SBML Model Report

Model name: "Sen2013 - Phospholipid Synthesis in P.knowlesi"



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah¹ and Partho Sen² at November 25th 2013 at 12:12 a.m. and last time modified at February 28th 2014 at 11:50 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	1
species types	0	species	11
events	0	constraints	0
reactions	17	function definitions	0
global parameters	34	unit definitions	4
rules	0	initial assignments	0

Model Notes

Sen2013 - Phospholipid Synthesis in P.knowlesi

The model describes the multiple phospholipid synthetic pathways in Plasmodium knowlesi.

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This model is described in the article: Kinetic modelling of phospholipid synthesis in Plasmodium knowlesi unravels crucial steps and relative importance of multiple pathways. Sen P, Vial HJ, Radulescu O.BMC Syst Biol 2013 Nov; 7(1): 123

Abstract:

BACKGROUND: Plasmodium is the causal parasite of malaria, infectious disease responsible for the death of up to one million people each year. Glycerophospholipid and consequently membrane biosynthesis are essential for the survival of the parasite and are targeted by a new class of antimalarial drugs developed in our lab. In order to understand the highly redundant phospholipid synthethic pathways and eventual mechanism of resistance to various drugs, an organism specific kinetic model of these metabolic pathways need to be developed in Plasmodium species. RESULTS: Fluxomic data were used to build a quantitative kinetic model of glycerophospholipid pathways in Plasmodium knowlesi. In vitro incorporation dynamics of phospholipids unravels multiple synthetic pathways. A detailed metabolic network with values of the kinetic parameters (maximum rates and Michaelis constants) has been built. In order to obtain a global search in the parameter space, we have designed a hybrid, discrete and continuous, optimization method. Discrete parameters were used to sample the cone of admissible fluxes, whereas the continuous Michaelis and maximum rates constants were obtained by local minimization of an objective function. The model was used to predict the distribution of fluxes within the network of various metabolic precursors. The quantitative analysis was used to understand eventual links between different pathways. The major source of phosphatidylcholine (PC) is the CDP-choline Kennedy pathway. In silico knock-out experiments showed comparable importance of phosphoethanolamine-N-methyltransferase (PMT) and phosphatidylethanolamine-N-methyltransferase (PEMT) for PC synthesis. The flux values indicate that, major part of serine derived phosphatidylethanolamine (PE) is formed via serine decarboxylation, whereas major part of phosphatidylserine (PS) is formed by base-exchange reactions. Sensitivity analysis of CDP-choline pathway shows that the carrier-mediated choline entry into the parasite and the phosphocholine cytidylyltransferase reaction have the largest sensitivity coefficients in this pathway, but does not distinguish a reaction as an unique rate-limiting step. CONCLUSION: We provide a fully parametrized kinetic model for the multiple phospholipid synthetic pathways in P. knowlesi. This model has been used to clarify the relative importance of the various reactions in these metabolic pathways. Future work extensions of this modelling strategy will serve to elucidate the regulatory mechanisms governing the development of Plasmodium during its blood stages, as well as the mechanisms of action of drugs on membrane biosynthetic pathways and eventual mechanisms of resistance.

This model is hosted on BioModels Database and identifiedby: BIOMD0000000495.

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

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2 Unit Definitions

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

2.1 Unit MWBUILTINUNIT_liter

Name liter

Definition $m^3 \cdot 0.0010$ dimensionless

2.2 Unit MWDERIVEDUNIT_mole_liter_minute

Name mole/liter/minute

2.3 Unit MWDERIVEDUNIT_mole__liter

Name mole/liter

Definition $m^{-3} \cdot mol \cdot 1000$ dimensionless

2.4 Unit MWDERIVEDUNIT_1_minute

Name 1/minute

2.5 Unit substance

Notes Mole is the predefined SBML unit for substance.

Definition mol

2.6 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition 1

2.7 Unit area

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

Definition m²

2.8 Unit length

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

Definition m

2.9 Unit time

Notes Second is the predefined SBML unit for time.

Definition s

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

*1			~	~.	
Id	Name	SBO	Spatial	Size	Unit
			Dimensions		
mw81b30d38_6ef3_4391_b826_e6c3cc210196	unnamed		3	1	$m^3 \cdot 0.0010$ dimension

3.1 Compartment mw81b30d38_6ef3_4391_b826_e6c3cc210196

This is a three dimensional compartment with a constant size of one $m^3 \cdot 0.0010$ dimensionless.

Name unnamed

4 Species

This model contains eleven species. The boundary condition of three of these species is set to true so that these species' amount cannot be changed by any reaction. Section 7 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit Constant	Boundary Condi-
				tion
mw73259e20-	SerE	mw81b30d38_6ef3_4391-	mol · m ⁻³ · ⊟	$ \overline{\checkmark} $
_240e_4f3a_b2e0- _9ca248658898		_b826_e6c3cc210196	$(0.0010 \text{ dimensionless})^{-1}$	
mw15abaa48-	Ser	mw81b30d38_6ef3_4391-	$mol \cdot m^{-3} \cdot \Box$	
_d7d0_4845_ae04- _c573d289d495		_b826_e6c3cc210196	$(0.0010 \text{ dimensionless})^{-1}$	
mwfcfaf604-	PS	mw81b30d38_6ef3_4391-	$\text{mol} \cdot \text{m}^{-3} \cdot \sqsubseteq$	
_14d4_47a6_b021- _226d1fb5497c		_b826_e6c3cc210196	$(0.0010 \text{ dimensionless})^{-1}$	
mw8796c919-	Etn	mw81b30d38_6ef3_4391-	$mol \cdot m^{-3} \cdot \Box$	\Box
_9251_4970_8f87- _0bca9ecfeb5c		_b826_e6c3cc210196	$(0.0010 \text{ dimensionless})^{-1}$	
mw849ed3fd-	PEtn	mw81b30d38_6ef3_4391-	$\text{mol} \cdot \text{m}^{-3} \cdot \boxminus$	
_87d9_44d2_9f3e- _4d631b900d41		_b826_e6c3cc210196	$(0.0010 \text{ dimensionless})^{-1}$	
mwcb834e43-	PCho	mw81b30d38_6ef3_4391-	$\text{mol} \cdot \text{m}^{-3} \cdot \square$	
_dc57_45ae_9452- _f4c10955caf1		_b826_e6c3cc210196	$(0.0010 \text{ dimensionless})^{-1}$	
mwf166ad55-	PE	mw81b30d38_6ef3_4391-	$\text{mol} \cdot \text{m}^{-3} \cdot \square$	\Box
_4ff0_49fb_95d2- _b657ad7653d5		_b826_e6c3cc210196	$(0.0010 \text{ dimensionless})^{-1}$	

Id	Name	Compartment	Derived Unit Constant	Boundary Condi- tion
mwee54b5b4- _b8c0_41df_8dda- _5b160c5e10a5	PC	mw81b30d38_6ef3_4391- _b826_e6c3cc210196	$\begin{array}{ccc} \text{mol} & \cdot & \text{m}^{-3} & \cdot & \\ (0.0010 \text{ dimensionless})^{-1} \end{array}$	В
mw919f8a86- _e702_4b24_9cd7- _adad694fcf9b	ChoE	mw81b30d38_6ef3_4391- _b826_e6c3cc210196	$\begin{array}{ccc} \text{mol} & \cdot & \text{m}^{-3} & \cdot & & \\ (0.0010 \text{ dimensionless})^{-1} & & & & \end{array}$	Ø
mw812f63db- _4cb0_40ad_b92b- _9874be969dfe	Cho	mw81b30d38_6ef3_4391- _b826_e6c3cc210196	$\begin{array}{ccc} \text{mol} & \cdot & \text{m}^{-3} & \cdot & \boxminus \\ \left(0.0010 \text{ dimensionless}\right)^{-1} \end{array}$	
mw08818dfe- _fb12_45cc_8c1d- _d965f142d0ce	EtnE	mw81b30d38_6ef3_4391- _b826_e6c3cc210196	$\begin{array}{ccc} \text{mol} & \cdot & \text{m}^{-3} & \cdot & \boxminus \\ (0.0010 \text{ dimensionless})^{-1} \end{array}$	Ø

5 Parameters

This model contains 34 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
mwee07eca4- _0806- _4cc3_a6ab-	Vm1		$3.40936490738966 \cdot 10^{-6}$	$\begin{array}{c} \text{m}^{-3} \cdot \text{mol} \cdot \text{s}^{-1} \cdot \\ 16.66666666666667 \text{di} \end{array}$	mensionless
_9226ee79be6c mw8f20c25d- _9700- _4822_b5f9-	km1		$3.62894258752347 \cdot 10^{-4}$	m^{-3} · mol · 1000 dimensionless	Ø
_fe243e001091 mw7ce1b6a3- _e65e- _4aaa_9c32-	Vm2		$1.30568052867489 \cdot 10^{-6}$	$m^{-3} \cdot mol \cdot s^{-1} \cdot 16.6666666666666666666666666666666666$	✓ mensionless
_aeefb420f0ea mw85485398- _9f97- _408c_bca6-	km2		$7.96722533770371 \cdot 10^{-4}$	m^{-3} · mol · 1000 dimensionless	Ø
_90f0a8377eae mw798d0b02- _925e- _471b_a372-	Vm3		$2.620389955953 \cdot 10^{-6}$	$m^{-3} \cdot mol \cdot s^{-1} \cdot 16.6666666666666666666666666666666666$	✓ mensionless
_526d681cc370 mwd3807289- _133c- _4621_8087-	km3		$2.39591245105385 \cdot 10^{-5}$	m^{-3} · mol · 1000 dimensionless	Ø
_366621f553d3 mw2439178f- _a48f- _4425_82f9-	Vm4		$8.62083015294042 \cdot 10^{-6}$	$m^{-3} \cdot mol \cdot s^{-1} \cdot 16.6666666666666666666666666666666666$	✓ mensionless
_13267b917b85 mw5c4edb54- _cfd9- _43af_b70b-	km4		$1.08608492867695 \cdot 10^{-4}$	m^{-3} · mol · 1000 dimensionless	Ø
_e9ff1b44dc55 mw961dacfa- _f443- _4814_ad6c- _a27c04e74268	Vm5		$1.0780611108133 \cdot 10^{-6}$	$m^{-3} \cdot mol \cdot s^{-1} \cdot 16.6666666666666666666666666666666666$	✓ mensionless

Id	Name	SBO	Value	Unit	Constant
mw15ba24b5- _7a87- _479e_9be7- _261b12cbdb63	km5		$1.22223738254533 \cdot 10^{-4}$	m^{-3} · mol · 1000 dimensionless	Ø
mw9f56ecc5- _c22b- _4f8c_8b82- _90e2a6d9e364	Vm6		$2.24518521682572 \cdot 10^{-6}$	$\begin{array}{c} \text{m}^{-3} \cdot \text{mol} \cdot \text{s}^{-1} \cdot \\ 16.666666666666667 \text{d} \end{array}$	✓ imensionless
mw18bbabcb- _d229- _4d91_99f1- _484f2ba8f020	km6		$2.03868171233541 \cdot 10^{-4}$	m^{-3} · mol · 1000 dimensionless	Ø
mwba0debe9- _c575- _4f5a_a980- _e2b6857ff053	Vm7		$5.61352652271706 \cdot 10^{-6}$	$\begin{array}{c} \text{m}^{-3} \cdot \text{mol} \cdot \text{s}^{-1} \cdot \\ 16.666666666666667 \text{d} \end{array}$	✓ imensionless
mwffba86ff- _a560- _401a_93d6- _c0e30bf42c87	km7		$2.27368268903121 \cdot 10^{-4}$	m^{-3} · mol · 1000 dimensionless	Ø
mw231a5907- _d1ee- _4a43_83ab- _abb72f19502c	Vm8		$4.12788404046025 \cdot 10^{-7}$	$\begin{array}{c} \text{m}^{-3} \cdot \text{mol} \cdot \text{s}^{-1} \cdot \\ 16.666666666666667 \text{d} \end{array}$	✓ imensionless
mwaf289d12- _4291- _4651_8bd1- _82e321e476a4	km8		$3.10498877738431 \cdot 10^{-5}$	m^{-3} · mol · 1000 dimensionless	Ø
mw1a53a2cb- _a3a7- _40d7_ae07- _4d93ad1123a3	Vm9		0.001	$\begin{array}{c} \text{m}^{-3} \cdot \text{mol} \cdot \text{s}^{-1} \cdot \\ 16.66666666666666667 \text{d} \end{array}$	✓ imensionless
mw4035a2c9- _3cda- _467c_83cc- _8f9c2902abaf	km9		0.321	m^{-3} · mol · 1000 dimensionless	Ø
mwf7d1ff9f- _1734- _4232_9a96- _037b31b193b0	Vm10		$6.97333029651601 \cdot 10^{-7}$	$\begin{array}{c} \text{m}^{-3} \cdot \text{mol} \cdot \text{s}^{-1} \cdot \\ 16.66666666666666667 \text{d} \end{array}$	☑ imensionless

Id	Name	SBO	Value	Unit	Constant
mw7d57aa6b- _1bfb- _4472_b555-	km10		$3.76085190209901 \cdot 10^{-6}$	m^{-3} · mol · $\mathrm{1000}$ dimensionless	✓
_5f02- _419d_ba99-	Vm11		$8.99054709659885 \cdot 10^{-5}$	$m^{-3} \cdot mol \cdot s^{-1} \cdot 16.6666666666666666666666666666666666$	mensionless
_6e1f9b7e6b7b mw3046ca21- _42a2- _4a4b_89c4-	km11		0.171	m^{-3} · mol · 1000 dimensionless	Ø
_9d6ca3d927c5 mw87bb1238- _3292- _467e_bfe3-	Vm12		$1.5662833197895 \cdot 10^{-6}$	$m^{-3} \cdot mol \cdot s^{-1} \cdot 16.6666666666666666666666666666666666$	✓ mensionless
_ff7f1e64a351 mw371071cd- _ec20- _4517_acc1-	km12		$2.41308392167819 \cdot 10^{-5}$	m^{-3} · mol · 1000 dimensionless	Ø
_08dfdc871e87 mw5b225cdc- _783f- _4a15_93db-	Vm13		$1.53754224136353 \cdot 10^{-6}$	$m^{-3} \cdot mol \cdot s^{-1} \cdot 16.6666666666666666666666666666666666$	✓ mensionless
_e960a2398b8e mw27f524cb- _75b3- _401c_8533-	km13		$2.03777063277265 \cdot 10^{-4}$	m^{-3} · mol · 1000 dimensionless	Ø
_99d6f27af654 mwc623d82f- _a94e- _4460_9aed-	Vm14		$7.7375270429582 \cdot 10^{-4}$	$m^{-3} \cdot mol \cdot s^{-1} \cdot 16.6666666666666666666666666666666666$	✓ mensionless
_444597a728c2 mwbf296afc- _5e4f- _4819_8028-	km14		0.155	m^{-3} · mol · 1000 dimensionless	Ø
_06b20d7af7ca mw91e15e1e- _c73e- _4866_ab2b- _8225a32b7610	Vm15		$2.32432741134546 \cdot 10^{-7}$	$m^{-3} \cdot mol \cdot s^{-1} \cdot 16.6666666666666666666666666666666666$	✓ mensionless

Id	Name	SBO	Value	Unit Constant
mwf5cecb8f- _89f8- _4fba_b39b-	km15		$1.02326862282225 \cdot 10^{-4}$	m^{-3} · mol · $\boxed{2}$ 1000 dimensionless
_b517d0bef2ce mwff26437c- _166b- _4946_ad35-	Vm16		$5.55658410000431 \cdot 10^{-7}$	$m^{-3} \cdot mol \cdot s^{-1} \cdot $ 7 16.6666666666666666666666666666666666
_f13df6145780 mw284c519a- _cc2b- _4a98_99ce-	km16		$3.04072645117622 \cdot 10^{-5}$	m^{-3} · mol · 1000 dimensionless
_5a4471af99e1 mw2cd81e51- _eb11- _4e2c_b609-	kf17		$5\cdot 10^{-4}$	s^{-1} . \checkmark 0.0166666666666666666666666666666666666
_b2f802438a6b mwff99ad6c- _8951- _4d58_a836- _cf2d3d08ac86	kb17		$1.32810241970949 \cdot 10^{-4}$	s^{-1}

6 Reactions

_2e06bedff243

This model contains 17 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

		ole 3. Overview of all feactions	140		
	SBO	Reaction Equation	Name	Id	N₀
		mw73259e20_240e_4f3a_b2e0_9ca248	R1	mw79830677- _2d7e- _4f49_9d0b- _f05fe026749f	1
		mw15abaa48_d7d0_4845_ae04_c573d	R2	mw155447fb- _ce5b- _4ba2_bd74- _434951481a78	2
		mw15abaa48_d7d0_4845_ae04_c573d	R3	mw4c9aa283- _577e- _4b6c_ae5a- _c96f62dbbb08	3
		mw8796c919_9251_4970_8f87_0bca9	R4	mw55fba323- _0865- _4254_a6e9- _09acd2b4a10f	4
.44d2_9f3e_4d631b	b900d41	mw849ed3fd_87d9_44d2_9f3e_4d6311	R5	mwb8420f59- _69c3- _4707_918c-	5

		_608b- _4bd7_b2d0- _f359d045da17	
	7	mwb47b4c45- _fac9- _49e6_a6a4- _87b9050ddfbb	R7
Produced b	8	mw4f62d07e- _217b- _4602_b6fe- _548af112eec8	R8
Produced by SBML2laTEX	9	mw307551ca- _91cc- _4634_bba5- _0e3ecd38cfdd	R9
	10	mw15bb92b6- _4cff- _4a41_b815- _c1d904618e57	R10
	11	mw106407fc-	R11

_258bd4790633

12

N⁰	Id	Name	Reaction Equation	SBO
	0.150 0.1	D.C.	mwfcfaf604_14d4_47a6_b021_226d1fb5497	 , mwfcfaf604_14d4_47a6_b021_226d1fb54
6	mwc9170c21- _608b- _4bd7_b2d0- _f359d045da17	R6		
7	mwb47b4c45- _fac9- _49e6_a6a4- _87b9050ddfbb	R7	mw849ed3fd_87d9_44d2_9f3e_4d631b900d-	
8	mw4f62d07e- _217b- _4602_b6fe- _548af112eec8	R8	mwcb834e43_dc57_45ae_9452_f4c10955caf	
9	mw307551ca- _91cc- _4634_bba5- _0e3ecd38cfdd	R9	mwf166ad55_4ff0_49fb_95d2_b657ad7653d	
10	mw15bb92b6- _4cff- _4a41_b815- _c1d904618e57	R10	mwee54b5b4_b8c0_41df_8dda_5b160c5e10a	
11	mw106407fc- _e33f- _45aa_b5ae-	R11	mwf166ad55_4ff0_49fb_95d2_b657ad7653d	.5 mwf166ad55_4ff0_49fb_95d2_b657ad765

No	Id	Name	Reaction Equation	SBO
12	mwfb854977- _51ea- _4daa_b84e- _3bcb2fcccd39	R12	mwee54b5b4_b8c0_41df_8dda_5b160c5e10a5	
13	mwd71cb6c2- _6420- _46b9_ab17- _eedc7b0fd8dc	R13	mwfcfaf604_14d4_47a6_b021_226d1fb5497c	
14	mwdd7079dc- _8d70- _41b7_a369- _3334522cdd13	R14	mwf166ad55_4ff0_49fb_95d2_b657ad7653d5	
15	mwa25d1a3d- _bbd9- _41b8_8274- _236f9d67bb60	R15	mw919f8a86_e702_4b24_9cd7_adad694fcf9b	
16	mw185e644d- _6f10- _499f_a3a6- _5a47d7ba2eef	R16	mw812f63db_4cb0_40ad_b92b_9874be969dfe = mv	
17	mw5194cffd- _f75a- _4c61_b60e- _23d5b0fea120	R17	mw08818dfe_fb12_45cc_8c1d_d965f142d0ce = mv	v08818dfe_fb12_45cc_8c1d_d965f142

6.1 Reaction mw79830677_2d7e_4f49_9d0b_f05fe026749f

This is an irreversible reaction of one reactant forming one product influenced by two modifiers.

Name R1

Reaction equation

 $mw73259e20_240e_4f3a_b2e0_9ca248658898 \\ \frac{mw73259e20_240e_4f3a_b2e0_9ca248658898}{mw73259e20_240e_4f3a_b2e0_9ca248658898} \\ \frac{mw73259e20_240e_4f3a_b2e0_9ca2486589}{mw73259e20_240e_4f3a_b2e0_9ca2486589} \\ \frac{mw73259e20_240e_4f3a_b2e0_9ca2486589}{mw73259e20_9ca2486658} \\ \frac{mw73259e20_240e_4f3a_b2e0_9ca2486589}{mw73259e20_9ca2486658} \\ \frac{mw73259e20_240e_4f3a_b2e0_9ca2486658}{mw73259e20_9ca248665} \\ \frac{mw73259e20_240e_4f3a_b2e0_9ca24666}{mw75666666} \\ \frac{mw73259e20_24666}{mw75666666} \\ \frac{mw73259e20_24666}{mw7566666} \\ \frac{mw73259e20_24666}{mw7566666} \\ \frac{mw73259e20_24666}{mw756666} \\ \frac{mw73259e20_24666}{mw756666} \\ \frac{mw756666}{mw756666} \\ \frac{mw756666}{mw756666} \\ \frac{mw756666}{mw756666} \\ \frac{mw756666}{mw756666} \\ \frac{mw756666}{mw756666} \\ \frac{mw756666}{mw756666} \\ \frac{mw756666}{mw75666} \\ \frac{mw756666}{mw756666} \\ \frac{mw756666}{mw75666} \\ \frac{mw756666}{mw7$

(1)

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
mw73259e20_240e_4f3a_b2e0_9ca248658898	SerE	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
mw73259e20_240e_4f3a_b2e0_9ca248658898	SerE	
mw73259e20_240e_4f3a_b2e0_9ca248658898	SerE	

Product

Table 8: Properties of each product.

Id			Name	SBO
mw15abaa48_d7d0_4845	_ae04_c573	d289d495	Ser	

Kinetic Law

Derived unit $m^{-3} \cdot mol \cdot s^{-1}$

 $v_1 = \frac{\text{mwee07eca4_0806_4cc3_a6ab_9226ee79be6c} \cdot [\text{mw73259e20_240e_4f3a_b2e0_9ca248658898}]}{\text{mw8f20c25d_9700_4822_b5f9_fe243e001091} + [\text{mw73259e20_240e_4f3a_b2e0_9ca248658898}]}$

6.2 Reaction mw155447fb_ce5b_4ba2_bd74_434951481a78

This is an irreversible reaction of one reactant forming one product influenced by two modifiers.

Name R2

Reaction equation

 $mw15abaa48_d7d0_4845_ae04_c573d289d495 \\ \underline{ mw15abaa48_d7d0_4845_ae04_c573d289d495}, \\ mw15abaa48_d7d0_4845_ae04_c573d289d495, \\ mw15abaa48_d7d0_4845_ae04_c573d289d495, \\ \underline{ mw15abaa48_d7d0_4845_ae04_c573d289d495}, \\ \underline{ mw15abaa48_d7d0_4845_ae04_c573d2896}, \\ \underline{ mw15abaa48_d7d0_4845_ae040_ae04_c573d2896}, \\ \underline{ mw15abaa48_d7d0_4845_ae040_ae04_ae04_ae04_ae04_ae040_ae0$

(3)

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
mw15abaa48_d7d0_4845_ae04_c573d289d495	Ser	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
mw15abaa48_d7d0_4845_ae04_c573d289d495	Ser	
${\tt mw15abaa48_d7d0_4845_ae04_c573d289d495}$	Ser	

Product

Table 11: Properties of each product.

Id			Name	SBO
mwfcfaf604_14d4_47a6	_b021_226d1	fb5497c	PS	

Kinetic Law

Derived unit $m^{-3} \cdot mol \cdot s^{-1}$

 $\frac{v_2}{\text{mw7ce1b6a3_e65e_4aaa_9c32_aeefb420f0ea} \cdot [\text{mw15abaa48_d7d0_4845_ae04_c573d289d495}]}{\text{mw85485398_9f97_408c_bca6_90f0a8377eae} + [\text{mw15abaa48_d7d0_4845_ae04_c573d289d495}]}$

6.3 Reaction mw4c9aa283_577e_4b6c_ae5a_c96f62dbbb08

This is an irreversible reaction of one reactant forming one product influenced by two modifiers.

Name R3

Reaction equation

(5)

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
mw15abaa48_d7d0_4845_ae04_c573d289d495	Ser	

Modifiers

Table 13: Properties of each modifier.

Id	Name	SBO
mw15abaa48_d7d0_4845_ae04_c573d289d495	Ser	
mw15abaa48_d7d0_4845_ae04_c573d289d495	Ser	

Product

Table 14: Properties of each product.

Id			Name	SBO
mw8796c919_9251_4970	_8f87_0bca9	ecfeb5c	Etn	

Kinetic Law

Derived unit $m^{-3} \cdot mol \cdot s^{-1}$

 $v_{3} = \frac{\text{mw798d0b02_925e_471b_a372_526d681cc370} \cdot [\text{mw15abaa48_d7d0_4845_ae04_c573d289d495}]}{\text{mwd3807289_133c_4621_8087_366621f553d3} + [\text{mw15abaa48_d7d0_4845_ae04_c573d289d495}]}$

6.4 Reaction mw55fba323_0865_4254_a6e9_09acd2b4a10f

This is an irreversible reaction of one reactant forming one product influenced by two modifiers.

Name R4

Reaction equation

 $mw8796c919_9251_4970_8f87_0bca9ecfeb5c \\ \frac{mw8796c919_9251_4970_8f87_0bca9ecfeb5c, \\ mw8796c919_9251_4970_8f87_0bca9ecfeb5c, \\ mw8796c919_0bca9ecfeb5c, \\ mw8796c919_0bca9ecfeb5c,$

(7)

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
mw8796c919_9251_4970_8f87_0bca9ecfeb5c	Etn	

Modifiers

Table 16: Properties of each modifier.

Id	Name	SBO
mw8796c919_9251_4970_8f87_0bca9ecfeb5c	Etn	
mw8796c919_9251_4970_8f87_0bca9ecfeb5c	Etn	

Product

Table 17: Properties of each product.

Id			Name	SBO
mw849ed3fd_87d9_44d2	_9f3e_4d631	lb900d41	PEtn	

Kinetic Law

Derived unit $m^{-3} \cdot mol \cdot s^{-1}$

 $v_4 = \frac{\text{mw2439178f_a48f_4425_82f9_13267b917b85} \cdot [\text{mw8796c919_9251_4970_8f87_0bca9ecfeb5c}]}{\text{mw5c4edb54_cfd9_43af_b70b_e9ff1b44dc55} + [\text{mw8796c919_9251_4970_8f87_0bca9ecfeb5c}]}$

6.5 Reaction mwb8420f59_69c3_4707_918c_2e06bedff243

This is an irreversible reaction of one reactant forming one product influenced by two modifiers.

Name R5

Reaction equation

 $mw849ed3fd_87d9_44d2_9f3e_4d631b900d41 \\ \frac{mw849ed3fd_87d9_44d2_9f3e_4d631b900d41, \\ mw849ed3fd_87d9_44d2_9f3e_4d631b900d41, \\ mw849ed3fd_87d9_44d2_9f3e_4d631b900d41, \\ mw849ed3fd_87d9_44d2_9f3e_4d631b900d41, \\ mw849ed3fd_87d9_4d631b900d41, \\ mw849ed3fd_87d9_4d631b9000d41, \\ mw849ed3fd_87d9_4d631b9000d41, \\ mw849ed$

(9)

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
mw849ed3fd_87d9_44d2_9f3e_4d631b900d41	PEtn	

Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
mw849ed3fd_87d9_44d2_9f3e_4d631b900d41	PEtn	
${\tt mw849ed3fd_87d9_44d2_9f3e_4d631b900d41}$	PEtn	

Product

Table 20: Properties of each product.

Id			Name	SBO
mwcb834e43_dc57_45ae	_9452_f4c1	10955caf1	PCho	

Kinetic Law

Derived unit $m^{-3} \cdot mol \cdot s^{-1}$

 $v_{5} = \frac{\text{mw961dacfa}_{\text{f443}}_{\text{4814}}_{\text{ad6c}}_{\text{a27c04e74268}} \cdot [\text{mw849ed3fd}_{\text{87d9}}_{\text{44d2}}_{\text{9f3e}}_{\text{4d631b900d41}}]}{\text{mw15ba24b5}_{\text{7a87}}_{\text{479e}}_{\text{9be7}}_{\text{261b12cbdb63}} + [\text{mw849ed3fd}_{\text{87d9}}_{\text{44d2}}_{\text{9f3e}}_{\text{4d631b900d41}}]}$

6.6 Reaction mwc9170c21_608b_4bd7_b2d0_f359d045da17

This is an irreversible reaction of one reactant forming one product influenced by two modifiers.

Name R6

Reaction equation

 $mwfcfaf604_14d4_47a6_b021_226d1fb5497c \\ \frac{mwfcfaf604_14d4_47a6_b021_226d1fb5497c, \\ mwfcfaf604_14d4_47a6_b021_226d1fb5497c, \\ mwfcfaf604_14d4_47a6_b020_226d1fb5497c, \\ mwfcfaf604_14d4_47a6_b020_226d1fb5497c, \\ mwfcfaf604_14d4_47a6_b020_226d1fb5497c, \\ mwfcfaf604_226d1fb5497c, \\ mwfcfaf604_226d1fb5497c, \\ mwfcfaf604_226d1fb5497c, \\ mwfcfaf604_226d1fb5497c, \\ mwfcfaf604_226d1fb5497c, \\ mwfcfaf604_226d1fb$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
mwfcfaf604_14d4_47a6_b021_226d1fb5497c	PS	

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
mwfcfaf604_14d4_47a6_b021_226d1fb5497c		
mwfcfaf604_14d4_47a6_b021_226d1fb5497c	PS	

Product

Table 23: Properties of each product.

Id		_	Name	SBO
mwf166ad55_4ff0_49fb	_95d2_b657a	17653d5	PE	

Kinetic Law

Derived unit $m^{-3} \cdot mol \cdot s^{-1}$

 $v_6 = \frac{\text{mw9f56ecc5_c22b_4f8c_8b82_90e2a6d9e364} \cdot [\text{mwfcfaf604_14d4_47a6_b021_226d1fb5497c}]}{\text{mw18bbabcb_d229_4d91_99f1_484f2ba8f020} + [\text{mwfcfaf604_14d4_47a6_b021_226d1fb5497c}]}$

6.7 Reaction mwb47b4c45_fac9_49e6_a6a4_87b9050ddfbb

This is an irreversible reaction of one reactant forming one product influenced by two modifiers.

Name R7

Reaction equation

 $mw849ed3fd_87d9_44d2_9f3e_4d631b900d41 \\ \frac{mw849ed3fd_87d9_44d2_9f3e_4d631b900d41, \\ mw849ed3fd_87d9_44d2_9f3e_4d631b900d41, \\ mw849ed3fd_87d9_4d2_9f3e_4d631b900d41, \\ mw849ed3fd_87d9_4d631b900d41, \\ mw849ed3fd_87d9_4d6$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
mw849ed3fd_87d9_44d2_9f3e_4d631b900d41	PEtn	

Modifiers

Table 25: Properties of each modifier.

Id	Name	SBO
mw849ed3fd_87d9_44d2_9f3e_4d631b900d41	PEtn	
${\tt mw849ed3fd_87d9_44d2_9f3e_4d631b900d41}$	PEtn	

Product

Table 26: Properties of each product.

Id			Name	SBO
mwf166ad55_4ff0_49fb	_95d2_b657a	d7653d5	PE	

Kinetic Law

Derived unit $m^{-3} \cdot mol \cdot s^{-1}$

 $v_7 = \frac{\text{mwba0debe9_c575_4f5a_a980_e2b6857ff053} \cdot [\text{mw849ed3fd_87d9_44d2_9f3e_4d631b900d41}]}{\text{mwffba86ff_a560_401a_93d6_c0e30bf42c87} + [\text{mw849ed3fd_87d9_44d2_9f3e_4d631b900d41}]}$

6.8 Reaction mw4f62d07e_217b_4602_b6fe_548af112eec8

This is an irreversible reaction of one reactant forming one product influenced by two modifiers.

Name R8

Reaction equation

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
mwcb834e43_dc57_45ae_9452_f4c10955caf1	PCho	

Modifiers

Table 28: Properties of each modifier.

Id	Name	SBO
mwcb834e43_dc57_45ae_9452_f4c10955caf1	PCho	
mwcb834e43_dc57_45ae_9452_f4c10955caf1	PCho	

Product

Table 29: Properties of each product.

Id		_	Name	SBO
mwee54b5b4_b8c0_41df	_8dda_5b16	0c5e10a5	PC	

Kinetic Law

Derived unit $m^{-3} \cdot mol \cdot s^{-1}$

 v_8 (16) $= \frac{\text{mw231a5907_d1ee_4a43_83ab_abb72f19502c} \cdot [\text{mwcb834e43_dc57_45ae_9452_f4c10955caf1}]}{\text{mwaf289d12_4291_4651_8bd1_82e321e476a4} + [\text{mwcb834e43_dc57_45ae_9452_f4c10955caf1}]}$

6.9 Reaction mw307551ca_91cc_4634_bba5_0e3ecd38cfdd

This is an irreversible reaction of one reactant forming one product influenced by two modifiers.

Name R9

Reaction equation

 $mwf166ad55_4ff0_49fb_95d2_b657ad7653d5 \xrightarrow{mwf166ad55_4ff0_49fb_95d2_b657ad7653d5, \ mwf166ad55_4ff0_49fb} (17)$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
mwf166ad55_4ff0_49fb_95d2_b657ad7653d5	PE	

Modifiers

Table 31: Properties of each modifier.

Id	Name	SBO
mwf166ad55_4ff0_49fb_95d2_b657ad7653d5	PE	
${\tt mwf166ad55_4ff0_49fb_95d2_b657ad7653d5}$	PE	

Product

Table 32: Properties of each product.

Id		_	Name	SBO
mwee54b5b4_b8c0_41df	_8dda_5b16	0c5e10a5	PC	

Kinetic Law

Derived unit $m^{-3} \cdot mol \cdot s^{-1}$

 $v_9 = \frac{\text{mw1a53a2cb_a3a7_40d7_ae07_4d93ad1123a3} \cdot [\text{mwf166ad55_4ff0_49fb_95d2_b657ad7653d5}]}{\text{mw4035a2c9_3cda_467c_83cc_8f9c2902abaf} + [\text{mwf166ad55_4ff0_49fb_95d2_b657ad7653d5}]}$

6.10 Reaction mw15bb92b6_4cff_4a41_b815_c1d904618e57

This is an irreversible reaction of one reactant forming one product influenced by two modifiers.

Name R10

Reaction equation

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
mwee54b5b4_b8c0_41df_8dda_5b160c5e10a5	PC	

Modifiers

Table 34: Properties of each modifier.

Id	Name	SBO
mwee54b5b4_b8c0_41df_8dda_5b160c5e10a5	PC	
${\tt mwee54b5b4_b8c0_41df_8dda_5b160c5e10a5}$	PC	

Product

Table 35: Properties of each product.

Id				Name	SBO
mwfcfaf604_14d4_47a6	_b021_226d	.1fb5497	7c	PS	

Kinetic Law

Derived unit $m^{-3} \cdot mol \cdot s^{-1}$

 $v_{10} = \frac{\text{mwf7d1ff9f}_{1734}_{4232}_{9a96}_{037b31b193b0} \cdot [\text{mwee54b5b4}_{b8c0}_{41df}_{8dda}_{5b160c5e10a5}]}{\text{mw7d57aa6b}_{1bfb}_{4472}_{b555}_{919263d9eaf9} + [\text{mwee54b5b4}_{b8c0}_{41df}_{8dda}_{5b160c5e10a5}]}$

6.11 Reaction mw106407fc_e33f_45aa_b5ae_258bd4790633

This is an irreversible reaction of one reactant forming one product influenced by two modifiers.

Name R11

Reaction equation

 $mwf166ad55_4ff0_49fb_95d2_b657ad7653d5 \xrightarrow{mwf166ad55_4ff0_49fb_95d2_b657ad7653d5, \ mwf166ad55_4ff0_49fb} (21)$

Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
mwf166ad55_4ff0_49fb_95d2_b657ad7653d5	PE	

Modifiers

Table 37: Properties of each modifier.

Id	Name	SBO
mwf166ad55_4ff0_49fb_95d2_b657ad7653d5	PE	
${\tt mwf166ad55_4ff0_49fb_95d2_b657ad7653d5}$	PE	

Product

Table 38: Properties of each product.

Id	_		Name	SBO
mwfcfaf604_14d4_47a6	_b021_226d	1fb5497c	PS	

Kinetic Law

Derived unit $m^{-3} \cdot mol \cdot s^{-1}$

 $v_{11} = \frac{\text{mw5ffad843_5f02_419d_ba99_6e1f9b7e6b7b} \cdot [\text{mwf166ad55_4ff0_49fb_95d2_b657ad7653d5}]}{\text{mw3046ca21_42a2_4a4b_89c4_9d6ca3d927c5} + [\text{mwf166ad55_4ff0_49fb_95d2_b657ad7653d5}]}$

6.12 Reaction mwfb854977_51ea_4daa_b84e_3bcb2fcccd39

This is an irreversible reaction of one reactant forming no product influenced by two modifiers.

Name R12

Reaction equation

 $mwee54b5b4_b8c0_41df_8dda_5b160c5e10a5 \xrightarrow{mwee54b5b4_b8c0_41df_8dda_5b160c5e10a5, \ mwee54b5b4_b8c0_41df_8dda_5b160c5e10a5} (23)$

Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
mwee54b5b4_b8c0_41df_8dda_5b160c5e10a5	PC	

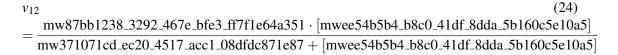
Modifiers

Table 40: Properties of each modifier.

Id	Name	SBO
mwee54b5b4_b8c0_41df_8dda_5b160c5e10a5	PC	
${\tt mwee54b5b4_b8c0_41df_8dda_5b160c5e10a5}$	PC	

Kinetic Law

Derived unit $m^{-3} \cdot mol \cdot s^{-1}$



6.13 Reaction mwd71cb6c2_6420_46b9_ab17_eedc7b0fd8dc

This is an irreversible reaction of one reactant forming no product influenced by two modifiers.

Name R13

Reaction equation

Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
mwfcfaf604_14d4_47a6_b021_226d1fb5497c	PS	

Modifiers

Table 42: Properties of each modifier.

Id	Name	SBO
mwfcfaf604_14d4_47a6_b021_226d1fb5497c mwfcfaf604_14d4_47a6_b021_226d1fb5497c		

Kinetic Law

Derived unit $m^{-3} \cdot mol \cdot s^{-1}$

```
v_{13} = \frac{\text{mw5b225cdc}_{783f}_{4a15}_{93db}_{e960a2398b8e} \cdot [\text{mwfcfaf604}_{14d4}_{47a6}_{b021}_{226d1fb5497c}]}{\text{mw27f524cb}_{75b3}_{401c}_{8533}_{99d6f27af654} + [\text{mwfcfaf604}_{14d4}_{47a6}_{b021}_{226d1fb5497c}]}
```

6.14 Reaction mwdd7079dc_8d70_41b7_a369_3334522cdd13

This is an irreversible reaction of one reactant forming no product influenced by two modifiers.

Name R14

Reaction equation

 $mwf166ad55_4ff0_49fb_95d2_b657ad7653d5 \xrightarrow{mwfcfaf604_14d4_47a6_b021_226d1fb5497c, \ mwfcfaf604_14d4_47a6_b021_226d1fb5497c, \ mwfcfaf604_226d1fb5497c, \ mwfcfaf6$

Reactant

Table 43: Properties of each reactant.

Id	Name	SBO
mwf166ad55_4ff0_49fb_95d2_b657ad7653d5	PE	

Modifiers

Table 44: Properties of each modifier.

Id	Name	SBO
mwfcfaf604_14d4_47a6_b021_226d1fb5497c	PS	
${\tt mwfcfaf604_14d4_47a6_b021_226d1fb5497c}$	PS	

Kinetic Law

Derived unit $m^{-3} \cdot mol \cdot s^{-1}$

$$v_{14} = \frac{\text{mwc623d82f_a94e_4460_9aed_444597a728c2} \cdot [\text{mwfcfaf604_14d4_47a6_b021_226d1fb5497c}]}{\text{mwbf296afc_5e4f_4819_8028_06b20d7af7ca} + [\text{mwfcfaf604_14d4_47a6_b021_226d1fb5497c}]}$$

6.15 Reaction mwa25d1a3d_bbd9_41b8_8274_236f9d67bb60

This is an irreversible reaction of one reactant forming one product influenced by two modifiers.

Name R15

Reaction equation

Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
mw919f8a86_e702_4b24_9cd7_adad694fcf9b	ChoE	

Modifiers

Table 46: Properties of each modifier.

Id	Name	SBO
mw919f8a86_e702_4b24_9cd7_adad694fcf9b mw919f8a86_e702_4b24_9cd7_adad694fcf9b		

Product

Table 47: Properties of each product.

	1		1		
Id				Name	SBO
mw812f63db_4cb0_40ad	_b92b_98	74be9	969dfe	Cho	

Kinetic Law

Derived unit $m^{-3} \cdot mol \cdot s^{-1}$

$$v_{15} = \frac{\text{mw91e15e1e_c73e_4866_ab2b_8225a32b7610} \cdot [\text{mw919f8a86_e702_4b24_9cd7_adad694fcf9b}]}{\text{mwf5cecb8f_89f8_4fba_b39b_b517d0bef2ce} + [\text{mw919f8a86_e702_4b24_9cd7_adad694fcf9b}]}$$

6.16 Reaction mw185e644d_6f10_499f_a3a6_5a47d7ba2eef

This is an irreversible reaction of one reactant forming one product influenced by two modifiers.

Name R16

Reaction equation

Reactant

Table 48: Properties of each reactant.

Id	Name	SBO
mw812f63db_4cb0_40ad_b92b_9874be969dfe	Cho	

Modifiers

Table 49: Properties of each modifier.

Id	Name	SBO
mw812f63db_4cb0_40ad_b92b_9874be969dfe	Cho	
mw812f63db_4cb0_40ad_b92b_9874be969dfe	Cho	

Product

Table 50: Properties of each product.

Id	1			Name	SBO
mwcb834e43_dc57_45ae	_9452_f4	:1095	5caf1	PCho	

Kinetic Law

Derived unit $m^{-3} \cdot mol \cdot s^{-1}$

$$= \frac{\text{mwff26437c_166b_4946_ad35_f13df6145780} \cdot [\text{mw812f63db_4cb0_40ad_b92b_9874be969dfe}]}{\text{mw284c519a_cc2b_4a98_99ce_5a4471af99e1} + [\text{mw812f63db_4cb0_40ad_b92b_9874be969dfe}]}$$

6.17 Reaction mw5194cffd_f75a_4c61_b60e_23d5b0fea120

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

Name R17

Reaction equation

Reactant

Table 51: Properties of each reactant.

Id	Name	SBO
mw08818dfe_fb12_45cc_8c1d_d965f142d0ce	EtnE	

Modifiers

Table 52: Properties of each modifier.

Id	Name	SBO
mw08818dfe_fb12_45cc_8c1d_d965f142d0ce	EtnE	
mw8796c919_9251_4970_8f87_0bca9ecfeb5c	Etn	
mw08818dfe_fb12_45cc_8c1d_d965f142d0ce	EtnE	
mw8796c919_9251_4970_8f87_0bca9ecfeb5c	Etn	

Product

Table 53: Properties of each product.

Id	-			Name	SBO
mw8796c919_9251_4970	_8f87_0b	ca9ec	feb5c	Etn	

Kinetic Law

Derived unit $s^{-1} \cdot mol \cdot m^{-3}$

$$v_{17} = \text{mw2cd81e51_eb11_4e2c_b609_b2f802438a6b}$$

$$\cdot [\text{mw08818dfe_fb12_45cc_8c1d_d965f142d0ce}]$$

$$- \text{mwff99ad6c_8951_4d58_a836_cf2d3d08ac86}$$

$$\cdot [\text{mw8796c919_9251_4970_8f87_0bca9ecfeb5c}]$$

$$(34)$$

7 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.

7.1 Species mw73259e20_240e_4f3a_b2e0_9ca248658898

Name SerE

Initial concentration $10^{-4} \text{ mol} \cdot \text{m}^{-3} \cdot (0.0010 \text{ dimensionless})^{-1}$

This species takes part in three reactions (as a reactant in mw79830677_2d7e_4f49_9d0b_f05fe026749f and as a modifier in mw79830677_2d7e_4f49_9d0b_f05fe026749f, mw79830677_2d7e_4f49_9d0b_f05fe026749f), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}mw73259e20_240e_4f3a_b2e0_9ca248658898 = 0$$
 (35)

7.2 Species mw15abaa48_d7d0_4845_ae04_c573d289d495

Name Ser

Initial amount 0 mol

This species takes part in seven reactions (as a reactant in mw155447fb_ce5b_4ba2_bd74-_434951481a78, mw4c9aa283_577e_4b6c_ae5a_c96f62dbbb08 and as a product in mw79830677-_2d7e_4f49_9d0b_f05fe026749f and as a modifier in mw155447fb_ce5b_4ba2_bd74_434951481a78, mw155447fb_ce5b_4ba2_bd74_434951481a78, mw4c9aa283_577e_4b6c_ae5a_c96f62dbbb08, mw4c9aa283_577e_4b6c_ae5a_c96f62dbbb08).

$$\frac{d}{dt} mw15abaa48_d7d0_4845_ae04_c573d289d495 = |v_1| - |v_2| - |v_3|$$
(36)

7.3 Species mwfcfaf604_14d4_47a6_b021_226d1fb5497c

Name PS

Initial amount 0 mol

This species takes part in eleven reactions (as a reactant in mwc9170c21_608b_4bd7_b2d0-_f359d045da17, mwd71cb6c2_6420_46b9_ab17_eedc7b0fd8dc and as a product in mw155447fb-_ce5b_4ba2_bd74_434951481a78, mw15bb92b6_4cff_4a41_b815_c1d904618e57, mw106407fc-_e33f_45aa_b5ae_258bd4790633 and as a modifier in mwc9170c21_608b_4bd7_b2d0_f359d045da17, mwc9170c21_608b_4bd7_b2d0_f359d045da17, mwd71cb6c2_6420_46b9_ab17_eedc7b0fd8dc, mwd71cb6c2_6420_46b9_ab17_eedc7b0fd8dc, mwdd7079dc_8d70_41b7_a369_3334522cdd13, mwdd7079dc_8d70_41b7_a369_3334522cdd13).

$$\frac{d}{dt} \text{mwfcfaf604_14d4_47a6_b021_226d1fb5497c} = v_2 + v_{10} + v_{11} - v_6 - v_{13}$$
 (37)

7.4 Species mw8796c919_9251_4970_8f87_0bca9ecfeb5c

Name Etn

Initial amount 0 mol

This species takes part in seven reactions (as a reactant in mw55fba323_0865_4254_a6e9-_09acd2b4a10f and as a product in mw4c9aa283_577e_4b6c_ae5a_c96f62dbbb08, mw5194cffd-_f75a_4c61_b60e_23d5b0fea120 and as a modifier in mw55fba323_0865_4254_a6e9_09acd2b4a10f, mw55fba323_0865_4254_a6e9_09acd2b4a10f, mw5194cffd_f75a_4c61_b60e_23d5b0fea120, mw5194cffd_f75a_4c61_b60e_23d5b0fea120).

$$\frac{d}{dt} mw8796c919_9251_4970_8f87_0bca9ecfeb5c = v_3 + v_{17} - v_4$$
(38)

7.5 Species mw849ed3fd_87d9_44d2_9f3e_4d631b900d41

Name PEtn

Initial amount 0 mol

This species takes part in seven reactions (as a reactant in mwb8420f59_69c3_4707_918c-_2e06bedff243, mwb47b4c45_fac9_49e6_a6a4_87b9050ddfbb and as a product in mw55fba323-_0865_4254_a6e9_09acd2b4a10f and as a modifier in mwb8420f59_69c3_4707_918c_2e06bedff243, mwb8420f59_69c3_4707_918c_2e06bedff243, mwb47b4c45_fac9_49e6_a6a4_87b9050ddfbb, mwb47b4c45_fac9_49e6_a6a4_87b9050ddfbb).

$$\frac{d}{dt} mw849 ed3 fd_87 d9_44 d2_9 f3 e_4 d631 b900 d41 = v_4 - v_5 - v_7$$
(39)

7.6 Species mwcb834e43_dc57_45ae_9452_f4c10955caf1

Name PCho

Initial amount 0 mol

This species takes part in five reactions (as a reactant in mw4f62d07e_217b_4602_b6fe_548af112eec8 and as a product in mwb8420f59_69c3_4707_918c_2e06bedff243, mw185e644d_6f10_499f-a3a6_5a47d7ba2eef and as a modifier in mw4f62d07e_217b_4602_b6fe_548af112eec8, mw4f62d07e_217b_4602_b6fe_548af112eec8).

$$\frac{d}{dt} \text{mwcb834e43_dc57_45ae_9452_f4c10955caf1} = v_5 + v_{16} - v_8$$
 (40)

7.7 Species mwf166ad55_4ff0_49fb_95d2_b657ad7653d5

Name PE

Initial amount 0 mol

This species takes part in nine reactions (as a reactant in mw307551ca_91cc_4634_bba5_0e3ecd38cfdd, mw106407fc_e33f_45aa_b5ae_258bd4790633, mwdd7079dc_8d70_41b7_a369_3334522cdd13 and as a product in mwc9170c21_608b_4bd7_b2d0_f359d045da17, mwb47b4c45_fac9_49e6-_a6a4_87b9050ddfbb and as a modifier in mw307551ca_91cc_4634_bba5_0e3ecd38cfdd, mw307551ca_91cc_4634_bba5_0e3ecd38cfdd, mw106407fc_e33f_45aa_b5ae_258bd4790633).

$$\frac{d}{dt} mwf166ad55_4ff0_49fb_95d2_b657ad7653d5 = |v_6| + |v_7| - |v_9| - |v_{11}| - |v_{14}|$$
 (41)

7.8 Species mwee54b5b4_b8c0_41df_8dda_5b160c5e10a5

Name PC

Initial amount 0 mol

This species takes part in eight reactions (as a reactant in mw15bb92b6_4cff_4a41_b815-_c1d904618e57, mwfb854977_51ea_4daa_b84e_3bcb2fcccd39 and as a product in mw4f62d07e-_217b_4602_b6fe_548af112eec8, mw307551ca_91cc_4634_bba5_0e3ecd38cfdd and as a modifier in mw15bb92b6_4cff_4a41_b815_c1d904618e57, mw15bb92b6_4cff_4a41_b815_c1d904618e57, mwfb854977_51ea_4daa_b84e_3bcb2fcccd39, mwfb854977_51ea_4daa_b84e_3bcb2fcccd39).

$$\frac{d}{dt} \text{mwee54b5b4_b8c0_41df_8dda_5b160c5e10a5} = |v_8| + |v_9| - |v_{10}| - |v_{12}|$$
 (42)

7.9 Species mw919f8a86_e702_4b24_9cd7_adad694fcf9b

Name ChoE

Initial concentration $5 \cdot 10^{-5} \text{ mol} \cdot \text{m}^{-3} \cdot (0.0010 \text{ dimensionless})^{-1}$

This species takes part in three reactions (as a reactant in mwa25d1a3d_bbd9_41b8_8274-236f9d67bb60 and as a modifier in mwa25d1a3d_bbd9_41b8_8274_236f9d67bb60, mwa25d1a3d_bbd9_41b8_8274_236f9d67bb60), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}mw919f8a86_e702_4b24_9cd7_adad694fcf9b = 0$$
 (43)

7.10 Species mw812f63db_4cb0_40ad_b92b_9874be969dfe

Name Cho

Initial amount 0 mol

This species takes part in four reactions (as a reactant in $mw185e644d_6f10_499f_a3a6_5a47d7ba2eef$ and as a product in $mwa25d1a3d_bbd9_41b8_8274_236f9d67bb60$ and as a modifier in $mw185e644d_6f10_499f_a3a6_5a47d7ba2eef$, $mw185e644d_6f10_499f_a3a6_5a47d7ba2eef$).

$$\frac{d}{dt} mw812f63db_4cb0_40ad_b92b_9874be969dfe = v_{15} - v_{16}$$
(44)

7.11 Species mw08818dfe_fb12_45cc_8c1d_d965f142d0ce

Name EtnE

Initial amount 0 mol

This species takes part in three reactions (as a reactant in mw5194cffd_f75a_4c61_b60e-_23d5b0fea120 and as a modifier in mw5194cffd_f75a_4c61_b60e_23d5b0fea120, mw5194cffd_f75a_4c61_b60e_23d5b0fea120), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt} mw08818 dfe_fb12_45 cc_8c1 d_d 965 f142 d0 ce = 0$$
 (45)

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

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