mathrm{C4AcylCarCYT} \rightleftharpoons \mathrm{CarMAT}, \mathrm{CarCYT}, \mathrm{C4AcylCarCYT}, \mathrm{CarMAT}, \mathrm{C4AcylCarMAT}, \mathrm{CarCYT}, \mathrm{C4AcylCarCYT}, \mathrm{CarM} \quad (36)$$

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
C4AcylCarCYT		

Id	Name	SBO

Modifiers

Table 34: Properties of each modifier.

Id	Name	SBO
CarMAT		
CarCYT		
C4AcylCarCYT		
CarMAT		
C4AcylCarMAT		
CarCYT		
C4AcylCarCYT		
CarMAT		
C4AcylCarMAT		
CarCYT		

Product

Table 35: Properties of each product.

Id	Name	SBO
C4AcylCarMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{CACT}(\mathrm{Vfcact}, \mathrm{Vrcact}, \mathrm{KmcactC4AcylCarCYT}, \mathrm{KmcactCarMAT}, \mathrm{KmcactC4AcylCarMAT}, \mathrm{KmcactCarCYT}, \mathrm{KicactC4AcylCarCYT}, \mathrm{KicactCarCYT}, \mathrm{Keqcact}, [\mathrm{C4AcylCarCYT}], [\mathrm{CarMAT}], [\mathrm{C4AcylCarMAT}], [\mathrm{CarCYT}]) \quad (37)$$

$$\mathrm{CACT}(\mathrm{Vf}, \mathrm{Vr}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kis1}, \mathrm{Kip2}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{P1}, \mathrm{P2}) \quad (38)$$
$$= \frac{\mathrm{Vf} \cdot \left(\mathrm{S1} \cdot \mathrm{S2} - \frac{\mathrm{P1} \cdot \mathrm{P2}}{\mathrm{Keq}}\right)}{\mathrm{S1} \cdot \mathrm{S2} + \mathrm{Kms2} \cdot \mathrm{S1} + \mathrm{Kms1} \cdot \mathrm{S2} \cdot \left(1 + \frac{\mathrm{P2}}{\mathrm{Kip2}}\right) + \frac{\mathrm{Vf}}{\mathrm{Vr} \cdot \mathrm{Keq}} \cdot \left(\mathrm{Kmp2} \cdot \mathrm{P1} \cdot \left(1 + \frac{\mathrm{S1}}{\mathrm{Kis1}}\right) + \mathrm{P2} \cdot (\mathrm{Kmp1} + \mathrm{P1})\right)}$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KicactC4AcylCarCYT			56.0	$\mu mol \cdot l^{-1}$	☑
KmcactC4AcylCarCYT			15.0	$\mu mol \cdot l^{-1}$	☑
KmcactC4AcylCarMAT			15.0	$\mu mol \cdot l^{-1}$	☑

8.9 Reaction vcpt2C16

This is a reversible reaction of one reactant forming one product influenced by 46 modifiers.

Reaction equation

$$\text{C16AcylCarMAT} \xrightleftharpoons{\text{C14AcylCarMAT, C12AcylCarMAT, C10AcylCarMAT, C8AcylCarMAT, C6AcylCarMAT, C4A}} \tag{39}$$

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		

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

$$v_9 = \mathrm{CPT2}\,(\mathrm{sfcpt2C16}, \mathrm{Vcpt2}, \mathrm{Kmcpt2C16AcylCarMAT}, \mathrm{Kmcpt2C14AcylCarMAT}, \mathrm{Kmcpt2C12AcylCarMAT}, \mathrm{Kmcpt2C10AcylCarMAT}, \mathrm{Kmcpt2C8AcylCarMAT}, \mathrm{Kmcpt2C6AcylCarMAT}, \mathrm{Kmcpt2C4AcylCarMAT}, \mathrm{Kmcpt2CoAMAT}, \mathrm{Kmcpt2C16AcylCoAMAT}, \mathrm{Kmcpt2C14AcylCoAMAT}, \mathrm{Kmcpt2C12AcylCoAMAT}, \mathrm{Kmcpt2C10AcylCoAMAT}, \mathrm{Kmcpt2C8AcylCoAMAT}, \mathrm{Kmcpt2C6AcylCoAMAT}, \mathrm{Kmcpt2C4AcylCoAMAT}, \mathrm{Kmcpt2CarMAT}, \mathrm{Keqcpt2}, [\mathrm{C16AcylCarMAT}], [\mathrm{C14AcylCarMAT}], [\mathrm{C12AcylCarMAT}], [\mathrm{C10AcylCarMAT}], [\mathrm{C8AcylCarMAT}], [\mathrm{C6AcylCarMAT}], [\mathrm{C4AcylCarMAT}], [\mathrm{CoAMAT}], [\mathrm{C16AcylCoAMAT}], [\mathrm{C14AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{C6AcylCoAMAT}], [\mathrm{C4AcylCoAMAT}], [\mathrm{CarMAT}]) \tag{40}$$

$$\mathrm{CPT2}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kms7}, \mathrm{Kms8}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Kmp7}, \mathrm{Kmp8}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{S7}, \mathrm{S8}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}, \mathrm{P7}, \mathrm{P8}) \tag{41}$$

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

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcpt2C16			0.85	dimensionless	☑

8.10 Reaction vcpt2C14

This is a reversible reaction of one reactant forming one product influenced by 46 modifiers.

Reaction equation

$$\mathrm{C14AcylCarMAT} \xrightleftharpoons{\mathrm{C16AcylCarMAT,\ C12AcylCarMAT,\ C10AcylCarMAT,\ C8AcylCarMAT,\ C6AcylCarMAT,\ C4A}} \tag{42}$$

Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
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		
C14AcylCarMAT		
C16AcylCarMAT		
C12AcylCarMAT		

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

Product

Table 43: Properties of each product.

Id	Name	SBO
C14AcylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{CPT2}\,(\mathrm{sfcpt2C14}, \mathrm{Vcpt2}, \mathrm{Kmcpt2C14AcylCarMAT}, \mathrm{Kmcpt2C16AcylCarMAT}, \mathrm{Kmcpt2C12AcylCarMAT}, \mathrm{Kmcpt2C10AcylCarMAT}, \mathrm{Kmcpt2C8AcylCarMAT}, \mathrm{Kmcpt2C6AcylCarMAT}, \mathrm{Kmcpt2C4AcylCoAMAT}, \mathrm{Kmcpt2CoAMAT}, \mathrm{Kmcpt2C14AcylCoAMAT}, \mathrm{Kmcpt2C16AcylCoAMAT}, \mathrm{Kmcpt2C12AcylCoAMAT}, \mathrm{Kmcpt2C10AcylCoAMAT}, \mathrm{Kmcpt2C8AcylCoAMAT}, \mathrm{Kmcpt2C6AcylCoAMAT}, \mathrm{Kmcpt2C4AcylCoAMAT}, \mathrm{Kmcpt2CarMAT}, \mathrm{Keqcpt2}, [\mathrm{C14AcylCarMAT}], [\mathrm{C16AcylCarMAT}], [\mathrm{C12AcylCarMAT}], [\mathrm{C10AcylCarMAT}], [\mathrm{C8AcylCarMAT}], [\mathrm{C6AcylCarMAT}], [\mathrm{C4AcylCarMAT}], [\mathrm{CoAMAT}], [\mathrm{C14AcylCoAMAT}], [\mathrm{C16AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{C6AcylCoAMAT}], [\mathrm{C4AcylCoAMAT}], [\mathrm{CarMAT}]) \quad (43)$$

$$\begin{aligned}&\mathrm{CPT2}\left(\mathrm{sf},\mathrm{V},\mathrm{Kms1},\mathrm{Kms2},\mathrm{Kms3},\mathrm{Kms4},\mathrm{Kms5},\mathrm{Kms6},\mathrm{Kms7},\right.\\&\left.\mathrm{Kms8},\mathrm{Kmp1},\mathrm{Kmp2},\mathrm{Kmp3},\mathrm{Kmp4},\mathrm{Kmp5},\mathrm{Kmp6},\mathrm{Kmp7},\mathrm{Kmp8},\right.\\&\left.\mathrm{Keq},\mathrm{S1},\mathrm{S2},\mathrm{S3},\mathrm{S4},\mathrm{S5},\mathrm{S6},\mathrm{S7},\mathrm{S8},\mathrm{P1},\mathrm{P2},\mathrm{P3},\mathrm{P4},\mathrm{P5},\mathrm{P6},\mathrm{P7},\mathrm{P8}\right)\\&=\frac{\mathrm{sf}\cdot\mathrm{V}\cdot\left(\frac{\mathrm{S1}\cdot\mathrm{S8}}{\mathrm{Kms1}\cdot\mathrm{Kms8}}-\frac{\mathrm{P1}\cdot\mathrm{P8}}{\mathrm{Kms1}\cdot\mathrm{Kms8}\cdot\mathrm{Keq}}\right)}{\left(1+\frac{\mathrm{S1}}{\mathrm{Kms1}}+\frac{\mathrm{P1}}{\mathrm{Kmp1}}+\frac{\mathrm{S2}}{\mathrm{Kms2}}+\frac{\mathrm{P2}}{\mathrm{Kmp2}}+\frac{\mathrm{S3}}{\mathrm{Kms3}}+\frac{\mathrm{P3}}{\mathrm{Kmp3}}+\frac{\mathrm{S4}}{\mathrm{Kms4}}+\frac{\mathrm{P4}}{\mathrm{Kmp4}}+\frac{\mathrm{S5}}{\mathrm{Kms5}}+\frac{\mathrm{P5}}{\mathrm{Kmp5}}+\frac{\mathrm{S6}}{\mathrm{Kms6}}+\frac{\mathrm{P6}}{\mathrm{Kmp6}}+\frac{\mathrm{S7}}{\mathrm{Kms7}}+\frac{\mathrm{P}}{\mathrm{Km}}\right.}\end{aligned}\tag{44}$$

Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcpt2C14			1.0	dimensionless	☑

8.11 Reaction vcpt2C12

This is a reversible reaction of one reactant forming one product influenced by 46 modifiers.

Reaction equation

$$\mathrm{C12AcylCarMAT}\ \underset{}{\overset{\mathrm{C16AcylCarMAT},\ \mathrm{C14AcylCarMAT},\ \mathrm{C10AcylCarMAT},\ \mathrm{C8AcylCarMAT},\ \mathrm{C6AcylCarMAT},\ \mathrm{C4A}}{\rightleftharpoons}}\tag{45}$$

Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
C12AcylCarMAT		

Modifiers

Table 46: Properties of each modifier.

Id	Name	SBO
C16AcylCarMAT		
C14AcylCarMAT		
C10AcylCarMAT		
C8AcylCarMAT		
C6AcylCarMAT		
C4AcylCarMAT		
CoAMAT		

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

Product

Table 47: Properties of each product.

Id	Name	SBO
C12AcylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{CPT2}\,(\mathrm{sfcpt2C12}, \mathrm{Vcpt2}, \mathrm{Kmcpt2C12AcylCarMAT}, \mathrm{Kmcpt2C16AcylCarMAT}, \mathrm{Kmcpt2C14AcylCarMAT}, \mathrm{Kmcpt2C10AcylCarMAT}, \mathrm{Kmcpt2C8AcylCarMAT}, \mathrm{Kmcpt2C6AcylCarMAT}, \mathrm{Kmcpt2C4AcylCarMAT}, \mathrm{Kmcpt2CoAMAT}, \mathrm{Kmcpt2C12AcylCoAMAT}, \mathrm{Kmcpt2C16AcylCoAMAT}, \mathrm{Kmcpt2C14AcylCoAMAT}, \mathrm{Kmcpt2C10AcylCoAMAT}, \mathrm{Kmcpt2C8AcylCoAMAT}, \mathrm{Kmcpt2C6AcylCoAMAT}, \mathrm{Kmcpt2C4AcylCoAMAT}, \mathrm{Kmcpt2CarMAT}, \mathrm{Keqcpt2}, [\mathrm{C12AcylCarMAT}], [\mathrm{C16AcylCarMAT}], [\mathrm{C14AcylCarMAT}], [\mathrm{C10AcylCarMAT}], [\mathrm{C8AcylCarMAT}], [\mathrm{C6AcylCarMAT}], [\mathrm{C4AcylCarMAT}], [\mathrm{CoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C16AcylCoAMAT}], [\mathrm{C14AcylCoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{C6AcylCoAMAT}], [\mathrm{C4AcylCoAMAT}], [\mathrm{CarMAT}]) \tag{46}$$

$$\mathrm{CPT2}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kms7}, \mathrm{Kms8}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Kmp7}, \mathrm{Kmp8}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{S7}, \mathrm{S8}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}, \mathrm{P7}, \mathrm{P8}) \tag{47}$$

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

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 46 modifiers.

Reaction equation

$$\text{C10AcylCarMAT} \rightleftharpoons \text{C16AcylCarMAT, C14AcylCarMAT, C12AcylCarMAT, C8AcylCarMAT, C6AcylCarMAT, C4A} \quad (48)$$

Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
C10AcylCarMAT		

Modifiers

Table 50: Properties of each modifier.

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

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

Product

Table 51: Properties of each product.

Id	Name	SBO
C10AcylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{CPT2}\,(\mathrm{sfcpt2C10}, \mathrm{Vcpt2}, \mathrm{Kmcpt2C10AcylCarMAT}, \mathrm{Kmcpt2C16AcylCarMAT}, \mathrm{Kmcpt2C14AcylCarMAT}, \mathrm{Kmcpt2C12AcylCarMAT}, \mathrm{Kmcpt2C8AcylCarMAT}, \mathrm{Kmcpt2C6AcylCarMAT}, \mathrm{Kmcpt2C4AcylCarMAT}, \mathrm{Kmcpt2CoAMAT}, \mathrm{Kmcpt2C10AcylCoAMAT}, \mathrm{Kmcpt2C16AcylCoAMAT}, \mathrm{Kmcpt2C14AcylCoAMAT}, \mathrm{Kmcpt2C12AcylCoAMAT}, \mathrm{Kmcpt2C8AcylCoAMAT}, \mathrm{Kmcpt2C6AcylCoAMAT}, \mathrm{Kmcpt2C4AcylCoAMAT}, \mathrm{Kmcpt2CarMAT}, \mathrm{Keqcpt2}, [\mathrm{C10AcylCarMAT}], [\mathrm{C16AcylCarMAT}], [\mathrm{C14AcylCarMAT}], [\mathrm{C12AcylCarMAT}], [\mathrm{C8AcylCarMAT}], [\mathrm{C6AcylCarMAT}], [\mathrm{C4AcylCarMAT}], [\mathrm{CoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C16AcylCoAMAT}], [\mathrm{C14AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{C6AcylCoAMAT}], [\mathrm{C4AcylCoAMAT}], [\mathrm{CarMAT}]) \tag{49}$$

$$\mathrm{CPT2}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kms7}, \mathrm{Kms8}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Kmp7}, \mathrm{Kmp8}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{S7}, \mathrm{S8}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}, \mathrm{P7}, \mathrm{P8}) \tag{50}$$

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

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 46 modifiers.

Reaction equation

$$\mathrm{C8AcylCarMAT} \rightleftharpoons \mathrm{C16AcylCarMAT},\ \mathrm{C14AcylCarMAT},\ \mathrm{C12AcylCarMAT},\ \mathrm{C10AcylCarMAT},\ \mathrm{C6AcylCarMAT},\ \mathrm{C4A} \tag{51}$$

Reactant

Table 53: Properties of each reactant.

Id	Name	SBO
C8AcylCarMAT		

Modifiers

Table 54: Properties of each modifier.

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

Id	Name	SBO
C8AcylCoAMAT		
C16AcylCoAMAT		
C14AcylCoAMAT		
C12AcylCoAMAT		
C10AcylCoAMAT		
C6AcylCoAMAT		
C4AcylCoAMAT		
CarMAT		

Product

Table 55: Properties of each product.

Id	Name	SBO
C8AcylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{CPT2}\,(\mathrm{sfcpt2C8}, \mathrm{Vcpt2}, \mathrm{Kmcpt2C8AcylCarMAT}, \mathrm{Kmcpt2C16AcylCarMAT}, \mathrm{Kmcpt2C14AcylCarMAT}, \mathrm{Kmcpt2C12AcylCarMAT}, \mathrm{Kmcpt2C10AcylCarMAT}, \mathrm{Kmcpt2C6AcylCarMAT}, \mathrm{Kmcpt2C4AcylCarMAT}, \mathrm{Kmcpt2CoAMAT}, \mathrm{Kmcpt2C8AcylCoAMAT}, \mathrm{Kmcpt2C16AcylCoAMAT}, \mathrm{Kmcpt2C14AcylCoAMAT}, \mathrm{Kmcpt2C12AcylCoAMAT}, \mathrm{Kmcpt2C10AcylCoAMAT}, \mathrm{Kmcpt2C6AcylCoAMAT}, \mathrm{Kmcpt2C4AcylCoAMAT}, \mathrm{Kmcpt2CarMAT}, \mathrm{Keqcpt2}, [\mathrm{C8AcylCarMAT}], [\mathrm{C16AcylCarMAT}], [\mathrm{C14AcylCarMAT}], [\mathrm{C12AcylCarMAT}], [\mathrm{C10AcylCarMAT}], [\mathrm{C6AcylCarMAT}], [\mathrm{C4AcylCarMAT}], [\mathrm{CoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{C16AcylCoAMAT}], [\mathrm{C14AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C6AcylCoAMAT}], [\mathrm{C4AcylCoAMAT}], [\mathrm{CarMAT}]) \tag{52}$$

$$\mathrm{CPT2}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kms7}, \mathrm{Kms8}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Kmp7}, \mathrm{Kmp8}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{S7}, \mathrm{S8}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}, \mathrm{P7}, \mathrm{P8}) \tag{53}$$

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

Table 56: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcpt2C8			0.35	dimensionless	☑

8.14 Reaction vcpt2C6

This is a reversible reaction of one reactant forming one product influenced by 46 modifiers.

Reaction equation

$$\text{C6AcylCarMAT} \rightleftharpoons \text{C16AcylCarMAT, C14AcylCarMAT, C12AcylCarMAT, C10AcylCarMAT, C8AcylCarMAT, C4A} \quad (54)$$

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		

Id	Name	SBO
C16AcylCarMAT		
C14AcylCarMAT		
C12AcylCarMAT		
C10AcylCarMAT		
C8AcylCarMAT		
C4AcylCarMAT		
CoAMAT		
C6AcylCoAMAT		
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

$$v_{14} = \mathrm{CPT2}\,(\mathrm{sfcpt2C6}, \mathrm{Vcpt2}, \mathrm{Kmcpt2C6AcylCarMAT}, \mathrm{Kmcpt2C16AcylCarMAT}, \mathrm{Kmcpt2C14AcylCarMAT}, \mathrm{Kmcpt2C12AcylCarMAT}, \mathrm{Kmcpt2C10AcylCarMAT}, \mathrm{Kmcpt2C8AcylCarMAT}, \mathrm{Kmcpt2C4AcylCarMAT}, \mathrm{Kmcpt2CoAMAT}, \mathrm{Kmcpt2C6AcylCoAMAT}, \mathrm{Kmcpt2C16AcylCoAMAT}, \mathrm{Kmcpt2C14AcylCoAMAT}, \mathrm{Kmcpt2C12AcylCoAMAT}, \mathrm{Kmcpt2C10AcylCoAMAT}, \mathrm{Kmcpt2C8AcylCoAMAT}, \mathrm{Kmcpt2C4AcylCoAMAT}, \mathrm{Kmcpt2CarMAT}, \mathrm{Keqcpt2}, [\mathrm{C6AcylCarMAT}], [\mathrm{C16AcylCarMAT}], [\mathrm{C14AcylCarMAT}], [\mathrm{C12AcylCarMAT}], [\mathrm{C10AcylCarMAT}], [\mathrm{C8AcylCarMAT}], [\mathrm{C4AcylCarMAT}], [\mathrm{CoAMAT}], [\mathrm{C6AcylCoAMAT}], [\mathrm{C16AcylCoAMAT}], [\mathrm{C14AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{C4AcylCoAMAT}], [\mathrm{CarMAT}]) \tag{55}$$

$$\mathrm{CPT2}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kms7}, \mathrm{Kms8}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Kmp7}, \mathrm{Kmp8}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{S7}, \mathrm{S8}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}, \mathrm{P7}, \mathrm{P8}) \tag{56}$$

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

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 46 modifiers.

Reaction equation

$$\mathrm{C4AcylCarMAT} \xrightleftharpoons{\mathrm{C16AcylCarMAT},\ \mathrm{C14AcylCarMAT},\ \mathrm{C12AcylCarMAT},\ \mathrm{C10AcylCarMAT},\ \mathrm{C8AcylCarMAT},\ \mathrm{C6A}} \tag{57}$$

Reactant

Table 61: Properties of each reactant.

Id	Name	SBO
C4AcylCarMAT		

Modifiers

Table 62: Properties of each modifier.

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

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

Product

Table 63: Properties of each product.

Id	Name	SBO
C4AcylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{CPT2}\,(\mathrm{sfcpt2C4}, \mathrm{Vcpt2}, \mathrm{Kmcpt2C4AcylCarMAT}, \mathrm{Kmcpt2C16AcylCarMAT}, \mathrm{Kmcpt2C14AcylCarMAT}, \mathrm{Kmcpt2C12AcylCarMAT}, \mathrm{Kmcpt2C10AcylCarMAT}, \mathrm{Kmcpt2C8AcylCarMAT}, \mathrm{Kmcpt2C6AcylCarMAT}, \mathrm{Kmcpt2CoAMAT}, \mathrm{Kmcpt2C4AcylCoAMAT}, \mathrm{Kmcpt2C16AcylCoAMAT}, \mathrm{Kmcpt2C14AcylCoAMAT}, \mathrm{Kmcpt2C12AcylCoAMAT}, \mathrm{Kmcpt2C10AcylCoAMAT}, \mathrm{Kmcpt2C8AcylCoAMAT}, \mathrm{Kmcpt2C6AcylCoAMAT}, \mathrm{Kmcpt2CarMAT}, \mathrm{Keqcpt2}, [\mathrm{C4AcylCarMAT}], [\mathrm{C16AcylCarMAT}], [\mathrm{C14AcylCarMAT}], [\mathrm{C12AcylCarMAT}], [\mathrm{C10AcylCarMAT}], [\mathrm{C8AcylCarMAT}], [\mathrm{C6AcylCarMAT}], [\mathrm{CoAMAT}], [\mathrm{C4AcylCoAMAT}], [\mathrm{C16AcylCoAMAT}], [\mathrm{C14AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{C6AcylCoAMAT}], [\mathrm{CarMAT}]) \tag{58}$$

$$\begin{aligned}&\mathrm{CPT2}\left(\mathrm{sf},\mathrm{V},\mathrm{Kms1},\mathrm{Kms2},\mathrm{Kms3},\mathrm{Kms4},\mathrm{Kms5},\mathrm{Kms6},\mathrm{Kms7},\right.\\&\left.\mathrm{Kms8},\mathrm{Kmp1},\mathrm{Kmp2},\mathrm{Kmp3},\mathrm{Kmp4},\mathrm{Kmp5},\mathrm{Kmp6},\mathrm{Kmp7},\mathrm{Kmp8},\right.\\&\left.\mathrm{Keq},\mathrm{S1},\mathrm{S2},\mathrm{S3},\mathrm{S4},\mathrm{S5},\mathrm{S6},\mathrm{S7},\mathrm{S8},\mathrm{P1},\mathrm{P2},\mathrm{P3},\mathrm{P4},\mathrm{P5},\mathrm{P6},\mathrm{P7},\mathrm{P8}\right)\\&=\frac{\mathrm{sf}\cdot\mathrm{V}\cdot\left(\frac{\mathrm{S1}\cdot\mathrm{S8}}{\mathrm{Kms1}\cdot\mathrm{Kms8}}-\frac{\mathrm{P1}\cdot\mathrm{P8}}{\mathrm{Kms1}\cdot\mathrm{Kms8}\cdot\mathrm{Keq}}\right)}{\left(1+\frac{\mathrm{S1}}{\mathrm{Kms1}}+\frac{\mathrm{P1}}{\mathrm{Kmp1}}+\frac{\mathrm{S2}}{\mathrm{Kms2}}+\frac{\mathrm{P2}}{\mathrm{Kmp2}}+\frac{\mathrm{S3}}{\mathrm{Kms3}}+\frac{\mathrm{P3}}{\mathrm{Kmp3}}+\frac{\mathrm{S4}}{\mathrm{Kms4}}+\frac{\mathrm{P4}}{\mathrm{Kmp4}}+\frac{\mathrm{S5}}{\mathrm{Kms5}}+\frac{\mathrm{P5}}{\mathrm{Kmp5}}+\frac{\mathrm{S6}}{\mathrm{Kms6}}+\frac{\mathrm{P6}}{\mathrm{Kmp6}}+\frac{\mathrm{S7}}{\mathrm{Kms7}}+\frac{\mathrm{P}}{\mathrm{Km}}\right.}\end{aligned}\tag{59}$$

Table 64: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcpt2C4			0.01	dimensionless	☑

8.16 Reaction vvlcadC16

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

Reaction equation

$$\mathrm{C16AcylCoAMAT} \rightleftharpoons \mathrm{C14AcylCoAMAT},\ \mathrm{C12AcylCoAMAT},\ \mathrm{FADtMAT},\ \mathrm{C14EnoylCoAMAT},\ \mathrm{C12EnoylCoAMAT},\ \mathrm{C}\tag{60}$$

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		

Id	Name	SBO
C12AcylCoAMAT		
FADtMAT		
C16EnoylCoAMAT		
C14EnoylCoAMAT		
C12EnoylCoAMAT		
FADHMAT		
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

$$v_{16} = \mathrm{VLCAD}\,(\mathrm{sfvlcadC16}, \mathrm{Vvlcad}, \mathrm{KmvlcadC16AcylCoAMAT}, \mathrm{KmvlcadC14AcylCoAMAT}, \mathrm{KmvlcadC12AcylCoAMAT}, \mathrm{KmvlcadFAD}, \mathrm{KmvlcadC16EnoylCoAMAT}, \mathrm{KmvlcadC14EnoylCoAMAT}, \mathrm{KmvlcadC12EnoylCoAMAT}, \mathrm{KmvlcadFADH}, \mathrm{Keqvlcad}, [\mathrm{C16AcylCoAMAT}], [\mathrm{C14AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{FADtMAT}], [\mathrm{C16EnoylCoAMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{FADHMAT}]) \tag{61}$$

$$\mathrm{VLCAD}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}) = \frac{\mathrm{sf} \cdot \mathrm{V} \cdot \left(\frac{\mathrm{S1} \cdot (\mathrm{S4} - \mathrm{P4})}{\mathrm{Kms1} \cdot \mathrm{Kms4}} - \frac{\mathrm{P1} \cdot \mathrm{P4}}{\mathrm{Kms1} \cdot \mathrm{Kms4} \cdot \mathrm{Keq}} \right)}{\left(1 + \frac{\mathrm{S1}}{\mathrm{Kms1}} + \frac{\mathrm{P1}}{\mathrm{Kmp1}} + \frac{\mathrm{S2}}{\mathrm{Kms2}} + \frac{\mathrm{P2}}{\mathrm{Kmp2}} + \frac{\mathrm{S3}}{\mathrm{Kms3}} + \frac{\mathrm{P3}}{\mathrm{Kmp3}} \right) \cdot \left(1 + \frac{\mathrm{S4} - \mathrm{P4}}{\mathrm{Kms4}} + \frac{\mathrm{P4}}{\mathrm{Kmp4}} \right)} \tag{62}$$

Table 68: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfvlcadC16			1.0	dimensionless	☑

8.17 Reaction vvlcadC14

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

Reaction equation

$$\text{C14AcylCoAMAT} \xrightleftharpoons{\text{C16AcylCoAMAT, C12AcylCoAMAT, FADtMAT, C16EnoylCoAMAT, C12EnoylCoAMAT, C} \quad \text{(63)}$$

Reactant

Table 69: Properties of each reactant.

Id	Name	SBO
C14AcylCoAMAT		

Modifiers

Table 70: Properties of each modifier.

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

Id	Name	SBO
C12AcylCoAMAT		
FADtMAT		
C14EnoylCoAMAT		
C16EnoylCoAMAT		
C12EnoylCoAMAT		
FADHMAT		

Products

Table 71: Properties of each product.

Id	Name	SBO
C14EnoylCoAMAT		
FADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{VLCAD}\,(\mathrm{sfvlcadC14}, \mathrm{Vvlcad}, \mathrm{KmvlcadC14AcylCoAMAT}, \mathrm{KmvlcadC16AcylCoAMAT}, \mathrm{KmvlcadC12AcylCoAMAT}, \mathrm{KmvlcadFAD}, \mathrm{KmvlcadC14EnoylCoAMAT}, \mathrm{KmvlcadC16EnoylCoAMAT}, \mathrm{KmvlcadC12EnoylCoAMAT}, \mathrm{KmvlcadFADH}, \mathrm{Keqvlcad}, [\mathrm{C14AcylCoAMAT}], [\mathrm{C16AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{FADtMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{C16EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{FADHMAT}]) \tag{64}$$

$$\mathrm{VLCAD}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}) = \frac{\mathrm{sf} \cdot \mathrm{V} \cdot \left(\frac{\mathrm{S1} \cdot (\mathrm{S4} - \mathrm{P4})}{\mathrm{Kms1} \cdot \mathrm{Kms4}} - \frac{\mathrm{P1} \cdot \mathrm{P4}}{\mathrm{Kms1} \cdot \mathrm{Kms4} \cdot \mathrm{Keq}}\right)}{\left(1 + \frac{\mathrm{S1}}{\mathrm{Kms1}} + \frac{\mathrm{P1}}{\mathrm{Kmp1}} + \frac{\mathrm{S2}}{\mathrm{Kms2}} + \frac{\mathrm{P2}}{\mathrm{Kmp2}} + \frac{\mathrm{S3}}{\mathrm{Kms3}} + \frac{\mathrm{P3}}{\mathrm{Kmp3}}\right) \cdot \left(1 + \frac{\mathrm{S4} - \mathrm{P4}}{\mathrm{Kms4}} + \frac{\mathrm{P4}}{\mathrm{Kmp4}}\right)} \tag{65}$$

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 21 modifiers.

Reaction equation

$$\text{C12AcylCoAMAT} \xrightleftharpoons{\text{C16AcylCoAMAT, C14AcylCoAMAT, FADtMAT, C16EnoylCoAMAT, C14EnoylCoAMAT, C}} \tag{66}$$

Reactant

Table 73: Properties of each reactant.

Id	Name	SBO
C12AcylCoAMAT		

Modifiers

Table 74: Properties of each modifier.

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

Products

Table 75: Properties of each product.

Id	Name	SBO
C12EnoylCoAMAT		
FADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \mathrm{VLCAD}\left(\mathrm{sfvlcadC12}, \mathrm{Vvlcad}, \mathrm{KmvlcadC12AcylCoAMAT}, \mathrm{KmvlcadC16AcylCoAMAT}, \mathrm{KmvlcadC14AcylCoAMAT}, \mathrm{KmvlcadFAD}, \mathrm{KmvlcadC12EnoylCoAMAT}, \mathrm{KmvlcadC16EnoylCoAMAT}, \mathrm{KmvlcadC14EnoylCoAMAT}, \mathrm{KmvlcadFADH}, \mathrm{Keqvlcad}, [\mathrm{C12AcylCoAMAT}], [\mathrm{C16AcylCoAMAT}], [\mathrm{C14AcylCoAMAT}], [\mathrm{FADtMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C16EnoylCoAMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{FADHMAT}]\right) \tag{67}$$

$$\mathrm{VLCAD}\left(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}\right) = \frac{\mathrm{sf} \cdot \mathrm{V} \cdot \left(\frac{\mathrm{S1} \cdot (\mathrm{S4} - \mathrm{P4})}{\mathrm{Kms1} \cdot \mathrm{Kms4}} - \frac{\mathrm{P1} \cdot \mathrm{P4}}{\mathrm{Kms1} \cdot \mathrm{Kms4} \cdot \mathrm{Keq}}\right)}{\left(1 + \frac{\mathrm{S1}}{\mathrm{Kms1}} + \frac{\mathrm{P1}}{\mathrm{Kmp1}} + \frac{\mathrm{S2}}{\mathrm{Kms2}} + \frac{\mathrm{P2}}{\mathrm{Kmp2}} + \frac{\mathrm{S3}}{\mathrm{Kms3}} + \frac{\mathrm{P3}}{\mathrm{Kmp3}}\right) \cdot \left(1 + \frac{\mathrm{S4} - \mathrm{P4}}{\mathrm{Kms4}} + \frac{\mathrm{P4}}{\mathrm{Kmp4}}\right)} \tag{68}$$

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 33 modifiers.

Reaction equation

$$\mathrm{C16AcylCoAMAT} \xrightleftharpoons{\mathrm{C14AcylCoAMAT,\ C12AcylCoAMAT,\ C10AcylCoAMAT,\ C8AcylCoAMAT,\ FADtMAT,\ C14} \quad \text{(69)}$$

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		
C16AcylCoAMAT		
C14AcylCoAMAT		
C12AcylCoAMAT		
C10AcylCoAMAT		
C8AcylCoAMAT		
FADtMAT		
C16EnoylCoAMAT		
C14EnoylCoAMAT		
C12EnoylCoAMAT		

Id	Name	SBO
C10EnoylCoAMAT		
C8EnoylCoAMAT		
FADHMAT		

Products

Table 79: Properties of each product.

Id	Name	SBO
C16EnoylCoAMAT		
FADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \mathrm{LCAD}\,(\mathrm{sflcadC16}, \mathrm{Vlcad}, \mathrm{KmlcadC16AcylCoAMAT}, \mathrm{KmlcadC14AcylCoAMAT}, \mathrm{KmlcadC12AcylCoAMAT}, \mathrm{KmlcadC10AcylCoAMAT}, \mathrm{KmlcadC8AcylCoAMAT}, \mathrm{KmlcadFAD}, \mathrm{KmlcadC16EnoylCoAMAT}, \mathrm{KmlcadC14EnoylCoAMAT}, \mathrm{KmlcadC12EnoylCoAMAT}, \mathrm{KmlcadC10EnoylCoAMAT}, \mathrm{KmlcadC8EnoylCoAMAT}, \mathrm{KmlcadFADH}, \mathrm{Keqlcad}, [\mathrm{C16AcylCoAMAT}], [\mathrm{C14AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{FADtMAT}], [\mathrm{C16EnoylCoAMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{FADHMAT}]) \tag{70}$$

$$\mathrm{LCAD}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}) \tag{71}$$

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

Table 80: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sflcadC16			0.9	dimensionless	☑

8.20 Reaction vlcadC14

This is a reversible reaction of one reactant forming two products influenced by 33 modifiers.

Reaction equation

$$\text{C14AcylCoAMAT} \xrightleftharpoons{\text{C16AcylCoAMAT, C12AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, FADtMAT, C16} \quad (72)$$

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		

Id	Name	SBO
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

Derived unit contains undeclared units

$$v_{20} = \mathrm{LCAD}\,(\mathrm{sflcadC14}, \mathrm{Vlcad}, \mathrm{KmlcadC14AcylCoAMAT}, \mathrm{KmlcadC16AcylCoAMAT}, \mathrm{KmlcadC12AcylCoAMAT}, \mathrm{KmlcadC10AcylCoAMAT}, \mathrm{KmlcadC8AcylCoAMAT}, \mathrm{KmlcadFAD}, \mathrm{KmlcadC14EnoylCoAMAT}, \mathrm{KmlcadC16EnoylCoAMAT}, \mathrm{KmlcadC12EnoylCoAMAT}, \mathrm{KmlcadC10EnoylCoAMAT}, \mathrm{KmlcadC8EnoylCoAMAT}, \mathrm{KmlcadFADH}, \mathrm{Keqlcad}, [\mathrm{C14AcylCoAMAT}], [\mathrm{C16AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{FADtMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{C16EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{FADHMAT}]) \tag{73}$$

$$\mathrm{LCAD}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}) \tag{74}$$

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

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 31 modifiers.

Reaction equation

$$\text{C12AcylCoAMAT} \xrightleftharpoons{\text{C16AcylCoAMAT, C14AcylCoAMAT, C10AcylCoAMAT, C8AcylCoAMAT, FADtMAT, C14}} \tag{75}$$

Reactant

Table 85: Properties of each reactant.

Id	Name	SBO
C12AcylCoAMAT		

Modifiers

Table 86: Properties of each modifier.

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

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

Products

Table 87: Properties of each product.

Id	Name	SBO
C12EnoylCoAMAT		
FADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \mathrm{LCAD}\,(\mathrm{sflcadC12}, \mathrm{Vlcad}, \mathrm{KmlcadC12AcylCoAMAT}, \mathrm{KmlcadC16AcylCoAMAT}, \mathrm{KmlcadC14AcylCoAMAT}, \mathrm{KmlcadC10AcylCoAMAT}, \mathrm{KmlcadC8AcylCoAMAT}, \mathrm{KmlcadFAD}, \mathrm{KmlcadC12EnoylCoAMAT}, \mathrm{KmlcadC16EnoylCoAMAT}, \mathrm{KmlcadC14EnoylCoAMAT}, \mathrm{KmlcadC10EnoylCoAMAT}, \mathrm{KmlcadC8EnoylCoAMAT}, \mathrm{KmlcadFADH}, \mathrm{Keqlcad}, [\mathrm{C12AcylCoAMAT}], [\mathrm{C16AcylCoAMAT}], [\mathrm{C14AcylCoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{FADtMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{C16EnoylCoAMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{FADHMAT}]) \quad (76)$$

$$\begin{aligned}&\mathrm{LCAD}\left(\mathrm{sf},\mathrm{V},\mathrm{Kms1},\mathrm{Kms2},\mathrm{Kms3},\mathrm{Kms4},\mathrm{Kms5},\mathrm{Kms6},\mathrm{Kmp1},\mathrm{Kmp2},\right. \qquad (77)\\ &\left.\mathrm{Kmp3},\mathrm{Kmp4},\mathrm{Kmp5},\mathrm{Kmp6},\mathrm{Keq},\mathrm{S1},\mathrm{S2},\mathrm{S3},\mathrm{S4},\mathrm{S5},\mathrm{S6},\mathrm{P1},\mathrm{P2},\mathrm{P3},\mathrm{P4},\mathrm{P5},\mathrm{P6}\right)\\ &= \frac{\mathrm{sf}\cdot\mathrm{V}\cdot\left(\frac{\mathrm{S1}\cdot(\mathrm{S6}-\mathrm{P6})}{\mathrm{Kms1}\cdot\mathrm{Kms6}}-\frac{\mathrm{P1}\cdot\mathrm{P6}}{\mathrm{Kms1}\cdot\mathrm{Kms6}\cdot\mathrm{Keq}}\right)}{\left(1+\frac{\mathrm{S1}}{\mathrm{Kms1}}+\frac{\mathrm{P1}}{\mathrm{Kmp1}}+\frac{\mathrm{S2}}{\mathrm{Kms2}}+\frac{\mathrm{P2}}{\mathrm{Kmp2}}+\frac{\mathrm{S3}}{\mathrm{Kms3}}+\frac{\mathrm{P3}}{\mathrm{Kmp3}}+\frac{\mathrm{S4}}{\mathrm{Kms4}}+\frac{\mathrm{P4}}{\mathrm{Kmp4}}+\frac{\mathrm{S5}}{\mathrm{Kms5}}+\frac{\mathrm{P5}}{\mathrm{Kmp5}}\right)\cdot\left(1+\frac{\mathrm{S6}-\mathrm{P6}}{\mathrm{Kms6}}+\frac{\mathrm{P6}}{\mathrm{Kmp6}}\right)}\end{aligned}$$

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 33 modifiers.

Reaction equation

$$\mathrm{C10AcylCoAMAT} \rightleftharpoons \mathrm{C16AcylCoAMAT},\ \mathrm{C14AcylCoAMAT},\ \mathrm{C12AcylCoAMAT},\ \mathrm{C8AcylCoAMAT},\ \mathrm{FADtMAT},\ \mathrm{C16} \qquad (78)$$

Reactant

Table 89: Properties of each reactant.

Id	Name	SBO
C10AcylCoAMAT		

Modifiers

Table 90: Properties of each modifier.

Id	Name	SBO
C16AcylCoAMAT		
C14AcylCoAMAT		
C12AcylCoAMAT		
C8AcylCoAMAT		
FADtMAT		
C16EnoylCoAMAT		
C14EnoylCoAMAT		
C12EnoylCoAMAT		

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

Products

Table 91: Properties of each product.

Id	Name	SBO
C10EnoylCoAMAT		
FADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \mathrm{LCAD}\,(\mathrm{sflcadC10}, \mathrm{Vlcad}, \mathrm{KmlcadC10AcylCoAMAT}, \mathrm{KmlcadC16AcylCoAMAT}, \mathrm{KmlcadC14AcylCoAMAT}, \mathrm{KmlcadC12AcylCoAMAT}, \mathrm{KmlcadC8AcylCoAMAT}, \mathrm{KmlcadFAD}, \mathrm{KmlcadC10EnoylCoAMAT}, \mathrm{KmlcadC16EnoylCoAMAT}, \mathrm{KmlcadC14EnoylCoAMAT}, \mathrm{KmlcadC12EnoylCoAMAT}, \mathrm{KmlcadC8EnoylCoAMAT}, \mathrm{KmlcadFADH}, \mathrm{Keqlcad}, [\mathrm{C10AcylCoAMAT}], [\mathrm{C16AcylCoAMAT}], [\mathrm{C14AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{FADtMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{C16EnoylCoAMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{FADHMAT}]) \tag{79}$$

$$\mathrm{LCAD}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}) \tag{80}$$
$$= \frac{\mathrm{sf} \cdot \mathrm{V} \cdot \left(\frac{\mathrm{S1} \cdot (\mathrm{S6} - \mathrm{P6})}{\mathrm{Kms1} \cdot \mathrm{Kms6}} - \frac{\mathrm{P1} \cdot \mathrm{P6}}{\mathrm{Kms1} \cdot \mathrm{Kms6} \cdot \mathrm{Keq}}\right)}{\left(1 + \frac{\mathrm{S1}}{\mathrm{Kms1}} + \frac{\mathrm{P1}}{\mathrm{Kmp1}} + \frac{\mathrm{S2}}{\mathrm{Kms2}} + \frac{\mathrm{P2}}{\mathrm{Kmp2}} + \frac{\mathrm{S3}}{\mathrm{Kms3}} + \frac{\mathrm{P3}}{\mathrm{Kmp3}} + \frac{\mathrm{S4}}{\mathrm{Kms4}} + \frac{\mathrm{P4}}{\mathrm{Kmp4}} + \frac{\mathrm{S5}}{\mathrm{Kms5}} + \frac{\mathrm{P5}}{\mathrm{Kmp5}}\right) \cdot \left(1 + \frac{\mathrm{S6} - \mathrm{P6}}{\mathrm{Kms6}} + \frac{\mathrm{P6}}{\mathrm{Kmp6}}\right)}$$

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 33 modifiers.

Reaction equation

$$\mathrm{C8AcylCoAMAT} \rightleftharpoons \mathrm{C16AcylCoAMAT},\ \mathrm{C14AcylCoAMAT},\ \mathrm{C12AcylCoAMAT},\ \mathrm{C10AcylCoAMAT},\ \mathrm{FADtMAT},\ \mathrm{C16} \tag{81}$$

Reactant

Table 93: Properties of each reactant.

Id	Name	SBO
`C8AcylCoAMAT`		

Modifiers

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

Products

Table 95: Properties of each product.

Id	Name	SBO
C8EnoylCoAMAT		

Id	Name	SBO
FADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \mathrm{LCAD}\,(\mathrm{sflcadC8}, \mathrm{Vlcad}, \mathrm{KmlcadC8AcylCoAMAT}, \mathrm{KmlcadC16AcylCoAMAT}, \mathrm{KmlcadC14AcylCoAMAT}, \mathrm{KmlcadC12AcylCoAMAT}, \mathrm{KmlcadC10AcylCoAMAT}, \mathrm{KmlcadFAD}, \mathrm{KmlcadC8EnoylCoAMAT}, \mathrm{KmlcadC16EnoylCoAMAT}, \mathrm{KmlcadC14EnoylCoAMAT}, \mathrm{KmlcadC12EnoylCoAMAT}, \mathrm{KmlcadC10EnoylCoAMAT}, \mathrm{KmlcadFADH}, \mathrm{Keqlcad}, [\mathrm{C8AcylCoAMAT}], [\mathrm{C16AcylCoAMAT}], [\mathrm{C14AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{FADtMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{C16EnoylCoAMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{FADHMAT}]) \tag{82}$$

$$\mathrm{LCAD}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}) \tag{83}$$
$$= \frac{\mathrm{sf} \cdot \mathrm{V} \cdot \left(\frac{\mathrm{S1} \cdot (\mathrm{S6} - \mathrm{P6})}{\mathrm{Kms1} \cdot \mathrm{Kms6}} - \frac{\mathrm{P1} \cdot \mathrm{P6}}{\mathrm{Kms1} \cdot \mathrm{Kms6} \cdot \mathrm{Keq}} \right)}{\left(1 + \frac{\mathrm{S1}}{\mathrm{Kms1}} + \frac{\mathrm{P1}}{\mathrm{Kmp1}} + \frac{\mathrm{S2}}{\mathrm{Kms2}} + \frac{\mathrm{P2}}{\mathrm{Kmp2}} + \frac{\mathrm{S3}}{\mathrm{Kms3}} + \frac{\mathrm{P3}}{\mathrm{Kmp3}} + \frac{\mathrm{S4}}{\mathrm{Kms4}} + \frac{\mathrm{P4}}{\mathrm{Kmp4}} + \frac{\mathrm{S5}}{\mathrm{Kms5}} + \frac{\mathrm{P5}}{\mathrm{Kmp5}} \right) \cdot \left(1 + \frac{\mathrm{S6} - \mathrm{P6}}{\mathrm{Kms6}} + \frac{\mathrm{P6}}{\mathrm{Kmp6}} \right)}$$

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 33 modifiers.

Reaction equation

$$\mathrm{C12AcylCoAMAT} \rightleftharpoons \mathrm{C10AcylCoAMAT},\ \mathrm{C8AcylCoAMAT},\ \mathrm{C6AcylCoAMAT},\ \mathrm{C4AcylCoAMAT},\ \mathrm{FADtMAT},\ \mathrm{C10En} \tag{84}$$

Reactant

Table 97: Properties of each reactant.

Id	Name	SBO
C12AcylCoAMAT		

Modifiers

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

Id	Name	SBO

Products

Table 99: Properties of each product.

Id	Name	SBO
C12EnoylCoAMAT		
FADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \mathrm{MCAD}(\mathrm{sfmcadC12}, \mathrm{Vmcad}, \mathrm{KmmcadC12AcylCoAMAT}, \mathrm{KmmcadC10AcylCoAMAT}, \mathrm{KmmcadC8AcylCoAMAT}, \mathrm{KmmcadC6AcylCoAMAT}, \mathrm{KmmcadC4AcylCoAMAT}, \mathrm{KmmcadFAD}, \mathrm{KmmcadC12EnoylCoAMAT}, \mathrm{KmmcadC10EnoylCoAMAT}, \mathrm{KmmcadC8EnoylCoAMAT}, \mathrm{KmmcadC6EnoylCoAMAT}, \mathrm{KmmcadC4EnoylCoAMAT}, \mathrm{KmmcadFADH}, \mathrm{Keqmcad}, [\mathrm{C12AcylCoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{C6AcylCoAMAT}], [\mathrm{C4AcylCoAMAT}], [\mathrm{FADtMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{C6EnoylCoAMAT}], [\mathrm{C4EnoylCoAMAT}], [\mathrm{FADHMAT}]) \tag{85}$$

$$\mathrm{MCAD}(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}) \tag{86}$$

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

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 33 modifiers.

Reaction equation

$$\text{C10AcylCoAMAT} \rightleftharpoons \text{C12AcylCoAMAT, C8AcylCoAMAT, C6AcylCoAMAT, C4AcylCoAMAT, FADtMAT, C12Er} \quad (87)$$

Reactant

Table 101: Properties of each reactant.

Id	Name	SBO
C10AcylCoAMAT		

Modifiers

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		
C10AcylCoAMAT		
C12AcylCoAMAT		
C8AcylCoAMAT		
C6AcylCoAMAT		

Id	Name	SBO
C4AcylCoAMAT		
FADtMAT		
C10EnoylCoAMAT		
C12EnoylCoAMAT		
C8EnoylCoAMAT		
C6EnoylCoAMAT		
C4EnoylCoAMAT		
FADHMAT		

Products

Table 103: Properties of each product.

Id	Name	SBO
C10EnoylCoAMAT		
FADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \mathrm{MCAD}\,(\mathrm{sfmcadC10}, \mathrm{Vmcad}, \mathrm{KmmcadC10AcylCoAMAT}, \mathrm{KmmcadC12AcylCoAMAT}, \mathrm{KmmcadC8AcylCoAMAT}, \mathrm{KmmcadC6AcylCoAMAT}, \mathrm{KmmcadC4AcylCoAMAT}, \mathrm{KmmcadFAD}, \mathrm{KmmcadC10EnoylCoAMAT}, \mathrm{KmmcadC12EnoylCoAMAT}, \mathrm{KmmcadC8EnoylCoAMAT}, \mathrm{KmmcadC6EnoylCoAMAT}, \mathrm{KmmcadC4EnoylCoAMAT}, \mathrm{KmmcadFADH}, \mathrm{Keqmcad}, [\mathrm{C10AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{C6AcylCoAMAT}], [\mathrm{C4AcylCoAMAT}], [\mathrm{FADtMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{C6EnoylCoAMAT}], [\mathrm{C4EnoylCoAMAT}], [\mathrm{FADHMAT}]) \tag{88}$$

$$\mathrm{MCAD}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}) \tag{89}$$

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

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 33 modifiers.

Reaction equation

$$\text{C8AcylCoAMAT} \xrightleftharpoons{\text{C12AcylCoAMAT, C10AcylCoAMAT, C6AcylCoAMAT, C4AcylCoAMAT, FADtMAT, C12En}} \tag{90}$$

Reactant

Table 105: Properties of each reactant.

Id	Name	SBO
C8AcylCoAMAT		

Modifiers

Table 106: Properties of each modifier.

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

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

Products

Table 107: Properties of each product.

Id	Name	SBO
C8EnoylCoAMAT		
FADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = \mathrm{MCAD}\,(\mathrm{sfmcadC8}, \mathrm{Vmcad}, \mathrm{KmmcadC8AcylCoAMAT}, \mathrm{KmmcadC12AcylCoAMAT}, \mathrm{KmmcadC10AcylCoAMAT}, \mathrm{KmmcadC6AcylCoAMAT}, \mathrm{KmmcadC4AcylCoAMAT}, \mathrm{KmmcadFAD}, \mathrm{KmmcadC8EnoylCoAMAT}, \mathrm{KmmcadC12EnoylCoAMAT}, \mathrm{KmmcadC10EnoylCoAMAT}, \mathrm{KmmcadC6EnoylCoAMAT}, \mathrm{KmmcadC4EnoylCoAMAT}, \mathrm{KmmcadFADH}, \mathrm{Keqmcad}, [\mathrm{C8AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C6AcylCoAMAT}], [\mathrm{C4AcylCoAMAT}], [\mathrm{FADtMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{C6EnoylCoAMAT}], [\mathrm{C4EnoylCoAMAT}], [\mathrm{FADHMAT}]) \quad (91)$$

$$\begin{aligned}&\mathrm{MCAD}\left(\mathrm{sf},\mathrm{V},\mathrm{Kms1},\mathrm{Kms2},\mathrm{Kms3},\mathrm{Kms4},\mathrm{Kms5},\mathrm{Kms6},\mathrm{Kmp1},\mathrm{Kmp2},\right. \qquad (92)\\ &\left.\mathrm{Kmp3},\mathrm{Kmp4},\mathrm{Kmp5},\mathrm{Kmp6},\mathrm{Keq},\mathrm{S1},\mathrm{S2},\mathrm{S3},\mathrm{S4},\mathrm{S5},\mathrm{S6},\mathrm{P1},\mathrm{P2},\mathrm{P3},\mathrm{P4},\mathrm{P5},\mathrm{P6}\right)\\ &= \frac{\mathrm{sf}\cdot\mathrm{V}\cdot\left(\frac{\mathrm{S1}\cdot(\mathrm{S6}-\mathrm{P6})}{\mathrm{Kms1}\cdot\mathrm{Kms6}}-\frac{\mathrm{P1}\cdot\mathrm{P6}}{\mathrm{Kms1}\cdot\mathrm{Kms6}\cdot\mathrm{Keq}}\right)}{\left(1+\frac{\mathrm{S1}}{\mathrm{Kms1}}+\frac{\mathrm{P1}}{\mathrm{Kmp1}}+\frac{\mathrm{S2}}{\mathrm{Kms2}}+\frac{\mathrm{P2}}{\mathrm{Kmp2}}+\frac{\mathrm{S3}}{\mathrm{Kms3}}+\frac{\mathrm{P3}}{\mathrm{Kmp3}}+\frac{\mathrm{S4}}{\mathrm{Kms4}}+\frac{\mathrm{P4}}{\mathrm{Kmp4}}+\frac{\mathrm{S5}}{\mathrm{Kms5}}+\frac{\mathrm{P5}}{\mathrm{Kmp5}}\right)\cdot\left(1+\frac{\mathrm{S6}-\mathrm{P6}}{\mathrm{Kms6}}+\frac{\mathrm{P6}}{\mathrm{Kmp6}}\right)}\end{aligned}$$

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 33 modifiers.

Reaction equation

$$\mathrm{C6AcylCoAMAT} \xrightleftharpoons{\mathrm{C12AcylCoAMAT},\ \mathrm{C10AcylCoAMAT},\ \mathrm{C8AcylCoAMAT},\ \mathrm{C4AcylCoAMAT},\ \mathrm{FADtMAT},\ \mathrm{C12En}} \qquad (93)$$

Reactant

Table 109: Properties of each reactant.

Id	Name	SBO
C6AcylCoAMAT		

Modifiers

Table 110: Properties of each modifier.

Id	Name	SBO
C12AcylCoAMAT		
C10AcylCoAMAT		
C8AcylCoAMAT		
C4AcylCoAMAT		
FADtMAT		
C12EnoylCoAMAT		
C10EnoylCoAMAT		
C8EnoylCoAMAT		

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

Products

Table 111: Properties of each product.

Id	Name	SBO
C6EnoylCoAMAT		
FADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{27} = \mathrm{MCAD}\,(\mathrm{sfmcadC6}, \mathrm{Vmcad}, \mathrm{KmmcadC6AcylCoAMAT}, \mathrm{KmmcadC12AcylCoAMAT}, \mathrm{KmmcadC10AcylCoAMAT}, \mathrm{KmmcadC8AcylCoAMAT}, \mathrm{KmmcadC4AcylCoAMAT}, \mathrm{KmmcadFAD}, \mathrm{KmmcadC6EnoylCoAMAT}, \mathrm{KmmcadC12EnoylCoAMAT}, \mathrm{KmmcadC10EnoylCoAMAT}, \mathrm{KmmcadC8EnoylCoAMAT}, \mathrm{KmmcadC4EnoylCoAMAT}, \mathrm{KmmcadFADH}, \mathrm{Keqmcad}, [\mathrm{C6AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{C4AcylCoAMAT}], [\mathrm{FADtMAT}], [\mathrm{C6EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{C4EnoylCoAMAT}], [\mathrm{FADHMAT}]) \tag{94}$$

$$\mathrm{MCAD}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}) \tag{95}$$
$$= \frac{\mathrm{sf} \cdot \mathrm{V} \cdot \left(\frac{\mathrm{S1} \cdot (\mathrm{S6} - \mathrm{P6})}{\mathrm{Kms1} \cdot \mathrm{Kms6}} - \frac{\mathrm{P1} \cdot \mathrm{P6}}{\mathrm{Kms1} \cdot \mathrm{Kms6} \cdot \mathrm{Keq}}\right)}{\left(1 + \frac{\mathrm{S1}}{\mathrm{Kms1}} + \frac{\mathrm{P1}}{\mathrm{Kmp1}} + \frac{\mathrm{S2}}{\mathrm{Kms2}} + \frac{\mathrm{P2}}{\mathrm{Kmp2}} + \frac{\mathrm{S3}}{\mathrm{Kms3}} + \frac{\mathrm{P3}}{\mathrm{Kmp3}} + \frac{\mathrm{S4}}{\mathrm{Kms4}} + \frac{\mathrm{P4}}{\mathrm{Kmp4}} + \frac{\mathrm{S5}}{\mathrm{Kms5}} + \frac{\mathrm{P5}}{\mathrm{Kmp5}}\right) \cdot \left(1 + \frac{\mathrm{S6} - \mathrm{P6}}{\mathrm{Kms6}} + \frac{\mathrm{P6}}{\mathrm{Kmp6}}\right)}$$

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 33 modifiers.

Reaction equation

$$\mathrm{C4AcylCoAMAT} \rightleftharpoons \mathrm{C12AcylCoAMAT}, \mathrm{C10AcylCoAMAT}, \mathrm{C8AcylCoAMAT}, \mathrm{C6AcylCoAMAT}, \mathrm{FADtMAT}, \mathrm{C12En} \tag{96}$$

Reactant

Table 113: Properties of each reactant.

Id	Name	SBO
C4AcylCoAMAT		

Modifiers

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

Products

Table 115: Properties of each product.

Id	Name	SBO
C4EnoylCoAMAT		

Id	Name	SBO
FADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \mathrm{MCAD}(\mathrm{sfmcadC4}, \mathrm{Vmcad}, \mathrm{KmmcadC4AcylCoAMAT}, \mathrm{KmmcadC12AcylCoAMAT}, \mathrm{KmmcadC10AcylCoAMAT}, \mathrm{KmmcadC8AcylCoAMAT}, \mathrm{KmmcadC6AcylCoAMAT}, \mathrm{KmmcadFAD}, \mathrm{KmmcadC4EnoylCoAMAT}, \mathrm{KmmcadC12EnoylCoAMAT}, \mathrm{KmmcadC10EnoylCoAMAT}, \mathrm{KmmcadC8EnoylCoAMAT}, \mathrm{KmmcadC6EnoylCoAMAT}, \mathrm{KmmcadFADH}, \mathrm{Keqmcad}, [\mathrm{C4AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{C6AcylCoAMAT}], [\mathrm{FADtMAT}], [\mathrm{C4EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{C6EnoylCoAMAT}], [\mathrm{FADHMAT}]) \tag{97}$$

$$\mathrm{MCAD}(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}) \tag{98}$$

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

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 15 modifiers.

Reaction equation

$$\mathrm{C6AcylCoAMAT} \rightleftharpoons \mathrm{C4AcylCoAMAT} + \mathrm{FADtMAT} + \mathrm{C4EnoylCoAMAT} + \mathrm{C6AcylCoAMAT} + \mathrm{C4AcylCoAMAT} + \mathrm{FADtM} \tag{99}$$

Reactant

Table 117: Properties of each reactant.

Id	Name	SBO
C6AcylCoAMAT		

Modifiers

Table 118: Properties of each modifier.

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

$$v_{29} = \mathrm{SCAD}\,(\mathrm{sfscadC6}, \mathrm{Vscad}, \mathrm{KmscadC6AcylCoAMAT}, \mathrm{KmscadC4AcylCoAMAT}, \mathrm{KmscadFAD}, \mathrm{KmscadC6EnoylCoAMAT}, \mathrm{KmscadC4EnoylCoAMAT}, \mathrm{KmscadFADH}, \mathrm{Keqscad}, [\mathrm{C6AcylCoAMAT}], [\mathrm{C4AcylCoAMAT}], [\mathrm{FADtMAT}], [\mathrm{C6EnoylCoAMAT}], [\mathrm{C4EnoylCoAMAT}], [\mathrm{FADHMAT}]) \tag{100}$$

$$\mathrm{SCAD}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}) = \frac{\mathrm{sf} \cdot \mathrm{V} \cdot \left(\frac{\mathrm{S1} \cdot (\mathrm{S3} - \mathrm{P3})}{\mathrm{Kms1} \cdot \mathrm{Kms3}} - \frac{\mathrm{P1} \cdot \mathrm{P3}}{\mathrm{Kms1} \cdot \mathrm{Kms3} \cdot \mathrm{Keq}}\right)}{\left(1 + \frac{\mathrm{S1}}{\mathrm{Kms1}} + \frac{\mathrm{P1}}{\mathrm{Kmp1}} + \frac{\mathrm{S2}}{\mathrm{Kms2}} + \frac{\mathrm{P2}}{\mathrm{Kmp2}}\right) \cdot \left(1 + \frac{\mathrm{S3} - \mathrm{P3}}{\mathrm{Kms3}} + \frac{\mathrm{P3}}{\mathrm{Kmp3}}\right)} \tag{101}$$

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 15 modifiers.

Reaction equation

$$\mathrm{C4AcylCoAMAT} \xrightleftharpoons{\mathrm{C6AcylCoAMAT},\ \mathrm{FADtMAT},\ \mathrm{C6EnoylCoAMAT},\ \mathrm{C4AcylCoAMAT},\ \mathrm{C6AcylCoAMAT},\ \mathrm{FADtM}} \tag{102}$$

Reactant

Table 121: Properties of each reactant.

Id	Name	SBO
C4AcylCoAMAT		

Modifiers

Table 122: Properties of each modifier.

Id	Name	SBO
C6AcylCoAMAT		
FADtMAT		

Id	Name	SBO
C6EnoylCoAMAT		
C4AcylCoAMAT		
C6AcylCoAMAT		
FADtMAT		
C4EnoylCoAMAT		
C6EnoylCoAMAT		
FADHMAT		
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

$$v_{30} = \mathrm{SCAD}\left(\mathrm{sfscadC4}, \mathrm{Vscad}, \mathrm{KmscadC4AcylCoAMAT}, \mathrm{KmscadC6AcylCoAMAT}, \mathrm{KmscadFAD}, \mathrm{KmscadC4EnoylCoAMAT}, \mathrm{KmscadC6EnoylCoAMAT}, \mathrm{KmscadFADH}, \mathrm{Keqscad}, [\mathrm{C4AcylCoAMAT}], [\mathrm{C6AcylCoAMAT}], [\mathrm{FADtMAT}], [\mathrm{C4EnoylCoAMAT}], [\mathrm{C6EnoylCoAMAT}], [\mathrm{FADHMAT}]\right) \tag{103}$$

$$\mathrm{SCAD}\left(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}\right) = \frac{\mathrm{sf} \cdot \mathrm{V} \cdot \left(\frac{\mathrm{S1} \cdot (\mathrm{S3} - \mathrm{P3})}{\mathrm{Kms1} \cdot \mathrm{Kms3}} - \frac{\mathrm{P1} \cdot \mathrm{P3}}{\mathrm{Kms1} \cdot \mathrm{Kms3} \cdot \mathrm{Keq}}\right)}{\left(1 + \frac{\mathrm{S1}}{\mathrm{Kms1}} + \frac{\mathrm{P1}}{\mathrm{Kmp1}} + \frac{\mathrm{S2}}{\mathrm{Kms2}} + \frac{\mathrm{P2}}{\mathrm{Kmp2}}\right) \cdot \left(1 + \frac{\mathrm{S3} - \mathrm{P3}}{\mathrm{Kms3}} + \frac{\mathrm{P3}}{\mathrm{Kmp3}}\right)} \tag{104}$$

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 43 modifiers.

Reaction equation

$$\text{C16EnoylCoAMAT} \xrightleftharpoons{\text{C14EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C8EnoylCoAMAT, C6EnoylC}} \quad (105)$$

Reactant

Table 125: Properties of each reactant.

Id	Name	SBO
C16EnoylCoAMAT		

Modifiers

Table 126: Properties of each modifier.

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

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

Kinetic Law

Derived unit contains undeclared units

$$v_{31} = \mathrm{CROT}\,(\mathrm{sfcrotC16}, \mathrm{Vcrot}, \mathrm{KmcrotC16EnoylCoAMAT}, \mathrm{KmcrotC14EnoylCoAMAT}, \mathrm{KmcrotC12EnoylCoAMAT}, \mathrm{KmcrotC10EnoylCoAMAT}, \mathrm{KmcrotC8EnoylCoAMAT}, \mathrm{KmcrotC6EnoylCoAMAT}, \mathrm{KmcrotC4EnoylCoAMAT}, \mathrm{KmcrotC16HydroxyacylCoAMAT}, \mathrm{KmcrotC14HydroxyacylCoAMAT}, \mathrm{KmcrotC12HydroxyacylCoAMAT}, \mathrm{KmcrotC10HydroxyacylCoAMAT}, \mathrm{KmcrotC8HydroxyacylCoAMAT}, \mathrm{KmcrotC6HydroxyacylCoAMAT}, \mathrm{KmcrotC4HydroxyacylCoAMAT}, \mathrm{KicrotC4AcetoacylCoA}, \mathrm{Keqcrot}, [\mathrm{C16EnoylCoAMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{C6EnoylCoAMAT}], [\mathrm{C4EnoylCoAMAT}], [\mathrm{C16HydroxyacylCoAMAT}], [\mathrm{C14HydroxyacylCoAMAT}], [\mathrm{C12HydroxyacylCoAMAT}], [\mathrm{C10HydroxyacylCoAMAT}], [\mathrm{C8HydroxyacylCoAMAT}], [\mathrm{C6HydroxyacylCoAMAT}], [\mathrm{C4HydroxyacylCoAMAT}], [\mathrm{C4AcetoacylCoAMAT}]) \tag{106}$$

$$\mathrm{CROT}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kms7}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Kmp7}, \mathrm{Ki1}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{S7}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}, \mathrm{P7}, \mathrm{I1}) \tag{107}$$

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

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 43 modifiers.

Reaction equation

$$\mathrm{C14EnoylCoAMAT} \rightleftharpoons \mathrm{C16EnoylCoAMAT},\ \mathrm{C12EnoylCoAMAT},\ \mathrm{C10EnoylCoAMAT},\ \mathrm{C8EnoylCoAMAT},\ \mathrm{C6EnoylC} \tag{108}$$

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

Id	Name	SBO
C14HydroxyacylCoAMAT		
C16HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
C4HydroxyacylCoAMAT		
C4AcetoacylCoAMAT		

Product

Table 131: Properties of each product.

Id	Name	SBO
C14HydroxyacylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{32} = \mathrm{CROT}(\mathrm{sfcrotC14}, \mathrm{Vcrot}, \mathrm{KmcrotC14EnoylCoAMAT}, \mathrm{KmcrotC16EnoylCoAMAT}, \mathrm{KmcrotC12EnoylCoAMAT}, \mathrm{KmcrotC10EnoylCoAMAT}, \mathrm{KmcrotC8EnoylCoAMAT}, \mathrm{KmcrotC6EnoylCoAMAT}, \mathrm{KmcrotC4EnoylCoAMAT}, \mathrm{KmcrotC14HydroxyacylCoAMAT}, \mathrm{KmcrotC16HydroxyacylCoAMAT}, \mathrm{KmcrotC12HydroxyacylCoAMAT}, \mathrm{KmcrotC10HydroxyacylCoAMAT}, \mathrm{KmcrotC8HydroxyacylCoAMAT}, \mathrm{KmcrotC6HydroxyacylCoAMAT}, \mathrm{KmcrotC4HydroxyacylCoAMAT}, \mathrm{KicrotC4AcetoacylCoA}, \mathrm{Keqcrot}, [\mathrm{C14EnoylCoAMAT}], [\mathrm{C16EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{C6EnoylCoAMAT}], [\mathrm{C4EnoylCoAMAT}], [\mathrm{C14HydroxyacylCoAMAT}], [\mathrm{C16HydroxyacylCoAMAT}], [\mathrm{C12HydroxyacylCoAMAT}], [\mathrm{C10HydroxyacylCoAMAT}], [\mathrm{C8HydroxyacylCoAMAT}], [\mathrm{C6HydroxyacylCoAMAT}], [\mathrm{C4HydroxyacylCoAMAT}], [\mathrm{C4AcetoacylCoAMAT}]) \tag{109}$$

$$\mathrm{CROT}(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kms7}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Kmp7}, \mathrm{Ki1}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{S7}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}, \mathrm{P7}, \mathrm{I1}) \tag{110}$$

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

Table 132: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcrotC14			0.2	dimensionless	☑

8.33 Reaction vcrotC12

This is a reversible reaction of one reactant forming one product influenced by 43 modifiers.

Reaction equation

$$\text{C12EnoylCoAMAT} \rightleftharpoons \text{C16EnoylCoAMAT, C14EnoylCoAMAT, C10EnoylCoAMAT, C8EnoylCoAMAT, C6EnoylC} \quad (111)$$

Reactant

Table 133: Properties of each reactant.

Id	Name	SBO
C12EnoylCoAMAT		

Modifiers

Table 134: Properties of each modifier.

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

Id	Name	SBO
C14EnoylCoAMAT		
C10EnoylCoAMAT		
C8EnoylCoAMAT		
C6EnoylCoAMAT		
C4EnoylCoAMAT		
C12HydroxyacylCoAMAT		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
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	SBO
C12HydroxyacylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{33} = \mathrm{CROT}\,(\mathrm{sfcrotC12}, \mathrm{Vcrot}, \mathrm{KmcrotC12EnoylCoAMAT}, \mathrm{KmcrotC16EnoylCoAMAT}, \mathrm{KmcrotC14EnoylCoAMAT}, \mathrm{KmcrotC10EnoylCoAMAT}, \mathrm{KmcrotC8EnoylCoAMAT}, \mathrm{KmcrotC6EnoylCoAMAT}, \mathrm{KmcrotC4EnoylCoAMAT}, \mathrm{KmcrotC12HydroxyacylCoAMAT}, \mathrm{KmcrotC16HydroxyacylCoAMAT}, \mathrm{KmcrotC14HydroxyacylCoAMAT}, \mathrm{KmcrotC10HydroxyacylCoAMAT}, \mathrm{KmcrotC8HydroxyacylCoAMAT}, \mathrm{KmcrotC6HydroxyacylCoAMAT}, \mathrm{KmcrotC4HydroxyacylCoAMAT}, \mathrm{KicrotC4AcetoacylCoA}, \mathrm{Keqcrot}, [\mathrm{C12EnoylCoAMAT}], [\mathrm{C16EnoylCoAMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{C6EnoylCoAMAT}], [\mathrm{C4EnoylCoAMAT}], [\mathrm{C12HydroxyacylCoAMAT}], [\mathrm{C16HydroxyacylCoAMAT}], [\mathrm{C14HydroxyacylCoAMAT}], [\mathrm{C10HydroxyacylCoAMAT}], [\mathrm{C8HydroxyacylCoAMAT}], [\mathrm{C6HydroxyacylCoAMAT}], [\mathrm{C4HydroxyacylCoAMAT}], [\mathrm{C4AcetoacylCoAMAT}]) \tag{112}$$

$$\begin{aligned}&\mathrm{CROT}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kms7}, \\ &\mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Kmp7}, \mathrm{Ki1}, \\ &\mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{S7}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}, \mathrm{P7}, \mathrm{I1}) \\ &= \frac{\mathrm{sf} \cdot \mathrm{V} \cdot \left(\frac{\mathrm{S1}}{\mathrm{Kms1}} - \frac{\mathrm{P1}}{\mathrm{Kms1} \cdot \mathrm{Keq}}\right)}{1 + \frac{\mathrm{S1}}{\mathrm{Kms1}} + \frac{\mathrm{P1}}{\mathrm{Kmp1}} + \frac{\mathrm{S2}}{\mathrm{Kms2}} + \frac{\mathrm{P2}}{\mathrm{Kmp2}} + \frac{\mathrm{S3}}{\mathrm{Kms3}} + \frac{\mathrm{P3}}{\mathrm{Kmp3}} + \frac{\mathrm{S4}}{\mathrm{Kms4}} + \frac{\mathrm{P4}}{\mathrm{Kmp4}} + \frac{\mathrm{S5}}{\mathrm{Kms5}} + \frac{\mathrm{P5}}{\mathrm{Kmp5}} + \frac{\mathrm{S6}}{\mathrm{Kms6}} + \frac{\mathrm{P6}}{\mathrm{Kmp6}} + \frac{\mathrm{S7}}{\mathrm{Kms7}} + \frac{\mathrm{P7}}{\mathrm{Kmp}}}\end{aligned} \tag{113}$$

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 43 modifiers.

Reaction equation

$$\mathrm{C10EnoylCoAMAT} \rightleftharpoons \mathrm{C16EnoylCoAMAT}, \mathrm{C14EnoylCoAMAT}, \mathrm{C12EnoylCoAMAT}, \mathrm{C8EnoylCoAMAT}, \mathrm{C6EnoylC} \tag{114}$$

Reactant

Table 137: Properties of each reactant.

Id	Name	SBO
`C10EnoylCoAMAT`		

Id	Name	SBO

Modifiers

Table 138: Properties of each modifier.

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

Id	Name	SBO
C10HydroxyacylCoAMAT		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
C4HydroxyacylCoAMAT		
C4AcetoacylCoAMAT		

Product

Table 139: Properties of each product.

Id	Name	SBO
C10HydroxyacylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{34} = \mathrm{CROT}(\mathrm{sfcrotC10}, \mathrm{Vcrot}, \mathrm{KmcrotC10EnoylCoAMAT}, \mathrm{KmcrotC16EnoylCoAMAT}, \mathrm{KmcrotC14EnoylCoAMAT}, \mathrm{KmcrotC12EnoylCoAMAT}, \mathrm{KmcrotC8EnoylCoAMAT}, \mathrm{KmcrotC6EnoylCoAMAT}, \mathrm{KmcrotC4EnoylCoAMAT}, \mathrm{KmcrotC10HydroxyacylCoAMAT}, \mathrm{KmcrotC16HydroxyacylCoAMAT}, \mathrm{KmcrotC14HydroxyacylCoAMAT}, \mathrm{KmcrotC12HydroxyacylCoAMAT}, \mathrm{KmcrotC8HydroxyacylCoAMAT}, \mathrm{KmcrotC6HydroxyacylCoAMAT}, \mathrm{KmcrotC4HydroxyacylCoAMAT}, \mathrm{KicrotC4AcetoacylCoA}, \mathrm{Keqcrot}, [\mathrm{C10EnoylCoAMAT}], [\mathrm{C16EnoylCoAMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{C6EnoylCoAMAT}], [\mathrm{C4EnoylCoAMAT}], [\mathrm{C10HydroxyacylCoAMAT}], [\mathrm{C16HydroxyacylCoAMAT}], [\mathrm{C14HydroxyacylCoAMAT}], [\mathrm{C12HydroxyacylCoAMAT}], [\mathrm{C8HydroxyacylCoAMAT}], [\mathrm{C6HydroxyacylCoAMAT}], [\mathrm{C4HydroxyacylCoAMAT}], [\mathrm{C4AcetoacylCoAMAT}]) \tag{115}$$

$$\begin{aligned}&\mathrm{CROT}(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kms7}, \\ &\mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Kmp7}, \mathrm{Ki1}, \\ &\mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{S7}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}, \mathrm{P7}, \mathrm{I1}) \\ &= \frac{\mathrm{sf} \cdot \mathrm{V} \cdot \left(\frac{\mathrm{S1}}{\mathrm{Kms1}} - \frac{\mathrm{P1}}{\mathrm{Kms1} \cdot \mathrm{Keq}}\right)}{1 + \frac{\mathrm{S1}}{\mathrm{Kms1}} + \frac{\mathrm{P1}}{\mathrm{Kmp1}} + \frac{\mathrm{S2}}{\mathrm{Kms2}} + \frac{\mathrm{P2}}{\mathrm{Kmp2}} + \frac{\mathrm{S3}}{\mathrm{Kms3}} + \frac{\mathrm{P3}}{\mathrm{Kmp3}} + \frac{\mathrm{S4}}{\mathrm{Kms4}} + \frac{\mathrm{P4}}{\mathrm{Kmp4}} + \frac{\mathrm{S5}}{\mathrm{Kms5}} + \frac{\mathrm{P5}}{\mathrm{Kmp5}} + \frac{\mathrm{S6}}{\mathrm{Kms6}} + \frac{\mathrm{P6}}{\mathrm{Kmp6}} + \frac{\mathrm{S7}}{\mathrm{Kms7}} + \frac{\mathrm{P7}}{\mathrm{Kmp}}}\end{aligned} \tag{116}$$

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 43 modifiers.

Reaction equation

$$\text{C8EnoylCoAMAT} \rightleftharpoons \text{C16EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C6EnoylC} \quad (117)$$

Reactant

Table 141: Properties of each reactant.

Id	Name	SBO
C8EnoylCoAMAT		

Modifiers

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

Product

Table 143: Properties of each product.

Id	Name	SBO
C8HydroxyacylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{35} = \mathrm{CROT}\,(\mathrm{sfcrotC8}, \mathrm{Vcrot}, \mathrm{KmcrotC8EnoylCoAMAT}, \mathrm{KmcrotC16EnoylCoAMAT}, \mathrm{KmcrotC14EnoylCoAMAT}, \mathrm{KmcrotC12EnoylCoAMAT}, \mathrm{KmcrotC10EnoylCoAMAT}, \mathrm{KmcrotC6EnoylCoAMAT}, \mathrm{KmcrotC4EnoylCoAMAT}, \mathrm{KmcrotC8HydroxyacylCoAMAT}, \mathrm{KmcrotC16HydroxyacylCoAMAT}, \mathrm{KmcrotC14HydroxyacylCoAMAT}, \mathrm{KmcrotC12HydroxyacylCoAMAT}, \mathrm{KmcrotC10HydroxyacylCoAMAT}, \mathrm{KmcrotC6HydroxyacylCoAMAT}, \mathrm{KmcrotC4HydroxyacylCoAMAT}, \mathrm{KicrotC4AcetoacylCoA}, \mathrm{Keqcrot}, [\mathrm{C8EnoylCoAMAT}], [\mathrm{C16EnoylCoAMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{C6EnoylCoAMAT}], [\mathrm{C4EnoylCoAMAT}], [\mathrm{C8HydroxyacylCoAMAT}], [\mathrm{C16HydroxyacylCoAMAT}], [\mathrm{C14HydroxyacylCoAMAT}], [\mathrm{C12HydroxyacylCoAMAT}], [\mathrm{C10HydroxyacylCoAMAT}], [\mathrm{C6HydroxyacylCoAMAT}], [\mathrm{C4HydroxyacylCoAMAT}], [\mathrm{C4AcetoacylCoAMAT}]) \tag{118}$$

$$\begin{aligned} &\mathrm{CROT}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kms7}, \\ &\mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Kmp7}, \mathrm{Ki1}, \\ &\mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{S7}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}, \mathrm{P7}, \mathrm{I1}) \end{aligned} \tag{119}$$

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

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 43 modifiers.

Reaction equation

$$\mathrm{C6EnoylCoAMAT} \rightleftharpoons \mathrm{C16EnoylCoAMAT},\ \mathrm{C14EnoylCoAMAT},\ \mathrm{C12EnoylCoAMAT},\ \mathrm{C10EnoylCoAMAT},\ \mathrm{C8EnoylC} \tag{120}$$

Reactant

Table 145: Properties of each reactant.

Id	Name	SBO
C6EnoylCoAMAT		

Id	Name	SBO

Modifiers

Table 146: Properties of each modifier.

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

Id	Name	SBO
C6HydroxyacylCoAMAT		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C4HydroxyacylCoAMAT		
C4AcetoacylCoAMAT		

Product

Table 147: Properties of each product.

Id	Name	SBO
C6HydroxyacylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{36} = \mathrm{CROT}\,(\mathrm{sfcrotC6}, \mathrm{Vcrot}, \mathrm{KmcrotC6EnoylCoAMAT}, \mathrm{KmcrotC16EnoylCoAMAT}, \mathrm{KmcrotC14EnoylCoAMAT}, \mathrm{KmcrotC12EnoylCoAMAT}, \mathrm{KmcrotC10EnoylCoAMAT}, \mathrm{KmcrotC8EnoylCoAMAT}, \mathrm{KmcrotC4EnoylCoAMAT}, \mathrm{KmcrotC6HydroxyacylCoAMAT}, \mathrm{KmcrotC16HydroxyacylCoAMAT}, \mathrm{KmcrotC14HydroxyacylCoAMAT}, \mathrm{KmcrotC12HydroxyacylCoAMAT}, \mathrm{KmcrotC10HydroxyacylCoAMAT}, \mathrm{KmcrotC8HydroxyacylCoAMAT}, \mathrm{KmcrotC4HydroxyacylCoAMAT}, \mathrm{KicrotC4AcetoacylCoA}, \mathrm{Keqcrot}, [\mathrm{C6EnoylCoAMAT}], [\mathrm{C16EnoylCoAMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{C4EnoylCoAMAT}], [\mathrm{C6HydroxyacylCoAMAT}], [\mathrm{C16HydroxyacylCoAMAT}], [\mathrm{C14HydroxyacylCoAMAT}], [\mathrm{C12HydroxyacylCoAMAT}], [\mathrm{C10HydroxyacylCoAMAT}], [\mathrm{C8HydroxyacylCoAMAT}], [\mathrm{C4HydroxyacylCoAMAT}], [\mathrm{C4AcetoacylCoAMAT}]) \tag{121}$$

$$\mathrm{CROT}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kms7}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Kmp7}, \mathrm{Ki1}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{S7}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}, \mathrm{P7}, \mathrm{I1}) \tag{122}$$

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

Table 148: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfcrotC6			0.83	dimensionless	☑

8.37 Reaction vcrotC4

This is a reversible reaction of one reactant forming one product influenced by 43 modifiers.

Reaction equation

$$\text{C4EnoylCoAMAT} \rightleftharpoons \text{C16EnoylCoAMAT, C14EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C8EnoylC} \quad (123)$$

Reactant

Table 149: Properties of each reactant.

Id	Name	SBO
C4EnoylCoAMAT		

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		

Id	Name	SBO
C14EnoylCoAMAT		
C12EnoylCoAMAT		
C10EnoylCoAMAT		
C8EnoylCoAMAT		
C6EnoylCoAMAT		
C4HydroxyacylCoAMAT		
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.

Id	Name	SBO
C4HydroxyacylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{37} = \mathrm{CROT}\,(\mathrm{sfcrotC4}, \mathrm{Vcrot}, \mathrm{KmcrotC4EnoylCoAMAT}, \mathrm{KmcrotC16EnoylCoAMAT}, \mathrm{KmcrotC14EnoylCoAMAT}, \mathrm{KmcrotC12EnoylCoAMAT}, \mathrm{KmcrotC10EnoylCoAMAT}, \mathrm{KmcrotC8EnoylCoAMAT}, \mathrm{KmcrotC6EnoylCoAMAT}, \mathrm{KmcrotC4HydroxyacylCoAMAT}, \mathrm{KmcrotC16HydroxyacylCoAMAT}, \mathrm{KmcrotC14HydroxyacylCoAMAT}, \mathrm{KmcrotC12HydroxyacylCoAMAT}, \mathrm{KmcrotC10HydroxyacylCoAMAT}, \mathrm{KmcrotC8HydroxyacylCoAMAT}, \mathrm{KmcrotC6HydroxyacylCoAMAT}, \mathrm{KicrotC4AcetoacylCoA}, \mathrm{Keqcrot}, [\mathrm{C4EnoylCoAMAT}], [\mathrm{C16EnoylCoAMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{C6EnoylCoAMAT}], [\mathrm{C4HydroxyacylCoAMAT}], [\mathrm{C16HydroxyacylCoAMAT}], [\mathrm{C14HydroxyacylCoAMAT}], [\mathrm{C12HydroxyacylCoAMAT}], [\mathrm{C10HydroxyacylCoAMAT}], [\mathrm{C8HydroxyacylCoAMAT}], [\mathrm{C6HydroxyacylCoAMAT}], [\mathrm{C4AcetoacylCoAMAT}]) \tag{124}$$

$$\mathrm{CROT}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms6}, \mathrm{Kms7}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Kmp7}, \mathrm{Ki1}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S6}, \mathrm{S7}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}, \mathrm{P7}, \mathrm{I1}) \tag{125}$$

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

Table 152: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`sfcrotC4`			1.0	dimensionless	☑

8.38 Reaction `vmschadC16`

This is a reversible reaction of one reactant forming two products influenced by 45 modifiers.

Reaction equation

$$\mathrm{C16HydroxyacylCoAMAT} \rightleftharpoons \mathrm{C14HydroxyacylCoAMAT},\ \mathrm{C12HydroxyacylCoAMAT},\ \mathrm{C10HydroxyacylCoAMAT},\ \mathrm{C8} \tag{126}$$

Reactant

Table 153: Properties of each reactant.

Id	Name	SBO
`C16HydroxyacylCoAMAT`		

Id	Name	SBO

Modifiers

Table 154: Properties of each modifier.

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

Id	Name	SBO
C4HydroxyacylCoAMAT		
NADtMAT		
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
C4AcetoacylCoAMAT		
NADHMAT		

Products

Table 155: Properties of each product.

Id	Name	SBO
C16KetoacylCoAMAT		
NADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{38} = \mathrm{MSCHAD}\,(\mathrm{sfmschadC16}, \mathrm{Vmschad}, \mathrm{KmmschadC16HydroxyacylCoAMAT}, \mathrm{KmmschadC14HydroxyacylCoAMAT}, \mathrm{KmmschadC12HydroxyacylCoAMAT}, \mathrm{KmmschadC10HydroxyacylCoAMAT}, \mathrm{KmmschadC8HydroxyacylCoAMAT}, \mathrm{KmmschadC6HydroxyacylCoAMAT}, \mathrm{KmmschadC4HydroxyacylCoAMAT}, \mathrm{KmmschadNADMAT}, \mathrm{KmmschadC16KetoacylCoAMAT}, \mathrm{KmmschadC14KetoacylCoAMAT}, \mathrm{KmmschadC12KetoacylCoAMAT}, \mathrm{KmmschadC10KetoacylCoAMAT}, \mathrm{KmmschadC8KetoacylCoAMAT}, \mathrm{KmmschadC6KetoacylCoAMAT}, \mathrm{KmmschadC4AcetoacylCoAMAT}, \mathrm{KmmschadNADHMAT}, \mathrm{Keqmschad}, [\mathrm{C16HydroxyacylCoAMAT}], [\mathrm{C14HydroxyacylCoAMAT}], [\mathrm{C12HydroxyacylCoAMAT}], [\mathrm{C10HydroxyacylCoAMAT}], [\mathrm{C8HydroxyacylCoAMAT}], [\mathrm{C6HydroxyacylCoAMAT}], [\mathrm{C4HydroxyacylCoAMAT}], [\mathrm{NADtMAT}], [\mathrm{C16KetoacylCoAMAT}], [\mathrm{C14KetoacylCoAMAT}], [\mathrm{C12KetoacylCoAMAT}], [\mathrm{C10KetoacylCoAMAT}], [\mathrm{C8KetoacylCoAMAT}], [\mathrm{C6KetoacylCoAMAT}], [\mathrm{C4AcetoacylCoAMAT}], [\mathrm{NADHMAT}]) \quad (127)$$

$$\begin{aligned}&\mathrm{MSCHAD}\left(\mathrm{sf},\mathrm{V},\mathrm{Kms1},\mathrm{Kms2},\mathrm{Kms3},\mathrm{Kms4},\mathrm{Kms5},\mathrm{Kms6},\mathrm{Kms7},\right.\\&\left.\mathrm{Kms8},\mathrm{Kmp1},\mathrm{Kmp2},\mathrm{Kmp3},\mathrm{Kmp4},\mathrm{Kmp5},\mathrm{Kmp6},\mathrm{Kmp7},\mathrm{Kmp8},\right.\\&\left.\mathrm{Keq},\mathrm{S1},\mathrm{S2},\mathrm{S3},\mathrm{S4},\mathrm{S5},\mathrm{S6},\mathrm{S7},\mathrm{S8},\mathrm{P1},\mathrm{P2},\mathrm{P3},\mathrm{P4},\mathrm{P5},\mathrm{P6},\mathrm{P7},\mathrm{P8}\right)\\&=\frac{\mathrm{sf}\cdot\mathrm{V}\cdot\left(\frac{\mathrm{S1}\cdot(\mathrm{S8}-\mathrm{P8})}{\mathrm{Kms1}\cdot\mathrm{Kms8}}-\frac{\mathrm{P1}\cdot\mathrm{P8}}{\mathrm{Kms1}\cdot\mathrm{Kms8}\cdot\mathrm{Keq}}\right)}{\left(1+\frac{\mathrm{S1}}{\mathrm{Kms1}}+\frac{\mathrm{P1}}{\mathrm{Kmp1}}+\frac{\mathrm{S2}}{\mathrm{Kms2}}+\frac{\mathrm{P2}}{\mathrm{Kmp2}}+\frac{\mathrm{S3}}{\mathrm{Kms3}}+\frac{\mathrm{P3}}{\mathrm{Kmp3}}+\frac{\mathrm{S4}}{\mathrm{Kms4}}+\frac{\mathrm{P4}}{\mathrm{Kmp4}}+\frac{\mathrm{S5}}{\mathrm{Kms5}}+\frac{\mathrm{P5}}{\mathrm{Kmp5}}+\frac{\mathrm{S6}}{\mathrm{Kms6}}+\frac{\mathrm{P6}}{\mathrm{Kmp6}}+\frac{\mathrm{S7}}{\mathrm{Kms7}}+\frac{\mathrm{P}}{\mathrm{Km}}\right.}\end{aligned}\tag{128}$$

Table 156: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmschadC16			0.6	dimensionless	☑

8.39 Reaction vmschadC14

This is a reversible reaction of one reactant forming two products influenced by 45 modifiers.

Reaction equation

$$\mathrm{C14HydroxyacylCoAMAT} \xrightleftharpoons{\mathrm{C16HydroxyacylCoAMAT},\ \mathrm{C12HydroxyacylCoAMAT},\ \mathrm{C10HydroxyacylCoAMAT},\ \mathrm{C8}}\tag{129}$$

Reactant

Table 157: Properties of each reactant.

Id	Name	SBO
C14HydroxyacylCoAMAT		

Modifiers

Table 158: Properties of each modifier.

Id	Name	SBO
C16HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
C4HydroxyacylCoAMAT		
NADtMAT		

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

$$v_{39} = \text{MSCHAD}(\text{sfmschadC14}, \text{Vmschad}, \text{KmmschadC14HydroxyacylCoAMAT}, \text{KmmschadC16HydroxyacylCoAMAT}, \text{KmmschadC12HydroxyacylCoAMAT}, \text{KmmschadC10HydroxyacylCoAMAT}, \text{KmmschadC8HydroxyacylCoAMAT}, \text{KmmschadC6HydroxyacylCoAMAT}, \text{KmmschadC4HydroxyacylCoAMAT}, \text{KmmschadNADMAT}, \text{KmmschadC14KetoacylCoAMAT}, \text{KmmschadC16KetoacylCoAMAT}, \text{KmmschadC12KetoacylCoAMAT}, \text{KmmschadC10KetoacylCoAMAT}, \text{KmmschadC8KetoacylCoAMAT}, \text{KmmschadC6KetoacylCoAMAT}, \text{KmmschadC4AcetoacylCoAMAT}, \text{KmmschadNADHMAT}, \text{Keqmschad}, [\text{C14HydroxyacylCoAMAT}], [\text{C16HydroxyacylCoAMAT}], [\text{C12HydroxyacylCoAMAT}], [\text{C10HydroxyacylCoAMAT}], [\text{C8HydroxyacylCoAMAT}], [\text{C6HydroxyacylCoAMAT}], [\text{C4HydroxyacylCoAMAT}], [\text{NADtMAT}], [\text{C14KetoacylCoAMAT}], [\text{C16KetoacylCoAMAT}], [\text{C12KetoacylCoAMAT}], [\text{C10KetoacylCoAMAT}], [\text{C8KetoacylCoAMAT}], [\text{C6KetoacylCoAMAT}], [\text{C4AcetoacylCoAMAT}], [\text{NADHMAT}]) \quad (130)$$

$$\text{MSCHAD}(\text{sf}, \text{V}, \text{Kms1}, \text{Kms2}, \text{Kms3}, \text{Kms4}, \text{Kms5}, \text{Kms6}, \text{Kms7}, \text{Kms8}, \text{Kmp1}, \text{Kmp2}, \text{Kmp3}, \text{Kmp4}, \text{Kmp5}, \text{Kmp6}, \text{Kmp7}, \text{Kmp8}, \text{Keq}, \text{S1}, \text{S2}, \text{S3}, \text{S4}, \text{S5}, \text{S6}, \text{S7}, \text{S8}, \text{P1}, \text{P2}, \text{P3}, \text{P4}, \text{P5}, \text{P6}, \text{P7}, \text{P8}) \quad (131)$$

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

Table 160: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmschadC14			0.5	dimensionless	☑

8.40 Reaction vmschadC12

This is a reversible reaction of one reactant forming two products influenced by 45 modifiers.

Reaction equation

$$\text{C12HydroxyacylCoAMAT} \xrightleftharpoons{\text{C16HydroxyacylCoAMAT, C14HydroxyacylCoAMAT, C10HydroxyacylCoAMAT, C8}} \tag{132}$$

Reactant

Table 161: Properties of each reactant.

Id	Name	SBO
C12HydroxyacylCoAMAT		

Modifiers

Table 162: Properties of each modifier.

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

Id	Name	SBO
C12KetoacylCoAMAT		
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
C4AcetoacylCoAMAT		
NADHMAT		
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

$$v_{40} = \text{MSCHAD}\,(\text{sfmschadC12}, \text{Vmschad}, \text{KmmschadC12HydroxyacylCoAMAT}, \text{KmmschadC16HydroxyacylCoAMAT}, \text{KmmschadC14HydroxyacylCoAMAT}, \text{KmmschadC10HydroxyacylCoAMAT}, \text{KmmschadC8HydroxyacylCoAMAT}, \text{KmmschadC6HydroxyacylCoAMAT}, \text{KmmschadC4HydroxyacylCoAMAT}, \text{KmmschadNADMAT}, \text{KmmschadC12KetoacylCoAMAT}, \text{KmmschadC16KetoacylCoAMAT}, \text{KmmschadC14KetoacylCoAMAT}, \text{KmmschadC10KetoacylCoAMAT}, \text{KmmschadC8KetoacylCoAMAT}, \text{KmmschadC6KetoacylCoAMAT}, \text{KmmschadC4AcetoacylCoAMAT}, \text{KmmschadNADHMAT}, \text{Keqmschad}, [\text{C12HydroxyacylCoAMAT}], [\text{C16HydroxyacylCoAMAT}], [\text{C14HydroxyacylCoAMAT}], [\text{C10HydroxyacylCoAMAT}], [\text{C8HydroxyacylCoAMAT}], [\text{C6HydroxyacylCoAMAT}], [\text{C4HydroxyacylCoAMAT}], [\text{NADtMAT}], [\text{C12KetoacylCoAMAT}], [\text{C16KetoacylCoAMAT}], [\text{C14KetoacylCoAMAT}], [\text{C10KetoacylCoAMAT}], [\text{C8KetoacylCoAMAT}], [\text{C6KetoacylCoAMAT}], [\text{C4AcetoacylCoAMAT}], [\text{NADHMAT}]) \tag{133}$$

$$\text{MSCHAD}\,(\text{sf}, \text{V}, \text{Kms1}, \text{Kms2}, \text{Kms3}, \text{Kms4}, \text{Kms5}, \text{Kms6}, \text{Kms7}, \text{Kms8}, \text{Kmp1}, \text{Kmp2}, \text{Kmp3}, \text{Kmp4}, \text{Kmp5}, \text{Kmp6}, \text{Kmp7}, \text{Kmp8}, \text{Keq}, \text{S1}, \text{S2}, \text{S3}, \text{S4}, \text{S5}, \text{S6}, \text{S7}, \text{S8}, \text{P1}, \text{P2}, \text{P3}, \text{P4}, \text{P5}, \text{P6}, \text{P7}, \text{P8}) \tag{134}$$

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

Table 164: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmschadC12			0.43	dimensionless	☑

8.41 Reaction vmschadC10

This is a reversible reaction of one reactant forming two products influenced by 45 modifiers.

Reaction equation

$$\text{C10HydroxyacylCoAMAT} \rightleftharpoons \text{C16HydroxyacylCoAMAT}, \text{C14HydroxyacylCoAMAT}, \text{C12HydroxyacylCoAMAT}, \text{C8} \tag{135}$$

Reactant

Table 165: Properties of each reactant.

Id	Name	SBO
C10HydroxyacylCoAMAT		

Modifiers

Table 166: Properties of each modifier.

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

Id	Name	SBO
C8HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
C4HydroxyacylCoAMAT		
NADtMAT		
C10KetoacylCoAMAT		
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
C4AcetoacylCoAMAT		
NADHMAT		

Products

Table 167: Properties of each product.

Id	Name	SBO
C10KetoacylCoAMAT		
NADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{41} = \text{MSCHAD}\,(\text{sfmschadC10}, \text{Vmschad}, \text{KmmschadC10HydroxyacylCoAMAT}, \text{KmmschadC16HydroxyacylCoAMAT}, \text{KmmschadC14HydroxyacylCoAMAT}, \text{KmmschadC12HydroxyacylCoAMAT}, \text{KmmschadC8HydroxyacylCoAMAT}, \text{KmmschadC6HydroxyacylCoAMAT}, \text{KmmschadC4HydroxyacylCoAMAT}, \text{KmmschadNADMAT}, \text{KmmschadC10KetoacylCoAMAT}, \text{KmmschadC16KetoacylCoAMAT}, \text{KmmschadC14KetoacylCoAMAT}, \text{KmmschadC12KetoacylCoAMAT}, \text{KmmschadC8KetoacylCoAMAT}, \text{KmmschadC6KetoacylCoAMAT}, \text{KmmschadC4AcetoacylCoAMAT}, \text{KmmschadNADHMAT}, \text{Keqmschad}, [\text{C10HydroxyacylCoAMAT}], [\text{C16HydroxyacylCoAMAT}], [\text{C14HydroxyacylCoAMAT}], [\text{C12HydroxyacylCoAMAT}], [\text{C8HydroxyacylCoAMAT}], [\text{C6HydroxyacylCoAMAT}], [\text{C4HydroxyacylCoAMAT}], [\text{NADtMAT}], [\text{C10KetoacylCoAMAT}], [\text{C16KetoacylCoAMAT}], [\text{C14KetoacylCoAMAT}], [\text{C12KetoacylCoAMAT}], [\text{C8KetoacylCoAMAT}], [\text{C6KetoacylCoAMAT}], [\text{C4AcetoacylCoAMAT}], [\text{NADHMAT}]) \quad (136)$$

$$\begin{aligned}&\mathrm{MSCHAD}\left(\mathrm{sf},\mathrm{V},\mathrm{Kms1},\mathrm{Kms2},\mathrm{Kms3},\mathrm{Kms4},\mathrm{Kms5},\mathrm{Kms6},\mathrm{Kms7},\right.\\&\left.\mathrm{Kms8},\mathrm{Kmp1},\mathrm{Kmp2},\mathrm{Kmp3},\mathrm{Kmp4},\mathrm{Kmp5},\mathrm{Kmp6},\mathrm{Kmp7},\mathrm{Kmp8},\right.\\&\left.\mathrm{Keq},\mathrm{S1},\mathrm{S2},\mathrm{S3},\mathrm{S4},\mathrm{S5},\mathrm{S6},\mathrm{S7},\mathrm{S8},\mathrm{P1},\mathrm{P2},\mathrm{P3},\mathrm{P4},\mathrm{P5},\mathrm{P6},\mathrm{P7},\mathrm{P8}\right)\\&=\frac{\mathrm{sf}\cdot\mathrm{V}\cdot\left(\frac{\mathrm{S1}\cdot(\mathrm{S8}-\mathrm{P8})}{\mathrm{Kms1}\cdot\mathrm{Kms8}}-\frac{\mathrm{P1}\cdot\mathrm{P8}}{\mathrm{Kms1}\cdot\mathrm{Kms8}\cdot\mathrm{Keq}}\right)}{\left(1+\frac{\mathrm{S1}}{\mathrm{Kms1}}+\frac{\mathrm{P1}}{\mathrm{Kmp1}}+\frac{\mathrm{S2}}{\mathrm{Kms2}}+\frac{\mathrm{P2}}{\mathrm{Kmp2}}+\frac{\mathrm{S3}}{\mathrm{Kms3}}+\frac{\mathrm{P3}}{\mathrm{Kmp3}}+\frac{\mathrm{S4}}{\mathrm{Kms4}}+\frac{\mathrm{P4}}{\mathrm{Kmp4}}+\frac{\mathrm{S5}}{\mathrm{Kms5}}+\frac{\mathrm{P5}}{\mathrm{Kmp5}}+\frac{\mathrm{S6}}{\mathrm{Kms6}}+\frac{\mathrm{P6}}{\mathrm{Kmp6}}+\frac{\mathrm{S7}}{\mathrm{Kms7}}+\frac{\mathrm{P}}{\mathrm{Km}}\right.}\end{aligned}\tag{137}$$

Table 168: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmschadC10			0.64	dimensionless	☑

8.42 Reaction vmschadC8

This is a reversible reaction of one reactant forming two products influenced by 45 modifiers.

Reaction equation

$$\mathrm{C8HydroxyacylCoAMAT} \rightleftharpoons \mathrm{C16HydroxyacylCoAMAT},\ \mathrm{C14HydroxyacylCoAMAT},\ \mathrm{C12HydroxyacylCoAMAT},\ \mathrm{C10}\tag{138}$$

Reactant

Table 169: Properties of each reactant.

Id	Name	SBO
C8HydroxyacylCoAMAT		

Modifiers

Table 170: Properties of each modifier.

Id	Name	SBO
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		
C10HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
C4HydroxyacylCoAMAT		
NADtMAT		

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

Products

Table 171: Properties of each product.

Id	Name	SBO
C8KetoacylCoAMAT		
NADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{42} = \text{MSCHAD}(\text{sfmschadC8}, \text{Vmschad}, \text{KmmschadC8HydroxyacylCoAMAT}, \text{KmmschadC16HydroxyacylCoAMAT}, \text{KmmschadC14HydroxyacylCoAMAT}, \text{KmmschadC12HydroxyacylCoAMAT}, \text{KmmschadC10HydroxyacylCoAMAT}, \text{KmmschadC6HydroxyacylCoAMAT}, \text{KmmschadC4HydroxyacylCoAMAT}, \text{KmmschadNADMAT}, \text{KmmschadC8KetoacylCoAMAT}, \text{KmmschadC16KetoacylCoAMAT}, \text{KmmschadC14KetoacylCoAMAT}, \text{KmmschadC12KetoacylCoAMAT}, \text{KmmschadC10KetoacylCoAMAT}, \text{KmmschadC6KetoacylCoAMAT}, \text{KmmschadC4AcetoacylCoAMAT}, \text{KmmschadNADHMAT}, \text{Keqmschad}, [\text{C8HydroxyacylCoAMAT}], [\text{C16HydroxyacylCoAMAT}], [\text{C14HydroxyacylCoAMAT}], [\text{C12HydroxyacylCoAMAT}], [\text{C10HydroxyacylCoAMAT}], [\text{C6HydroxyacylCoAMAT}], [\text{C4HydroxyacylCoAMAT}], [\text{NADtMAT}], [\text{C8KetoacylCoAMAT}], [\text{C16KetoacylCoAMAT}], [\text{C14KetoacylCoAMAT}], [\text{C12KetoacylCoAMAT}], [\text{C10KetoacylCoAMAT}], [\text{C6KetoacylCoAMAT}], [\text{C4AcetoacylCoAMAT}], [\text{NADHMAT}]) \tag{139}$$

$$\text{MSCHAD}(\text{sf}, \text{V}, \text{Kms1}, \text{Kms2}, \text{Kms3}, \text{Kms4}, \text{Kms5}, \text{Kms6}, \text{Kms7}, \text{Kms8}, \text{Kmp1}, \text{Kmp2}, \text{Kmp3}, \text{Kmp4}, \text{Kmp5}, \text{Kmp6}, \text{Kmp7}, \text{Kmp8}, \text{Keq}, \text{S1}, \text{S2}, \text{S3}, \text{S4}, \text{S5}, \text{S6}, \text{S7}, \text{S8}, \text{P1}, \text{P2}, \text{P3}, \text{P4}, \text{P5}, \text{P6}, \text{P7}, \text{P8}) \tag{140}$$

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

Table 172: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmschadC8			0.89	dimensionless	☑

8.43 Reaction vmschadC6

This is a reversible reaction of one reactant forming two products influenced by 45 modifiers.

Reaction equation

$$\text{C6HydroxyacylCoAMAT} \rightleftharpoons \text{C16HydroxyacylCoAMAT, C14HydroxyacylCoAMAT, C12HydroxyacylCoAMAT, C10} \quad (141)$$

Reactant

Table 173: Properties of each reactant.

Id	Name	SBO
C6HydroxyacylCoAMAT		

Modifiers

Table 174: Properties of each modifier.

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

Id	Name	SBO
C6KetoacylCoAMAT		
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
C4AcetoacylCoAMAT		
NADHMAT		
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		
NADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{43} = \text{MSCHAD}(\text{sfmschadC6}, \text{Vmschad}, \text{KmmschadC6HydroxyacylCoAMAT}, \text{KmmschadC16HydroxyacylCoAMAT}, \text{KmmschadC14HydroxyacylCoAMAT}, \text{KmmschadC12HydroxyacylCoAMAT}, \text{KmmschadC10HydroxyacylCoAMAT}, \text{KmmschadC8HydroxyacylCoAMAT}, \text{KmmschadC4HydroxyacylCoAMAT}, \text{KmmschadNADMAT}, \text{KmmschadC6KetoacylCoAMAT}, \text{KmmschadC16KetoacylCoAMAT}, \text{KmmschadC14KetoacylCoAMAT}, \text{KmmschadC12KetoacylCoAMAT}, \text{KmmschadC10KetoacylCoAMAT}, \text{KmmschadC8KetoacylCoAMAT}, \text{KmmschadC4AcetoacylCoAMAT}, \text{KmmschadNADHMAT}, \text{Keqmschad}, [\text{C6HydroxyacylCoAMAT}], [\text{C16HydroxyacylCoAMAT}], [\text{C14HydroxyacylCoAMAT}], [\text{C12HydroxyacylCoAMAT}], [\text{C10HydroxyacylCoAMAT}], [\text{C8HydroxyacylCoAMAT}], [\text{C4HydroxyacylCoAMAT}], [\text{NADtMAT}], [\text{C6KetoacylCoAMAT}], [\text{C16KetoacylCoAMAT}], [\text{C14KetoacylCoAMAT}], [\text{C12KetoacylCoAMAT}], [\text{C10KetoacylCoAMAT}], [\text{C8KetoacylCoAMAT}], [\text{C4AcetoacylCoAMAT}], [\text{NADHMAT}]) \tag{142}$$

$$\text{MSCHAD}(\text{sf}, \text{V}, \text{Kms1}, \text{Kms2}, \text{Kms3}, \text{Kms4}, \text{Kms5}, \text{Kms6}, \text{Kms7}, \text{Kms8}, \text{Kmp1}, \text{Kmp2}, \text{Kmp3}, \text{Kmp4}, \text{Kmp5}, \text{Kmp6}, \text{Kmp7}, \text{Kmp8}, \text{Keq}, \text{S1}, \text{S2}, \text{S3}, \text{S4}, \text{S5}, \text{S6}, \text{S7}, \text{S8}, \text{P1}, \text{P2}, \text{P3}, \text{P4}, \text{P5}, \text{P6}, \text{P7}, \text{P8}) \tag{143}$$

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

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 45 modifiers.

Reaction equation

$$\text{C4HydroxyacylCoAMAT} \rightleftharpoons \text{C16HydroxyacylCoAMAT}, \text{C14HydroxyacylCoAMAT}, \text{C12HydroxyacylCoAMAT}, \text{C10} \tag{144}$$

Reactant

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		
C6HydroxyacylCoAMAT		
NADtMAT		
C4AcetoacylCoAMAT		
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
NADHMAT		
C4HydroxyacylCoAMAT		
C16HydroxyacylCoAMAT		
C14HydroxyacylCoAMAT		
C12HydroxyacylCoAMAT		

Id	Name	SBO
C10HydroxyacylCoAMAT		
C8HydroxyacylCoAMAT		
C6HydroxyacylCoAMAT		
NADtMAT		
C4AcetoacylCoAMAT		
C16KetoacylCoAMAT		
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
NADHMAT		

Products

Table 179: Properties of each product.

Id	Name	SBO
C4AcetoacylCoAMAT		
NADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{44} = \text{MSCHAD}\,(\text{sfmschadC4}, \text{Vmschad}, \text{KmmschadC4HydroxyacylCoAMAT}, \text{KmmschadC16HydroxyacylCoAMAT}, \text{KmmschadC14HydroxyacylCoAMAT}, \text{KmmschadC12HydroxyacylCoAMAT}, \text{KmmschadC10HydroxyacylCoAMAT}, \text{KmmschadC8HydroxyacylCoAMAT}, \text{KmmschadC6HydroxyacylCoAMAT}, \text{KmmschadNADMAT}, \text{KmmschadC4AcetoacylCoAMAT}, \text{KmmschadC16KetoacylCoAMAT}, \text{KmmschadC14KetoacylCoAMAT}, \text{KmmschadC12KetoacylCoAMAT}, \text{KmmschadC10KetoacylCoAMAT}, \text{KmmschadC8KetoacylCoAMAT}, \text{KmmschadC6KetoacylCoAMAT}, \text{KmmschadNADHMAT}, \text{Keqmschad}, [\text{C4HydroxyacylCoAMAT}], [\text{C16HydroxyacylCoAMAT}], [\text{C14HydroxyacylCoAMAT}], [\text{C12HydroxyacylCoAMAT}], [\text{C10HydroxyacylCoAMAT}], [\text{C8HydroxyacylCoAMAT}], [\text{C6HydroxyacylCoAMAT}], [\text{NADtMAT}], [\text{C4AcetoacylCoAMAT}], [\text{C16KetoacylCoAMAT}], [\text{C14KetoacylCoAMAT}], [\text{C12KetoacylCoAMAT}], [\text{C10KetoacylCoAMAT}], [\text{C8KetoacylCoAMAT}], [\text{C6KetoacylCoAMAT}], [\text{NADHMAT}]) \quad (145)$$

$$\begin{aligned}&\mathrm{MSCHAD}\left(\mathrm{sf},\mathrm{V},\mathrm{Kms1},\mathrm{Kms2},\mathrm{Kms3},\mathrm{Kms4},\mathrm{Kms5},\mathrm{Kms6},\mathrm{Kms7},\right.\\&\left.\mathrm{Kms8},\mathrm{Kmp1},\mathrm{Kmp2},\mathrm{Kmp3},\mathrm{Kmp4},\mathrm{Kmp5},\mathrm{Kmp6},\mathrm{Kmp7},\mathrm{Kmp8},\right.\\&\left.\mathrm{Keq},\mathrm{S1},\mathrm{S2},\mathrm{S3},\mathrm{S4},\mathrm{S5},\mathrm{S6},\mathrm{S7},\mathrm{S8},\mathrm{P1},\mathrm{P2},\mathrm{P3},\mathrm{P4},\mathrm{P5},\mathrm{P6},\mathrm{P7},\mathrm{P8}\right)\\&=\frac{\mathrm{sf}\cdot\mathrm{V}\cdot\left(\frac{\mathrm{S1}\cdot(\mathrm{S8}-\mathrm{P8})}{\mathrm{Kms1}\cdot\mathrm{Kms8}}-\frac{\mathrm{P1}\cdot\mathrm{P8}}{\mathrm{Kms1}\cdot\mathrm{Kms8}\cdot\mathrm{Keq}}\right)}{\left(1+\frac{\mathrm{S1}}{\mathrm{Kms1}}+\frac{\mathrm{P1}}{\mathrm{Kmp1}}+\frac{\mathrm{S2}}{\mathrm{Kms2}}+\frac{\mathrm{P2}}{\mathrm{Kmp2}}+\frac{\mathrm{S3}}{\mathrm{Kms3}}+\frac{\mathrm{P3}}{\mathrm{Kmp3}}+\frac{\mathrm{S4}}{\mathrm{Kms4}}+\frac{\mathrm{P4}}{\mathrm{Kmp4}}+\frac{\mathrm{S5}}{\mathrm{Kms5}}+\frac{\mathrm{P5}}{\mathrm{Kmp5}}+\frac{\mathrm{S6}}{\mathrm{Kms6}}+\frac{\mathrm{P6}}{\mathrm{Kmp6}}+\frac{\mathrm{S7}}{\mathrm{Kms7}}+\frac{\mathrm{P}}{\mathrm{Km}}\right.}\end{aligned}\tag{146}$$

Table 180: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmschadC4			0.67	dimensionless	☑

8.45 Reaction vmckatC16

This is a reversible reaction of one reactant forming two products influenced by 45 modifiers.

Reaction equation

$$\mathrm{C16KetoacylCoAMAT} \rightleftharpoons \mathrm{C14KetoacylCoAMAT},\ \mathrm{C12KetoacylCoAMAT},\ \mathrm{C10KetoacylCoAMAT},\ \mathrm{C8KetoacylCoAM}\tag{147}$$

Reactant

Table 181: Properties of each reactant.

Id	Name	SBO
C16KetoacylCoAMAT		

Modifiers

Table 182: Properties of each modifier.

Id	Name	SBO
C14KetoacylCoAMAT		
C12KetoacylCoAMAT		
C10KetoacylCoAMAT		
C8KetoacylCoAMAT		
C6KetoacylCoAMAT		
C4AcetoacylCoAMAT		
CoAMAT		

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

Products

Table 183: Properties of each product.

Id	Name	SBO
C14AcylCoAMAT		
AcetylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{45} = \text{MCKATA}(\text{sfmckatC16}, \text{Vmckat}, \text{KmmckatC16KetoacylCoAMAT}, \text{KmmckatC14KetoacylCoAMAT}, \text{KmmckatC12KetoacylCoAMAT}, \text{KmmckatC10KetoacylCoAMAT}, \text{KmmckatC8KetoacylCoAMAT}, \text{KmmckatC6KetoacylCoAMAT}, \text{KmmckatC4AcetoacylCoAMAT}, \text{KmmckatCoAMAT}, \text{KmmckatC14AcylCoAMAT}, \text{KmmckatC16AcylCoAMAT}, \text{KmmckatC12AcylCoAMAT}, \text{KmmckatC10AcylCoAMAT}, \text{KmmckatC8AcylCoAMAT}, \text{KmmckatC6AcylCoAMAT}, \text{KmmckatC4AcylCoAMAT}, \text{KmmckatAcetylCoAMAT}, \text{Keqmckat}, [\text{C16KetoacylCoAMAT}], [\text{C14KetoacylCoAMAT}], [\text{C12KetoacylCoAMAT}], [\text{C10KetoacylCoAMAT}], [\text{C8KetoacylCoAMAT}], [\text{C6KetoacylCoAMAT}], [\text{C4AcetoacylCoAMAT}], [\text{CoAMAT}], [\text{C14AcylCoAMAT}], [\text{C16AcylCoAMAT}], [\text{C12AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C8AcylCoAMAT}], [\text{C6AcylCoAMAT}], [\text{C4AcylCoAMAT}], [\text{AcetylCoAMAT}]) \quad (148)$$

$$\text{MCKATA}(\text{sf}, \text{V}, \text{Kms1}, \text{Kms2}, \text{Kms3}, \text{Kms4}, \text{Kms5}, \text{Kms6}, \text{Kms7}, \text{Kms8}, \text{Kmp1}, \text{Kmp2}, \text{Kmp3}, \text{Kmp4}, \text{Kmp5}, \text{Kmp6}, \text{Kmp7}, \text{Kmp8}, \text{Keq}, \text{S1}, \text{S2}, \text{S3}, \text{S4}, \text{S5}, \text{S6}, \text{S7}, \text{S8}, \text{P1}, \text{P2}, \text{P3}, \text{P4}, \text{P5}, \text{P6}, \text{P7}, \text{P8}) \quad (149)$$

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

Table 184: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmckatC16			0.0	dimensionless	☑

8.46 Reaction vmckatC14

This is a reversible reaction of one reactant forming two products influenced by 45 modifiers.

Reaction equation

$$\text{C14KetoacylCoAMAT} \rightleftharpoons \text{C16KetoacylCoAMAT, C12KetoacylCoAMAT, C10KetoacylCoAMAT, C8KetoacylCoAM} \quad (150)$$

Reactant

Table 185: Properties of each reactant.

Id	Name	SBO
C14KetoacylCoAMAT		

Modifiers

Table 186: Properties of each modifier.

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

Id	Name	SBO
C8AcylCoAMAT		
C6AcylCoAMAT		
C4AcylCoAMAT		
AcetylCoAMAT		
C14KetoacylCoAMAT		
C16KetoacylCoAMAT		
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

$$v_{46} = \text{MCKATA}\,(\text{sfmckatC14}, \text{Vmckat}, \text{KmmckatC14KetoacylCoAMAT}, \text{KmmckatC16KetoacylCoAMAT}, \text{KmmckatC12KetoacylCoAMAT}, \text{KmmckatC10KetoacylCoAMAT}, \text{KmmckatC8KetoacylCoAMAT}, \text{KmmckatC6KetoacylCoAMAT}, \text{KmmckatC4AcetoacylCoAMAT}, \text{KmmckatCoAMAT}, \text{KmmckatC12AcylCoAMAT}, \text{KmmckatC16AcylCoAMAT}, \text{KmmckatC14AcylCoAMAT}, \text{KmmckatC10AcylCoAMAT}, \text{KmmckatC8AcylCoAMAT}, \text{KmmckatC6AcylCoAMAT}, \text{KmmckatC4AcylCoAMAT}, \text{KmmckatAcetylCoAMAT}, \text{Keqmckat}, [\text{C14KetoacylCoAMAT}], [\text{C16KetoacylCoAMAT}], [\text{C12KetoacylCoAMAT}], [\text{C10KetoacylCoAMAT}], [\text{C8KetoacylCoAMAT}], [\text{C6KetoacylCoAMAT}], [\text{C4AcetoacylCoAMAT}], [\text{CoAMAT}], [\text{C12AcylCoAMAT}], [\text{C16AcylCoAMAT}], [\text{C14AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C8AcylCoAMAT}], [\text{C6AcylCoAMAT}], [\text{C4AcylCoAMAT}], [\text{AcetylCoAMAT}]) \tag{151}$$

$$\text{MCKATA}\,(\text{sf}, \text{V}, \text{Kms1}, \text{Kms2}, \text{Kms3}, \text{Kms4}, \text{Kms5}, \text{Kms6}, \text{Kms7}, \text{Kms8}, \text{Kmp1}, \text{Kmp2}, \text{Kmp3}, \text{Kmp4}, \text{Kmp5}, \text{Kmp6}, \text{Kmp7}, \text{Kmp8}, \text{Keq}, \text{S1}, \text{S2}, \text{S3}, \text{S4}, \text{S5}, \text{S6}, \text{S7}, \text{S8}, \text{P1}, \text{P2}, \text{P3}, \text{P4}, \text{P5}, \text{P6}, \text{P7}, \text{P8}) \tag{152}$$

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

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 45 modifiers.

Reaction equation

$$\text{C12KetoacylCoAMAT} \rightleftharpoons \text{C16KetoacylCoAMAT, C14KetoacylCoAMAT, C10KetoacylCoAMAT, C8KetoacylCoAM} \tag{153}$$

Reactant

Table 189: Properties of each reactant.

Id	Name	SBO
C12KetoacylCoAMAT		

Id	Name	SBO

Modifiers

Table 190: Properties of each modifier.

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

Id	Name	SBO
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

$$v_{47} = \text{MCKATA}\,(\text{sfmckatC12}, \text{Vmckat}, \text{KmmckatC12KetoacylCoAMAT}, \text{KmmckatC16KetoacylCoAMAT}, \text{KmmckatC14KetoacylCoAMAT}, \text{KmmckatC10KetoacylCoAMAT}, \text{KmmckatC8KetoacylCoAMAT}, \text{KmmckatC6KetoacylCoAMAT}, \text{KmmckatC4AcetoacylCoAMAT}, \text{KmmckatCoAMAT}, \text{KmmckatC10AcylCoAMAT}, \text{KmmckatC16AcylCoAMAT}, \text{KmmckatC14AcylCoAMAT}, \text{KmmckatC12AcylCoAMAT}, \text{KmmckatC8AcylCoAMAT}, \text{KmmckatC6AcylCoAMAT}, \text{KmmckatC4AcylCoAMAT}, \text{KmmckatAcetylCoAMAT}, \text{Keqmckat}, [\text{C12KetoacylCoAMAT}], [\text{C16KetoacylCoAMAT}], [\text{C14KetoacylCoAMAT}], [\text{C10KetoacylCoAMAT}], [\text{C8KetoacylCoAMAT}], [\text{C6KetoacylCoAMAT}], [\text{C4AcetoacylCoAMAT}], [\text{CoAMAT}], [\text{C10AcylCoAMAT}], [\text{C16AcylCoAMAT}], [\text{C14AcylCoAMAT}], [\text{C12AcylCoAMAT}], [\text{C8AcylCoAMAT}], [\text{C6AcylCoAMAT}], [\text{C4AcylCoAMAT}], [\text{AcetylCoAMAT}]) \quad (154)$$

$$\begin{aligned}&\mathrm{MCKATA}\left(\mathrm{sf},\mathrm{V},\mathrm{Kms1},\mathrm{Kms2},\mathrm{Kms3},\mathrm{Kms4},\mathrm{Kms5},\mathrm{Kms6},\mathrm{Kms7},\right.\\&\left.\mathrm{Kms8},\mathrm{Kmp1},\mathrm{Kmp2},\mathrm{Kmp3},\mathrm{Kmp4},\mathrm{Kmp5},\mathrm{Kmp6},\mathrm{Kmp7},\mathrm{Kmp8},\right.\\&\left.\mathrm{Keq},\mathrm{S1},\mathrm{S2},\mathrm{S3},\mathrm{S4},\mathrm{S5},\mathrm{S6},\mathrm{S7},\mathrm{S8},\mathrm{P1},\mathrm{P2},\mathrm{P3},\mathrm{P4},\mathrm{P5},\mathrm{P6},\mathrm{P7},\mathrm{P8}\right)\\&=\frac{\mathrm{sf}\cdot\mathrm{V}\cdot\left(\frac{\mathrm{S1}\cdot\mathrm{S8}}{\mathrm{Kms1}\cdot\mathrm{Kms8}}-\frac{\mathrm{P1}\cdot\mathrm{P8}}{\mathrm{Kms1}\cdot\mathrm{Kms8}\cdot\mathrm{Keq}}\right)}{\left(1+\frac{\mathrm{S1}}{\mathrm{Kms1}}+\frac{\mathrm{P1}}{\mathrm{Kmp1}}+\frac{\mathrm{S2}}{\mathrm{Kms2}}+\frac{\mathrm{P2}}{\mathrm{Kmp2}}+\frac{\mathrm{S3}}{\mathrm{Kms3}}+\frac{\mathrm{P3}}{\mathrm{Kmp3}}+\frac{\mathrm{S4}}{\mathrm{Kms4}}+\frac{\mathrm{P4}}{\mathrm{Kmp4}}+\frac{\mathrm{S5}}{\mathrm{Kms5}}+\frac{\mathrm{P5}}{\mathrm{Kmp5}}+\frac{\mathrm{S6}}{\mathrm{Kms6}}+\frac{\mathrm{P6}}{\mathrm{Kmp6}}+\frac{\mathrm{S7}}{\mathrm{Kms7}}+\frac{\mathrm{P}}{\mathrm{Km}}\right.}\end{aligned}\tag{155}$$

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 45 modifiers.

Reaction equation

$$\mathrm{C10KetoacylCoAMAT} \rightleftharpoons \mathrm{C16KetoacylCoAMAT},\ \mathrm{C14KetoacylCoAMAT},\ \mathrm{C12KetoacylCoAMAT},\ \mathrm{C8KetoacylCoAM}\tag{156}$$

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		
C4AcetoacylCoAMAT		
CoAMAT		

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

$$v_{48} = \text{MCKATA}(\text{sfmckatC10}, \text{Vmckat}, \text{KmmckatC10KetoacylCoAMAT}, \text{KmmckatC16KetoacylCoAMAT}, \text{KmmckatC14KetoacylCoAMAT}, \text{KmmckatC12KetoacylCoAMAT}, \text{KmmckatC8KetoacylCoAMAT}, \text{KmmckatC6KetoacylCoAMAT}, \text{KmmckatC4AcetoacylCoAMAT}, \text{KmmckatCoAMAT}, \text{KmmckatC8AcylCoAMAT}, \text{KmmckatC16AcylCoAMAT}, \text{KmmckatC14AcylCoAMAT}, \text{KmmckatC12AcylCoAMAT}, \text{KmmckatC10AcylCoAMAT}, \text{KmmckatC6AcylCoAMAT}, \text{KmmckatC4AcylCoAMAT}, \text{KmmckatAcetylCoAMAT}, \text{Keqmckat}, [\text{C10KetoacylCoAMAT}], [\text{C16KetoacylCoAMAT}], [\text{C14KetoacylCoAMAT}], [\text{C12KetoacylCoAMAT}], [\text{C8KetoacylCoAMAT}], [\text{C6KetoacylCoAMAT}], [\text{C4AcetoacylCoAMAT}], [\text{CoAMAT}], [\text{C8AcylCoAMAT}], [\text{C16AcylCoAMAT}], [\text{C14AcylCoAMAT}], [\text{C12AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C6AcylCoAMAT}], [\text{C4AcylCoAMAT}], [\text{AcetylCoAMAT}]) \quad (157)$$

$$\text{MCKATA}(\text{sf}, \text{V}, \text{Kms1}, \text{Kms2}, \text{Kms3}, \text{Kms4}, \text{Kms5}, \text{Kms6}, \text{Kms7}, \text{Kms8}, \text{Kmp1}, \text{Kmp2}, \text{Kmp3}, \text{Kmp4}, \text{Kmp5}, \text{Kmp6}, \text{Kmp7}, \text{Kmp8}, \text{Keq}, \text{S1}, \text{S2}, \text{S3}, \text{S4}, \text{S5}, \text{S6}, \text{S7}, \text{S8}, \text{P1}, \text{P2}, \text{P3}, \text{P4}, \text{P5}, \text{P6}, \text{P7}, \text{P8}) \quad (158)$$

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

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 45 modifiers.

Reaction equation

$$\text{C8KetoacylCoAMAT} \rightleftharpoons \text{C16KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCoAMAT, C10KetoacylCoAM} \quad (159)$$

Reactant

Table 197: Properties of each reactant.

Id	Name	SBO
C8KetoacylCoAMAT		

Modifiers

Table 198: Properties of each modifier.

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

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

Products

Table 199: Properties of each product.

Id	Name	SBO
C6AcylCoAMAT		
AcetylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{49} = \text{MCKATA}\,(\text{sfmckatC8}, \text{Vmckat}, \text{KmmckatC8KetoacylCoAMAT}, \text{KmmckatC16KetoacylCoAMAT}, \text{KmmckatC14KetoacylCoAMAT}, \text{KmmckatC12KetoacylCoAMAT}, \text{KmmckatC10KetoacylCoAMAT}, \text{KmmckatC6KetoacylCoAMAT}, \text{KmmckatC4AcetoacylCoAMAT}, \text{KmmckatCoAMAT}, \text{KmmckatC6AcylCoAMAT}, \text{KmmckatC16AcylCoAMAT}, \text{KmmckatC14AcylCoAMAT}, \text{KmmckatC12AcylCoAMAT}, \text{KmmckatC10AcylCoAMAT}, \text{KmmckatC8AcylCoAMAT}, \text{KmmckatC4AcylCoAMAT}, \text{KmmckatAcetylCoAMAT}, \text{Keqmckat}, [\text{C8KetoacylCoAMAT}], [\text{C16KetoacylCoAMAT}], [\text{C14KetoacylCoAMAT}], [\text{C12KetoacylCoAMAT}], [\text{C10KetoacylCoAMAT}], [\text{C6KetoacylCoAMAT}], [\text{C4AcetoacylCoAMAT}], [\text{CoAMAT}], [\text{C6AcylCoAMAT}], [\text{C16AcylCoAMAT}], [\text{C14AcylCoAMAT}], [\text{C12AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C8AcylCoAMAT}], [\text{C4AcylCoAMAT}], [\text{AcetylCoAMAT}]) \tag{160}$$

$$\text{MCKATA}\,(\text{sf}, \text{V}, \text{Kms1}, \text{Kms2}, \text{Kms3}, \text{Kms4}, \text{Kms5}, \text{Kms6}, \text{Kms7}, \text{Kms8}, \text{Kmp1}, \text{Kmp2}, \text{Kmp3}, \text{Kmp4}, \text{Kmp5}, \text{Kmp6}, \text{Kmp7}, \text{Kmp8}, \text{Keq}, \text{S1}, \text{S2}, \text{S3}, \text{S4}, \text{S5}, \text{S6}, \text{S7}, \text{S8}, \text{P1}, \text{P2}, \text{P3}, \text{P4}, \text{P5}, \text{P6}, \text{P7}, \text{P8}) \tag{161}$$

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

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 45 modifiers.

Reaction equation

$$\text{C6KetoacylCoAMAT} \rightleftharpoons \text{C16KetoacylCoAMAT, C14KetoacylCoAMAT, C12KetoacylCoAMAT, C10KetoacylCoAM} \tag{162}$$

Reactant

Table 201: Properties of each reactant.

Id	Name	SBO
C6KetoacylCoAMAT		

Id	Name	SBO

Modifiers

Table 202: Properties of each modifier.

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

Id	Name	SBO
C4AcetoacylCoAMAT		
CoAMAT		
C4AcylCoAMAT		
C16AcylCoAMAT		
C14AcylCoAMAT		
C12AcylCoAMAT		
C10AcylCoAMAT		
C8AcylCoAMAT		
C6AcylCoAMAT		
AcetylCoAMAT		

Products

Table 203: Properties of each product.

Id	Name	SBO
C4AcylCoAMAT		
AcetylCoAMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{50} = \text{MCKATA}\,(\text{sfmckatC6}, \text{Vmckat}, \text{KmmckatC6KetoacylCoAMAT}, \text{KmmckatC16KetoacylCoAMAT}, \text{KmmckatC14KetoacylCoAMAT}, \text{KmmckatC12KetoacylCoAMAT}, \text{KmmckatC10KetoacylCoAMAT}, \text{KmmckatC8KetoacylCoAMAT}, \text{KmmckatC4AcetoacylCoAMAT}, \text{KmmckatCoAMAT}, \text{KmmckatC4AcylCoAMAT}, \text{KmmckatC16AcylCoAMAT}, \text{KmmckatC14AcylCoAMAT}, \text{KmmckatC12AcylCoAMAT}, \text{KmmckatC10AcylCoAMAT}, \text{KmmckatC8AcylCoAMAT}, \text{KmmckatC6AcylCoAMAT}, \text{KmmckatAcetylCoAMAT}, \text{Keqmckat}, [\text{C6KetoacylCoAMAT}], [\text{C16KetoacylCoAMAT}], [\text{C14KetoacylCoAMAT}], [\text{C12KetoacylCoAMAT}], [\text{C10KetoacylCoAMAT}], [\text{C8KetoacylCoAMAT}], [\text{C4AcetoacylCoAMAT}], [\text{CoAMAT}], [\text{C4AcylCoAMAT}], [\text{C16AcylCoAMAT}], [\text{C14AcylCoAMAT}], [\text{C12AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C8AcylCoAMAT}], [\text{C6AcylCoAMAT}], [\text{AcetylCoAMAT}]) \quad (163)$$

$$\begin{aligned}&\mathrm{MCKATA}\left(\mathrm{sf},\mathrm{V},\mathrm{Kms1},\mathrm{Kms2},\mathrm{Kms3},\mathrm{Kms4},\mathrm{Kms5},\mathrm{Kms6},\mathrm{Kms7},\right.\\&\left.\mathrm{Kms8},\mathrm{Kmp1},\mathrm{Kmp2},\mathrm{Kmp3},\mathrm{Kmp4},\mathrm{Kmp5},\mathrm{Kmp6},\mathrm{Kmp7},\mathrm{Kmp8},\right.\\&\left.\mathrm{Keq},\mathrm{S1},\mathrm{S2},\mathrm{S3},\mathrm{S4},\mathrm{S5},\mathrm{S6},\mathrm{S7},\mathrm{S8},\mathrm{P1},\mathrm{P2},\mathrm{P3},\mathrm{P4},\mathrm{P5},\mathrm{P6},\mathrm{P7},\mathrm{P8}\right)\\&=\frac{\mathrm{sf}\cdot\mathrm{V}\cdot\left(\frac{\mathrm{S1}\cdot\mathrm{S8}}{\mathrm{Kms1}\cdot\mathrm{Kms8}}-\frac{\mathrm{P1}\cdot\mathrm{P8}}{\mathrm{Kms1}\cdot\mathrm{Kms8}\cdot\mathrm{Keq}}\right)}{\left(1+\frac{\mathrm{S1}}{\mathrm{Kms1}}+\frac{\mathrm{P1}}{\mathrm{Kmp1}}+\frac{\mathrm{S2}}{\mathrm{Kms2}}+\frac{\mathrm{P2}}{\mathrm{Kmp2}}+\frac{\mathrm{S3}}{\mathrm{Kms3}}+\frac{\mathrm{P3}}{\mathrm{Kmp3}}+\frac{\mathrm{S4}}{\mathrm{Kms4}}+\frac{\mathrm{P4}}{\mathrm{Kmp4}}+\frac{\mathrm{S5}}{\mathrm{Kms5}}+\frac{\mathrm{P5}}{\mathrm{Kmp5}}+\frac{\mathrm{S6}}{\mathrm{Kms6}}+\frac{\mathrm{P6}}{\mathrm{Kmp6}}+\frac{\mathrm{S7}}{\mathrm{Kms7}}+\frac{\mathrm{P}}{\mathrm{Km}}\right.}\end{aligned}\tag{164}$$

Table 204: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmckatC6			1.0	dimensionless	☑

8.51 Reaction vmckatC4

This is a reversible reaction of one reactant forming one product influenced by 46 modifiers.

Reaction equation

$$\mathrm{C4AcetoacylCoAMAT}\ \underset{}{\overset{\mathrm{C16KetoacylCoAMAT},\ \mathrm{C14KetoacylCoAMAT},\ \mathrm{C12KetoacylCoAMAT},\ \mathrm{C10KetoacylCoAM}}{\rightleftharpoons}}\tag{165}$$

Reactant

Table 205: Properties of each reactant.

Id	Name	SBO
C4AcetoacylCoAMAT		

Modifiers

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		
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

$$v_{51} = \text{MCKATB}\,(\text{sfmckatC4}, \text{Vmckat}, \text{KmmckatC4AcetoacylCoAMAT}, \text{KmmckatC16KetoacylCoAMAT}, \text{KmmckatC14KetoacylCoAMAT}, \text{KmmckatC12KetoacylCoAMAT}, \text{KmmckatC10KetoacylCoAMAT}, \text{KmmckatC8KetoacylCoAMAT}, \text{KmmckatC6KetoacylCoAMAT}, \text{KmmckatCoAMAT}, \text{KmmckatC4AcylCoAMAT}, \text{KmmckatC16AcylCoAMAT}, \text{KmmckatC14AcylCoAMAT}, \text{KmmckatC12AcylCoAMAT}, \text{KmmckatC10AcylCoAMAT}, \text{KmmckatC8AcylCoAMAT}, \text{KmmckatC6AcylCoAMAT}, \text{KmmckatAcetylCoAMAT}, \text{Keqmckat}, [\text{C4AcetoacylCoAMAT}], [\text{C16KetoacylCoAMAT}], [\text{C14KetoacylCoAMAT}], [\text{C12KetoacylCoAMAT}], [\text{C10KetoacylCoAMAT}], [\text{C8KetoacylCoAMAT}], [\text{C6KetoacylCoAMAT}], [\text{CoAMAT}], [\text{C4AcylCoAMAT}], [\text{C16AcylCoAMAT}], [\text{C14AcylCoAMAT}], [\text{C12AcylCoAMAT}], [\text{C10AcylCoAMAT}], [\text{C8AcylCoAMAT}], [\text{C6AcylCoAMAT}], [\text{AcetylCoAMAT}]) \tag{166}$$

$$\text{MCKATB}\,(\text{sf}, \text{V}, \text{Kms1}, \text{Kms2}, \text{Kms3}, \text{Kms4}, \text{Kms5}, \text{Kms6}, \text{Kms7}, \text{Kms8}, \text{Kmp1}, \text{Kmp2}, \text{Kmp3}, \text{Kmp4}, \text{Kmp5}, \text{Kmp6}, \text{Kmp7}, \text{Kmp8}, \text{Keq}, \text{S1}, \text{S2}, \text{S3}, \text{S4}, \text{S5}, \text{S6}, \text{S7}, \text{S8}, \text{P1}, \text{P2}, \text{P3}, \text{P4}, \text{P5}, \text{P6}, \text{P7}, \text{P8}) \tag{167}$$

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

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 44 modifiers.

Reaction equation

$$\text{C16EnoylCoAMAT} \rightleftharpoons \text{C14EnoylCoAMAT, C12EnoylCoAMAT, C10EnoylCoAMAT, C8EnoylCoAMAT, NADtMAT} \quad (168)$$

Reactant

Table 209: Properties of each reactant.

Id	Name	SBO
C16EnoylCoAMAT		

Modifiers

Table 210: Properties of each modifier.

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

Id	Name	SBO
NADHMAT		
AcetylCoAMAT		
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		
AcetylCoAMAT		
NADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{52} = \mathrm{MTP}(\mathrm{sfmtpC16}, \mathrm{Vmtp}, \mathrm{KmmtpC16EnoylCoAMAT}, \mathrm{KmmtpC14EnoylCoAMAT}, \mathrm{KmmtpC12EnoylCoAMAT}, \mathrm{KmmtpC10EnoylCoAMAT}, \mathrm{KmmtpC8EnoylCoAMAT}, \mathrm{KmmtpNADMAT}, \mathrm{KmmtpCoAMAT}, \mathrm{KmmtpC14AcylCoAMAT}, \mathrm{KmmtpC16AcylCoAMAT}, \mathrm{KmmtpC12AcylCoAMAT}, \mathrm{KmmtpC10AcylCoAMAT}, \mathrm{KmmtpC8AcylCoAMAT}, \mathrm{KmmtpC6AcylCoAMAT}, \mathrm{KmmtpNADHMAT}, \mathrm{KmmtpAcetylCoAMAT}, \mathrm{KicrotC4AcetoacylCoA}, \mathrm{Keqmtp}, [\mathrm{C16EnoylCoAMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{NADtMAT}], [\mathrm{CoAMAT}], [\mathrm{C14AcylCoAMAT}], [\mathrm{C16AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{C6AcylCoAMAT}], [\mathrm{NADHMAT}], [\mathrm{AcetylCoAMAT}], [\mathrm{C4AcetoacylCoAMAT}]) \quad (169)$$

$$\mathrm{MTP}(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms7}, \mathrm{Kms8}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Kmp7}, \mathrm{Kmp8}, \mathrm{Ki1}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S7}, \mathrm{S8}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}, \mathrm{P7}, \mathrm{P8}, \mathrm{I1}) \quad (170)$$

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

Table 212: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmtpC16			1.0	dimensionless	☑

8.53 Reaction vmtpC14

This is a reversible reaction of one reactant forming three products influenced by 44 modifiers.

Reaction equation

$$\mathrm{C14EnoylCoAMAT} \rightleftharpoons \mathrm{C16EnoylCoAMAT}, \mathrm{C12EnoylCoAMAT}, \mathrm{C10EnoylCoAMAT}, \mathrm{C8EnoylCoAMAT}, \mathrm{NADtMAT} \quad (171)$$

Reactant

Table 213: Properties of each reactant.

Id	Name	SBO
C14EnoylCoAMAT		

Modifiers

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		
C14EnoylCoAMAT		
C16EnoylCoAMAT		
C12EnoylCoAMAT		
C10EnoylCoAMAT		
C8EnoylCoAMAT		
NADtMAT		
CoAMAT		
C12AcylCoAMAT		
C16AcylCoAMAT		
C14AcylCoAMAT		

Id	Name	SBO
C10AcylCoAMAT		
C8AcylCoAMAT		
C6AcylCoAMAT		
NADHMAT		
AcetylCoAMAT		
C4AcetoacylCoAMAT		

Products

Table 215: Properties of each product.

Id	Name	SBO
C12AcylCoAMAT		
AcetylCoAMAT		
NADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{53} = \mathrm{MTP}\,(\mathrm{sfmtpC14}, \mathrm{Vmtp}, \mathrm{KmmtpC14EnoylCoAMAT}, \mathrm{KmmtpC16EnoylCoAMAT}, \mathrm{KmmtpC12EnoylCoAMAT}, \mathrm{KmmtpC10EnoylCoAMAT}, \mathrm{KmmtpC8EnoylCoAMAT}, \mathrm{KmmtpNADMAT}, \mathrm{KmmtpCoAMAT}, \mathrm{KmmtpC12AcylCoAMAT}, \mathrm{KmmtpC16AcylCoAMAT}, \mathrm{KmmtpC14AcylCoAMAT}, \mathrm{KmmtpC10AcylCoAMAT}, \mathrm{KmmtpC8AcylCoAMAT}, \mathrm{KmmtpC6AcylCoAMAT}, \mathrm{KmmtpNADHMAT}, \mathrm{KmmtpAcetylCoAMAT}, \mathrm{KicrotC4AcetoacylCoA}, \mathrm{Keqmtp}, [\mathrm{C14EnoylCoAMAT}], [\mathrm{C16EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{NADtMAT}], [\mathrm{CoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C16AcylCoAMAT}], [\mathrm{C14AcylCoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{C6AcylCoAMAT}], [\mathrm{NADHMAT}], [\mathrm{AcetylCoAMAT}], [\mathrm{C4AcetoacylCoAMAT}]) \tag{172}$$

$$\mathrm{MTP}\,(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms7}, \mathrm{Kms8}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Kmp7}, \mathrm{Kmp8}, \mathrm{Ki1}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S7}, \mathrm{S8}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}, \mathrm{P7}, \mathrm{P8}, \mathrm{I1}) \tag{173}$$

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

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 44 modifiers.

Reaction equation

$$\text{C12EnoylCoAMAT} \rightleftharpoons \text{C16EnoylCoAMAT, C14EnoylCoAMAT, C10EnoylCoAMAT, C8EnoylCoAMAT, NADtMAT} \quad (174)$$

Reactant

Table 217: Properties of each reactant.

Id	Name	SBO
C12EnoylCoAMAT		

Modifiers

Table 218: Properties of each modifier.

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

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

Products

Table 219: Properties of each product.

Id	Name	SBO
C10AcylCoAMAT		
AcetylCoAMAT		
NADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{54} = \mathrm{MTP}(\mathrm{sfmtpC12}, \mathrm{Vmtp}, \mathrm{KmmtpC12EnoylCoAMAT}, \mathrm{KmmtpC16EnoylCoAMAT}, \mathrm{KmmtpC14EnoylCoAMAT}, \mathrm{KmmtpC10EnoylCoAMAT}, \mathrm{KmmtpC8EnoylCoAMAT}, \mathrm{KmmtpNADMAT}, \mathrm{KmmtpCoAMAT}, \mathrm{KmmtpC10AcylCoAMAT}, \mathrm{KmmtpC16AcylCoAMAT}, \mathrm{KmmtpC14AcylCoAMAT}, \mathrm{KmmtpC12AcylCoAMAT}, \mathrm{KmmtpC8AcylCoAMAT}, \mathrm{KmmtpC6AcylCoAMAT}, \mathrm{KmmtpNADHMAT}, \mathrm{KmmtpAcetylCoAMAT}, \mathrm{KicrotC4AcetoacylCoA}, \mathrm{Keqmtp}, [\mathrm{C12EnoylCoAMAT}], [\mathrm{C16EnoylCoAMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{NADtMAT}], [\mathrm{CoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C16AcylCoAMAT}], [\mathrm{C14AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{C6AcylCoAMAT}], [\mathrm{NADHMAT}], [\mathrm{AcetylCoAMAT}], [\mathrm{C4AcetoacylCoAMAT}]) \tag{175}$$

$$\mathrm{MTP}(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms7}, \mathrm{Kms8}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Kmp7}, \mathrm{Kmp8}, \mathrm{Ki1}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S7}, \mathrm{S8}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}, \mathrm{P7}, \mathrm{P8}, \mathrm{I1}) \tag{176}$$

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

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 44 modifiers.

Reaction equation

$$\mathrm{C10EnoylCoAMAT} \xrightleftharpoons{\mathrm{C16EnoylCoAMAT},\ \mathrm{C14EnoylCoAMAT},\ \mathrm{C12EnoylCoAMAT},\ \mathrm{C8EnoylCoAMAT},\ \mathrm{NADtMAT}} \tag{177}$$

Reactant

Table 221: Properties of each reactant.

Id	Name	SBO
C10EnoylCoAMAT		

Modifiers

Table 222: Properties of each modifier.

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

Id	Name	SBO
NADtMAT		
CoAMAT		
C8AcylCoAMAT		
C16AcylCoAMAT		
C14AcylCoAMAT		
C12AcylCoAMAT		
C10AcylCoAMAT		
C6AcylCoAMAT		
NADHMAT		
AcetylCoAMAT		
C4AcetoacylCoAMAT		

Products

Table 223: Properties of each product.

Id	Name	SBO
C8AcylCoAMAT		
AcetylCoAMAT		
NADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{55} = \mathrm{MTP}\,(\mathrm{sfmtpC10}, \mathrm{Vmtp}, \mathrm{KmmtpC10EnoylCoAMAT}, \mathrm{KmmtpC16EnoylCoAMAT}, \mathrm{KmmtpC14EnoylCoAMAT}, \mathrm{KmmtpC12EnoylCoAMAT}, \mathrm{KmmtpC8EnoylCoAMAT}, \mathrm{KmmtpNADMAT}, \mathrm{KmmtpCoAMAT}, \mathrm{KmmtpC8AcylCoAMAT}, \mathrm{KmmtpC16AcylCoAMAT}, \mathrm{KmmtpC14AcylCoAMAT}, \mathrm{KmmtpC12AcylCoAMAT}, \mathrm{KmmtpC10AcylCoAMAT}, \mathrm{KmmtpC6AcylCoAMAT}, \mathrm{KmmtpNADHMAT}, \mathrm{KmmtpAcetylCoAMAT}, \mathrm{KicrotC4AcetoacylCoA}, \mathrm{Keqmtp}, [\mathrm{C10EnoylCoAMAT}], [\mathrm{C16EnoylCoAMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C8EnoylCoAMAT}], [\mathrm{NADtMAT}], [\mathrm{CoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{C16AcylCoAMAT}], [\mathrm{C14AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C6AcylCoAMAT}], [\mathrm{NADHMAT}], [\mathrm{AcetylCoAMAT}], [\mathrm{C4AcetoacylCoAMAT}]) \quad (178)$$

$$\begin{aligned}&\mathrm{MTP}\left(\mathrm{sf},\mathrm{V},\mathrm{Kms1},\mathrm{Kms2},\mathrm{Kms3},\mathrm{Kms4},\mathrm{Kms5},\mathrm{Kms7},\mathrm{Kms8},\right.\\&\left.\mathrm{Kmp1},\mathrm{Kmp2},\mathrm{Kmp3},\mathrm{Kmp4},\mathrm{Kmp5},\mathrm{Kmp6},\mathrm{Kmp7},\mathrm{Kmp8},\mathrm{Ki1},\right.\\&\left.\mathrm{Keq},\mathrm{S1},\mathrm{S2},\mathrm{S3},\mathrm{S4},\mathrm{S5},\mathrm{S7},\mathrm{S8},\mathrm{P1},\mathrm{P2},\mathrm{P3},\mathrm{P4},\mathrm{P5},\mathrm{P6},\mathrm{P7},\mathrm{P8},\mathrm{I1}\right)\\&=\frac{\mathrm{sf}\cdot\mathrm{V}\cdot\left(\frac{\mathrm{S1}\cdot(\mathrm{S7}-\mathrm{P7})\cdot\mathrm{S8}}{\mathrm{Kms1}\cdot\mathrm{Kms7}\cdot\mathrm{Kms8}}-\frac{\mathrm{P1}\cdot\mathrm{P7}\cdot\mathrm{P8}}{\mathrm{Kms1}\cdot\mathrm{Kms7}\cdot\mathrm{Kms8}\cdot\mathrm{Keq}}\right)}{\left(1+\frac{\mathrm{S1}}{\mathrm{Kms1}}+\frac{\mathrm{P1}}{\mathrm{Kmp1}}+\frac{\mathrm{S2}}{\mathrm{Kms2}}+\frac{\mathrm{P2}}{\mathrm{Kmp2}}+\frac{\mathrm{S3}}{\mathrm{Kms3}}+\frac{\mathrm{P3}}{\mathrm{Kmp3}}+\frac{\mathrm{S4}}{\mathrm{Kms4}}+\frac{\mathrm{P4}}{\mathrm{Kmp4}}+\frac{\mathrm{S5}}{\mathrm{Kms5}}+\frac{\mathrm{P5}}{\mathrm{Kmp5}}+\frac{\mathrm{P6}}{\mathrm{Kmp6}}+\frac{\mathrm{I1}}{\mathrm{Ki1}}\right)\cdot\left(1+\frac{\mathrm{S7}-\mathrm{P7}}{\mathrm{Kms7}}\right.}\end{aligned}\tag{179}$$

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 44 modifiers.

Reaction equation

$$\mathrm{C8EnoylCoAMAT}\rightleftharpoons\mathrm{C16EnoylCoAMAT},\ \mathrm{C14EnoylCoAMAT},\ \mathrm{C12EnoylCoAMAT},\ \mathrm{C10EnoylCoAMAT},\ \mathrm{NADtMAT}\tag{180}$$

Reactant

Table 225: Properties of each reactant.

Id	Name	SBO
C8EnoylCoAMAT		

Modifiers

Table 226: Properties of each modifier.

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		
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		
AcetylCoAMAT		
NADHMAT		

Kinetic Law

Derived unit contains undeclared units

$$v_{56} = \mathrm{MTP}(\mathrm{sfmtpC8}, \mathrm{Vmtp}, \mathrm{KmmtpC8EnoylCoAMAT}, \mathrm{KmmtpC16EnoylCoAMAT}, \mathrm{KmmtpC14EnoylCoAMAT}, \mathrm{KmmtpC12EnoylCoAMAT}, \mathrm{KmmtpC10EnoylCoAMAT}, \mathrm{KmmtpNADMAT}, \mathrm{KmmtpCoAMAT}, \mathrm{KmmtpC6AcylCoAMAT}, \mathrm{KmmtpC16AcylCoAMAT}, \mathrm{KmmtpC14AcylCoAMAT}, \mathrm{KmmtpC12AcylCoAMAT}, \mathrm{KmmtpC10AcylCoAMAT}, \mathrm{KmmtpC8AcylCoAMAT}, \mathrm{KmmtpNADHMAT}, \mathrm{KmmtpAcetylCoAMAT}, \mathrm{KicrotC4AcetoacylCoA}, \mathrm{Keqmtp}, [\mathrm{C8EnoylCoAMAT}], [\mathrm{C16EnoylCoAMAT}], [\mathrm{C14EnoylCoAMAT}], [\mathrm{C12EnoylCoAMAT}], [\mathrm{C10EnoylCoAMAT}], [\mathrm{NADtMAT}], [\mathrm{CoAMAT}], [\mathrm{C6AcylCoAMAT}], [\mathrm{C16AcylCoAMAT}], [\mathrm{C14AcylCoAMAT}], [\mathrm{C12AcylCoAMAT}], [\mathrm{C10AcylCoAMAT}], [\mathrm{C8AcylCoAMAT}], [\mathrm{NADHMAT}], [\mathrm{AcetylCoAMAT}], [\mathrm{C4AcetoacylCoAMAT}]) \quad (181)$$

$$\mathrm{MTP}(\mathrm{sf}, \mathrm{V}, \mathrm{Kms1}, \mathrm{Kms2}, \mathrm{Kms3}, \mathrm{Kms4}, \mathrm{Kms5}, \mathrm{Kms7}, \mathrm{Kms8}, \mathrm{Kmp1}, \mathrm{Kmp2}, \mathrm{Kmp3}, \mathrm{Kmp4}, \mathrm{Kmp5}, \mathrm{Kmp6}, \mathrm{Kmp7}, \mathrm{Kmp8}, \mathrm{Ki1}, \mathrm{Keq}, \mathrm{S1}, \mathrm{S2}, \mathrm{S3}, \mathrm{S4}, \mathrm{S5}, \mathrm{S7}, \mathrm{S8}, \mathrm{P1}, \mathrm{P2}, \mathrm{P3}, \mathrm{P4}, \mathrm{P5}, \mathrm{P6}, \mathrm{P7}, \mathrm{P8}, \mathrm{I1}) \quad (182)$$

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

Table 228: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
sfmtpC8			0.34	dimensionless	☑

8.57 Reaction vacesink

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

Reaction equation

$$\text{AcetylCoAMAT} \xrightleftharpoons{\text{AcetylCoAMAT, AcetylCoAMAT}} \emptyset \tag{183}$$

Reactant

Table 229: Properties of each reactant.

Id	Name	SBO
AcetylCoAMAT		

Modifiers

Table 230: Properties of each modifier.

Id	Name	SBO
AcetylCoAMAT		
AcetylCoAMAT		

Kinetic Law

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

$$v_{57} = \text{RES}\left(\text{Ksacesink}, [\text{AcetylCoAMAT}], \text{K1acesink}\right) \tag{184}$$

$$\text{RES}\left(\text{Ks}, \text{S}, \text{K1}\right) = \text{Ks} \cdot (\text{S} - \text{K1}) \tag{185}$$

Table 231: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K1acesink			70.0	$\mu\text{mol} \cdot 1^{-1}$	☑
Ksacesink			6000000.0	$1 \cdot (60\ \text{s})^{-1}$	☑

8.58 Reaction vfadhsink

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

Reaction equation

$$\text{FADHMAT} \xrightleftharpoons{\text{FADHMAT, FADHMAT}} \emptyset \tag{186}$$

Reactant

Table 232: Properties of each reactant.

Id	Name	SBO
FADHMAT		

Modifiers

Table 233: Properties of each modifier.

Id	Name	SBO
FADHMAT		
FADHMAT		

Kinetic Law

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

$$v_{58} = \mathrm{RES}\left(\mathrm{Ksfadhsink}, [\mathrm{FADHMAT}], \mathrm{K1fadhsink}\right) \tag{187}$$

$$\mathrm{RES}\left(\mathrm{Ks}, \mathrm{S}, \mathrm{K1}\right) = \mathrm{Ks} \cdot \left(\mathrm{S} - \mathrm{K1}\right) \tag{188}$$

Table 234: Properties of each parameter.

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

8.59 Reaction vnadhsink

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

Reaction equation

$$\mathrm{NADHMAT} \xrightleftharpoons{\text{NADHMAT, NADHMAT}} \emptyset \tag{189}$$

Reactant

Table 235: Properties of each reactant.

Id	Name	SBO
NADHMAT		

Modifiers

Table 236: Properties of each modifier.

Id	Name	SBO
NADHMAT		
NADHMAT		

Kinetic Law

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

$$v_{59} = \mathrm{RES}\left(\mathrm{Ksnadhsink}, [\mathrm{NADHMAT}], \mathrm{K1nadhsink}\right) \tag{190}$$

$$\mathrm{RES}\left(\mathrm{Ks}, \mathrm{S}, \mathrm{K1}\right) = \mathrm{Ks} \cdot (\mathrm{S} - \mathrm{K1}) \tag{191}$$

Table 237: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K1nadhsink			16.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
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 $0\ \mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{\text{d}}{\text{d}t}\text{C16AcylCarCYT} = v_1 - v_2 \tag{192}$$

9.2 Species C16AcylCarMAT

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

This species takes part in 24 reactions (as a reactant in vcpt2C16 and as a product in vcactC16 and as a modifier in vcactC16, vcactC16, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vcpt2C4).

$$\frac{\text{d}}{\text{d}t}\text{C16AcylCarMAT} = v_2 - v_9 \tag{193}$$

9.3 Species C16AcylCoAMAT

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

This species takes part in 81 reactions (as a reactant in vvlcadC16, vlcadC16 and as a product in vcpt2C16 and as a modifier in vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vcpt2C4, vvlcadC16, vvlcadC16, vvlcadC14, vvlcadC14, vvlcadC14, vvlcadC12, vvlcadC12, vvlcadC12, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC12, vlcadC10, vlcadC10, vlcadC10, vlcadC8, vlcadC8, vlcadC8, vmckatC16, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmckatC4, vmtpC16, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC10, vmtpC8, vmtpC8, vmtpC8).

$$\frac{\text{d}}{\text{d}t}\text{C16AcylCoAMAT} = v_9 - v_{16} - v_{19} \tag{194}$$

9.4 Species C16EnoylCoAMAT

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

This species takes part in 60 reactions (as a reactant in vcrotC16, vmtpC16 and as a product in vvlcadC16, vlcadC16 and as a modifier in vvlcadC16, vvlcadC16, vvlcadC14, vvlcadC14, vvlcadC14, vvlcadC12, vvlcadC12, vvlcadC12, vlcadC16, vlcadC16, vlcadC14, vlcadC14,

vlcadC14, vlcadC12, vlcadC12, vlcadC12, vlcadC10, vlcadC10, vlcadC10, vlcadC8, vlcadC8, vlcadC8, vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vcrotC4, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC10, vmtpC8, vmtpC8, vmtpC8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C16EnoylCoAMAT} = v_{16} + v_{19} - v_{31} - v_{52} \tag{195}$$

9.5 Species C16HydroxyacylCoAMAT

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

This species takes part in 42 reactions (as a reactant in vmschadC16 and as a product in vcrotC16 and as a modifier in vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vcrotC4, vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC10, vmschadC8, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmschadC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C16HydroxyacylCoAMAT} = v_{31} - v_{38} \tag{196}$$

9.6 Species C16KetoacylCoAMAT

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

This species takes part in 42 reactions (as a reactant in vmckatC16 and as a product in vmschadC16 and as a modifier in vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC10, vmschadC8, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmschadC4, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmckatC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C16KetoacylCoAMAT} = v_{38} - v_{45} \tag{197}$$

9.7 Species C14AcylCarCYT

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C14AcylCarCYT} = -v_{3} \tag{198}$$

9.8 Species C14AcylCarMAT

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

This species takes part in 24 reactions (as a reactant in vcpt2C14 and as a product in vcactC14 and as a modifier in vcactC14, vcactC14, vcpt2C16, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vcpt2C4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{C14AcylCarMAT} = v_3 - v_{10} \tag{199}$$

9.9 Species C14AcylCoAMAT

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

This species takes part in 81 reactions (as a reactant in vvlcadC14, vlcadC14 and as a product in vcpt2C14, vmckatC16, vmtpC16 and as a modifier in vcpt2C16, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vcpt2C4, vvlcadC16, vvlcadC16, vvlcadC16, vvlcadC14, vvlcadC14, vvlcadC12, vvlcadC12, vvlcadC12, vlcadC16, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC12, vlcadC10, vlcadC10, vlcadC10, vlcadC8, vlcadC8, vlcadC8, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmckatC4, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC10, vmtpC8, vmtpC8, vmtpC8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{C14AcylCoAMAT} = v_{10} + v_{45} + v_{52} - v_{17} - v_{20} \tag{200}$$

9.10 Species C14EnoylCoAMAT

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

This species takes part in 60 reactions (as a reactant in vcrotC14, vmtpC14 and as a product in vvlcadC14, vlcadC14 and as a modifier in vvlcadC16, vvlcadC16, vvlcadC16, vvlcadC14, vvlcadC14, vvlcadC12, vvlcadC12, vvlcadC12, vlcadC16, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC12, vlcadC10, vlcadC10, vlcadC10, vlcadC8, vlcadC8, vlcadC8, vcrotC16, vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vcrotC4, vmtpC16, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC10, vmtpC8, vmtpC8, vmtpC8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{C14EnoylCoAMAT} = v_{17} + v_{20} - v_{32} - v_{53} \tag{201}$$

9.11 Species C14HydroxyacylCoAMAT

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

This species takes part in 42 reactions (as a reactant in vmschadC14 and as a product in vcrotC14 and as a modifier in vcrotC16, vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vcrotC4, vmschadC16, vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC10, vmschadC8, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmschadC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{C14HydroxyacylCoAMAT} = v_{32} - v_{39} \tag{202}$$

9.12 Species C14KetoacylCoAMAT

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

This species takes part in 42 reactions (as a reactant in vmckatC14 and as a product in vmschadC14 and as a modifier in vmschadC16, vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC10, vmschadC8, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmschadC4, vmckatC16, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmckatC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{C14KetoacylCoAMAT} = v_{39} - v_{46} \tag{203}$$

9.13 Species C12AcylCarCYT

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{C12AcylCarCYT} = -v_{4} \tag{204}$$

9.14 Species C12AcylCarMAT

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

This species takes part in 24 reactions (as a reactant in vcpt2C12 and as a product in vcactC12 and as a modifier in vcactC12, vcactC12, vcpt2C16, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vcpt2C4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{C12AcylCarMAT} = v_{4} - v_{11} \tag{205}$$

9.15 Species C12AcylCoAMAT

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

This species takes part in 96 reactions (as a reactant in vvlcadC12, vlcadC12, vmcadC12 and as a product in vcpt2C12, vmckatC14, vmtpC14 and as a modifier in vcpt2C16, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vcpt2C4, vvlcadC16, vvlcadC16, vvlcadC16, vvlcadC14, vvlcadC14, vvlcadC14, vvlcadC12, vvlcadC12, vlcadC16, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC10, vlcadC10, vlcadC10, vlcadC8, vlcadC8, vlcadC8, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC10, vmcadC8, vmcadC8, vmcadC8, vmcadC6, vmcadC6, vmcadC6, vmcadC4, vmcadC4, vmcadC4, vmckatC16, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmckatC4, vmtpC16, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC10, vmtpC8, vmtpC8, vmtpC8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C12AcylCoAMAT} = v_{11} + v_{46} + v_{53} - v_{18} - v_{21} - v_{24} \tag{206}$$

9.16 Species C12EnoylCoAMAT

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

This species takes part in 73 reactions (as a reactant in vcrotC12, vmtpC12 and as a product in vvlcadC12, vlcadC12, vmcadC12 and as a modifier in vvlcadC16, vvlcadC16, vvlcadC16, vvlcadC14, vvlcadC14, vvlcadC14, vvlcadC12, vvlcadC12, vlcadC16, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC14, vlcadC10, vlcadC10, vlcadC10, vlcadC8, vlcadC8, vlcadC8, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC10, vmcadC8, vmcadC8, vmcadC8, vmcadC6, vmcadC6, vmcadC6, vmcadC4, vmcadC4, vmcadC4, vcrotC16, vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vcrotC4, vmtpC16, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC10, vmtpC8, vmtpC8, vmtpC8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C12EnoylCoAMAT} = v_{18} + v_{21} + v_{24} - v_{33} - v_{54} \tag{207}$$

9.17 Species C12HydroxyacylCoAMAT

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

This species takes part in 42 reactions (as a reactant in vmschadC12 and as a product in vcrotC12 and as a modifier in vcrotC16, vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC8, vcrotC6,

vcrotC6, vcrotC6, vcrotC4, vcrotC4, vcrotC4, vmschadC16, vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC10, vmschadC8, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmschadC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C12HydroxyacylCoAMAT} = v_{33} - v_{40} \tag{208}$$

9.18 Species C12KetoacylCoAMAT

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

This species takes part in 42 reactions (as a reactant in vmckatC12 and as a product in vmschadC12 and as a modifier in vmschadC16, vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC10, vmschadC8, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmschadC4, vmckatC16, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmckatC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C12KetoacylCoAMAT} = v_{40} - v_{47} \tag{209}$$

9.19 Species C10AcylCarCYT

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C10AcylCarCYT} = -v_{5} \tag{210}$$

9.20 Species C10AcylCarMAT

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

This species takes part in 24 reactions (as a reactant in vcpt2C10 and as a product in vcactC10 and as a modifier in vcactC10, vcactC10, vcpt2C16, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vcpt2C4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C10AcylCarMAT} = v_{5} - v_{12} \tag{211}$$

9.21 Species C10AcylCoAMAT

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

This species takes part in 87 reactions (as a reactant in vlcadC10, vmcadC10 and as a product in vcpt2C10, vmckatC12, vmtpC12 and as a modifier in vcpt2C16, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vcpt2C4, vlcadC16, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC12, vlcadC10, vlcadC10, vlcadC8, vlcadC8, vlcadC8, vmcadC12, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC8, vmcadC8, vmcadC8, vmcadC6, vmcadC6, vmcadC6, vmcadC4, vmcadC4, vmcadC4, vmckatC16, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmckatC4, vmtpC16, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC10, vmtpC8, vmtpC8, vmtpC8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C10AcylCoAMAT} = v_{12} + v_{47} + v_{54} - v_{22} - v_{25} \tag{212}$$

9.22 Species C10EnoylCoAMAT

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

This species takes part in 66 reactions (as a reactant in vcrotC10, vmtpC10 and as a product in vlcadC10, vmcadC10 and as a modifier in vlcadC16, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC12, vlcadC10, vlcadC10, vlcadC8, vlcadC8, vlcadC8, vmcadC12, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC8, vmcadC8, vmcadC8, vmcadC6, vmcadC6, vmcadC6, vmcadC4, vmcadC4, vmcadC4, vcrotC16, vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vcrotC4, vmtpC16, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC8, vmtpC8, vmtpC8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C10EnoylCoAMAT} = v_{22} + v_{25} - v_{34} - v_{55} \tag{213}$$

9.23 Species C10HydroxyacylCoAMAT

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

This species takes part in 42 reactions (as a reactant in vmschadC10 and as a product in vcrotC10 and as a modifier in vcrotC16, vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vcrotC4, vmschadC16, vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC12, vmschadC10,

vmschadC10, vmschadC8, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmschadC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C10HydroxyacylCoAMAT} = v_{34} - v_{41} \tag{214}$$

9.24 Species C10KetoacylCoAMAT

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

This species takes part in 42 reactions (as a reactant in vmckatC10 and as a product in vmschadC10 and as a modifier in vmschadC16, vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC8, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmschadC4, vmckatC16, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmckatC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C10KetoacylCoAMAT} = v_{41} - v_{48} \tag{215}$$

9.25 Species C8AcylCarCYT

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C8AcylCarCYT} = -v_{6} \tag{216}$$

9.26 Species C8AcylCarMAT

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

This species takes part in 24 reactions (as a reactant in vcpt2C8 and as a product in vcactC8 and as a modifier in vcactC8, vcactC8, vcpt2C16, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vcpt2C4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C8AcylCarMAT} = v_{6} - v_{13} \tag{217}$$

9.27 Species C8AcylCoAMAT

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

This species takes part in 87 reactions (as a reactant in vlcadC8, vmcadC8 and as a product in vcpt2C8, vmckatC10, vmtpC10 and as a modifier in vcpt2C16, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vcpt2C4, vlcadC16, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC12, vlcadC10, vlcadC10, vlcadC10, vlcadC8, vlcadC8, vmcadC12, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC10, vmcadC8, vmcadC8, vmcadC6, vmcadC6, vmcadC6, vmcadC4, vmcadC4, vmcadC4, vmckatC16, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmckatC4, vmtpC16, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC8, vmtpC8, vmtpC8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C8AcylCoAMAT} = v_{13} + v_{48} + v_{55} - v_{23} - v_{26} \tag{218}$$

9.28 Species C8EnoylCoAMAT

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

This species takes part in 66 reactions (as a reactant in vcrotC8, vmtpC8 and as a product in vlcadC8, vmcadC8 and as a modifier in vlcadC16, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC12, vlcadC10, vlcadC10, vlcadC10, vlcadC8, vlcadC8, vmcadC12, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC10, vmcadC8, vmcadC8, vmcadC6, vmcadC6, vmcadC6, vmcadC4, vmcadC4, vmcadC4, vcrotC16, vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vcrotC4, vmtpC16, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC10, vmtpC8, vmtpC8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C8EnoylCoAMAT} = v_{23} + v_{26} - v_{35} - v_{56} \tag{219}$$

9.29 Species C8HydroxyacylCoAMAT

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

This species takes part in 42 reactions (as a reactant in vmschadC8 and as a product in vcrotC8 and as a modifier in vcrotC16, vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vcrotC4, vmschadC16, vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC12, vmschadC10,

vmschadC10, vmschadC10, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmschadC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C8HydroxyacylCoAMAT} = v_{35} - v_{42} \tag{220}$$

9.30 Species C8KetoacylCoAMAT

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

This species takes part in 42 reactions (as a reactant in vmckatC8 and as a product in vmschadC8 and as a modifier in vmschadC16, vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC10, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmschadC4, vmckatC16, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmckatC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C8KetoacylCoAMAT} = v_{42} - v_{49} \tag{221}$$

9.31 Species C6AcylCarCYT

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C6AcylCarCYT} = -v_{7} \tag{222}$$

9.32 Species C6AcylCarMAT

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

This species takes part in 24 reactions (as a reactant in vcpt2C6 and as a product in vcactC6 and as a modifier in vcactC6, vcactC6, vcpt2C16, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vcpt2C4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C6AcylCarMAT} = v_{7} - v_{14} \tag{223}$$

9.33 Species C6AcylCoAMAT

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

This species takes part in 78 reactions (as a reactant in vmcadC6, vscadC6 and as a product in vcpt2C6, vmckatC8, vmtpC8 and as a modifier in vcpt2C16, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vcpt2C4, vmcadC12, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC10, vmcadC8, vmcadC8, vmcadC8, vmcadC6, vmcadC6, vmcadC4, vmcadC4, vmcadC4, vscadC6, vscadC6, vscadC4, vscadC4, vscadC4, vmckatC16, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmckatC4, vmtpC16, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC10, vmtpC8, vmtpC8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{C6AcylCoAMAT} = v_{14} + v_{49} + v_{56} - v_{27} - v_{29} \tag{224}$$

9.34 Species C6EnoylCoAMAT

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

This species takes part in 42 reactions (as a reactant in vcrotC6 and as a product in vmcadC6, vscadC6 and as a modifier in vmcadC12, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC10, vmcadC8, vmcadC8, vmcadC8, vmcadC6, vmcadC6, vmcadC4, vmcadC4, vmcadC4, vscadC6, vscadC6, vscadC4, vscadC4, vscadC4, vcrotC16, vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vcrotC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{C6EnoylCoAMAT} = v_{27} + v_{29} - v_{36} \tag{225}$$

9.35 Species C6HydroxyacylCoAMAT

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

This species takes part in 42 reactions (as a reactant in vmschadC6 and as a product in vcrotC6 and as a modifier in vcrotC16, vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vcrotC4, vmschadC16, vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC10, vmschadC8, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmschadC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{C6HydroxyacylCoAMAT} = v_{36} - v_{43} \tag{226}$$

9.36 Species C6KetoacylCoAMAT

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

This species takes part in 42 reactions (as a reactant in vmckatC6 and as a product in vmschadC6 and as a modifier in vmschadC16, vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC10, vmschadC8, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmschadC4, vmckatC16, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmckatC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{C6KetoacylCoAMAT} = v_{43} - v_{50} \tag{227}$$

9.37 Species C4AcylCarCYT

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{C4AcylCarCYT} = -v_{8} \tag{228}$$

9.38 Species C4AcylCarMAT

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

This species takes part in 24 reactions (as a reactant in vcpt2C4 and as a product in vcactC4 and as a modifier in vcactC4, vcactC4, vcpt2C16, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{C4AcylCarMAT} = v_{8} - v_{15} \tag{229}$$

9.39 Species C4AcylCoAMAT

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

This species takes part in 63 reactions (as a reactant in vmcadC4, vscadC4 and as a product in vcpt2C4, vmckatC6 and as a modifier in vcpt2C16, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vmcadC12, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC10, vmcadC8, vmcadC8, vmcadC8, vmcadC6, vmcadC6, vmcadC6, vmcadC4, vmcadC4, vscadC6, vscadC6, vscadC6, vscadC4, vscadC4, vmckatC16, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC14, vmckatC12, vmckatC12,

vmckatC12, vmckatC10, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmckatC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C4AcylCoAMAT} = v_{15} + v_{50} - v_{28} - v_{30} \tag{230}$$

9.40 Species C4EnoylCoAMAT

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

This species takes part in 42 reactions (as a reactant in vcrotC4 and as a product in vmcadC4, vscadC4 and as a modifier in vmcadC12, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC10, vmcadC8, vmcadC8, vmcadC8, vmcadC6, vmcadC6, vmcadC6, vmcadC4, vmcadC4, vscadC6, vscadC6, vscadC6, vscadC4, vscadC4, vcrotC16, vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC6, vcrotC4, vcrotC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C4EnoylCoAMAT} = v_{28} + v_{30} - v_{37} \tag{231}$$

9.41 Species C4HydroxyacylCoAMAT

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

This species takes part in 42 reactions (as a reactant in vmschadC4 and as a product in vcrotC4 and as a modifier in vcrotC16, vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vmschadC16, vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC10, vmschadC8, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC6, vmschadC4, vmschadC4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C4HydroxyacylCoAMAT} = v_{37} - v_{44} \tag{232}$$

9.42 Species C4AcetoacylCoAMAT

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

This species takes part in 78 reactions (as a reactant in vmckatC4 and as a product in vmschadC4 and as a modifier in vcrotC16, vcrotC16, vcrotC16, vcrotC14, vcrotC14, vcrotC14, vcrotC12, vcrotC12, vcrotC12, vcrotC10, vcrotC10, vcrotC10, vcrotC8, vcrotC8, vcrotC8, vcrotC6, vcrotC6, vcrotC6, vcrotC4, vcrotC4, vcrotC4, vmschadC16, vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC10, vmschadC8, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmckatC16, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC10, vmckatC8,

vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmtpC16, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC10, vmtpC8, vmtpC8, vmtpC8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C4AcetoacylCoAMAT} = v_{44} - v_{51} \tag{233}$$

9.43 Species AcetylCoAMAT

Initial concentration $70\ \mu\mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in 39 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, vmckatC16, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC8, vmtpC8, vacesink, vacesink).

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AcetylCoAMAT} = {} & v_{45} + v_{46} + v_{47} + v_{48} + v_{49} + v_{50} + 2\,v_{51} \\ & + v_{52} + v_{53} + v_{54} + v_{55} + v_{56} - v_{57}\end{aligned} \tag{234}$$

9.44 Species FADHMAT

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

This species takes part in 48 reactions (as a reactant in vfadhsink and as a product in vvlcadC16, vvlcadC14, vvlcadC12, vlcadC16, vlcadC14, vlcadC12, vlcadC10, vlcadC8, vmcadC12, vmcadC10, vmcadC8, vmcadC6, vmcadC4, vscadC6, vscadC4 and as a modifier in vvlcadC16, vvlcadC16, vvlcadC14, vvlcadC14, vvlcadC12, vvlcadC12, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC10, vlcadC10, vlcadC8, vlcadC8, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC8, vmcadC8, vmcadC6, vmcadC6, vmcadC4, vmcadC4, vscadC6, vscadC6, vscadC4, vscadC4, vfadhsink, vfadhsink).

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{FADHMAT} = {} & v_{16} + v_{17} + v_{18} + v_{19} + v_{20} + v_{21} + v_{22} + v_{23} \\ & + v_{24} + v_{25} + v_{26} + v_{27} + v_{28} + v_{29} + v_{30} - v_{58}\end{aligned} \tag{235}$$

9.45 Species NADHMAT

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

This species takes part in 39 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, vmschadC16, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC8, vmschadC8,

vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC8, vmtpC8, vnadhsink, vnadhsink).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADHMAT} = v_{38} + v_{39} + v_{40} + v_{41} + v_{42} + v_{43} + v_{44} + v_{52} + v_{53} + v_{54} + v_{55} + v_{56} - v_{59} \tag{236}$$

9.46 Species CoAMAT

Initial concentration $4930\ \mu\mathrm{mol}\cdot\mathrm{l}^{-1}$

Involved in rule CoAMAT

This species takes part in 57 reactions (as a modifier in vcpt2C16, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4, vcpt2C4, vcpt2C4, vmckatC16, vmckatC16, vmckatC16, vmckatC14, vmckatC14, vmckatC14, vmckatC12, vmckatC12, vmckatC12, vmckatC10, vmckatC10, vmckatC10, vmckatC8, vmckatC8, vmckatC8, vmckatC6, vmckatC6, vmckatC6, vmckatC4, vmckatC4, vmckatC4, vmtpC16, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC10, vmtpC8, 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 $25\ \mu\mathrm{mol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C16AcylCoACYT} = 0 \tag{237}$$

9.48 Species CarCYT

Initial concentration $200\ \mu\mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in 24 reactions (as a modifier in vcpt1C16, vcpt1C16, vcpt1C16, vcactC16, vcactC16, vcactC16, vcactC14, vcactC14, vcactC14, vcactC12, vcactC12, vcactC12, vcactC10, vcactC10, vcactC10, vcactC8, vcactC8, vcactC8, vcactC6, vcactC6, vcactC6, vcactC4, 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 $140\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in three reactions (as a modifier in vcpt1C16, 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 $0\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in three reactions (as a modifier in vcpt1C16, 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 $950\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in 42 reactions (as a modifier in vcactC16, vcactC16, vcactC16, vcactC14, vcactC14, vcactC14, vcactC12, vcactC12, vcactC12, vcactC10, vcactC10, vcactC10, vcactC8, vcactC8, vcactC8, vcactC6, vcactC6, vcactC6, vcactC4, vcactC4, vcactC4, vcpt2C16, vcpt2C16, vcpt2C16, vcpt2C14, vcpt2C14, vcpt2C14, vcpt2C12, vcpt2C12, vcpt2C12, vcpt2C10, vcpt2C10, vcpt2C10, vcpt2C8, vcpt2C8, vcpt2C8, vcpt2C6, vcpt2C6, vcpt2C6, vcpt2C4, 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 $0.77\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in 45 reactions (as a modifier in vvlcadC16, vvlcadC16, vvlcadC16, vvlcadC14, vvlcadC14, vvlcadC14, vvlcadC12, vvlcadC12, vvlcadC12, vlcadC16, vlcadC16, vlcadC16, vlcadC14, vlcadC14, vlcadC14, vlcadC12, vlcadC12, vlcadC12, vlcadC10, vlcadC10, vlcadC10, vlcadC8, vlcadC8, vlcadC8, vmcadC12, vmcadC12, vmcadC12, vmcadC10, vmcadC10, vmcadC10, vmcadC8, vmcadC8, vmcadC8, vmcadC6, vmcadC6, vmcadC6, vmcadC4, vmcadC4, vmcadC4, vscadC6, vscadC6, vscadC6, vscadC4, 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 $250\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in 36 reactions (as a modifier in vmschadC16, vmschadC16, vmschadC16, vmschadC14, vmschadC14, vmschadC14, vmschadC12, vmschadC12, vmschadC12, vmschadC10, vmschadC10, vmschadC10, vmschadC8, vmschadC8, vmschadC8, vmschadC6, vmschadC6, vmschadC6, vmschadC4, vmschadC4, vmschadC4, vmtpC16, vmtpC16, vmtpC16, vmtpC14, vmtpC14, vmtpC14, vmtpC12, vmtpC12, vmtpC12, vmtpC10, vmtpC10, vmtpC10, vmtpC8, vmtpC8, vmtpC8), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

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

9.54 Species CoAMATt

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

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

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