

SBML Model Report

Model name: “Salcedo-Sora2016 - Microbial folate biosynthesis and utilisation”



February 10, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: J. Enrique Salcedo-Sora¹ and Mark T. McAuley² at June 28th 2015 at 2:24 p. m. and last time modified at June 28th 2015 at 2:24 p. m. Table 1 gives an overview of the quantities of all components of this model.

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

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	51
events	0	constraints	0
reactions	31	function definitions	24
global parameters	0	unit definitions	2
rules	0	initial assignments	0

Model Notes

Salcedo-Sora2016 - Microbial folate biosynthesis and utilisation

This model is described in the article: [A mathematical model of microbial folate biosynthesis and utilisation: implications for antifolate development](#). Enrique Salcedo-Sora J, Mc Auley MT. Mol Biosyst. 2016 Jan 21.

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Abstract:

The metabolic biochemistry of folate biosynthesis and utilisation has evolved into a complex network of reactions. Although this complexity represents challenges to the field of folate research it has also provided a renewed source for antimetabolite targets. A range of improved folate chemotherapy continues to be developed and applied particularly to cancer and chronic inflammatory diseases. However, new or better antifolates against infectious diseases remain much more elusive. In this paper we describe the assembly of a generic deterministic mathematical model of microbial folate metabolism. Our aim is to explore how a mathematical model could be used to explore the dynamics of this inherently complex set of biochemical reactions. Using the model it was found that: (1) a particular small set of folate intermediates are overrepresented, (2) inhibitory profiles can be quantified by the level of key folate products, (3) using the model to scan for the most effective combinatorial inhibitions of folate enzymes we identified specific targets which could complement current antifolates, and (4) the model substantiates the case for a substrate cycle in the folinic acid biosynthesis reaction. Our model is coded in the systems biology markup language and has been deposited in the BioModels Database (MODEL1511020000), this makes it accessible to the community as a whole.

This model is hosted on [BioModels Database](#) and identified by: [MODEL1511020000](#).

To cite BioModels Database, please use: [BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models](#).

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2 Unit Definitions

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

2.1 Unit `time`

Name `time`

Definition 60 s

2.2 Unit `substance`

Name `substance`

Definition μmol

2.3 Unit `volume`

Notes Litre is the predefined SBML unit for volume.

Definition 1

2.4 Unit `area`

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

Definition m^2

2.5 Unit `length`

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

Definition m

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
compartment	compartment		3	1	litre	<input checked="" type="checkbox"/>	

3.1 Compartment `compartment`

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

Name `compartment`

4 Species

This model contains 51 species. The boundary condition of 13 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
DAHP	DAHP	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
PEP	PEP	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Pi	Pi	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
DHQ	DHQ	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
EP	EP	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
DHSK	DHSK	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
SK	SK	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
SKP	SKP	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
CVPSK	CVPSK	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
CM	CM	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Gln	Gln	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Glu	Glu	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
ADC	ADC	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Pyr	Pyr	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
pABA	pABA	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
DHNTp	DHNTp	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
GTP	GTP	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
AHMDHP	AHMDHP	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
HAD	HAD	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
PTHP	PTHP	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
AHMDPP	AHMDPP	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
DHP	DHP	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
DHF	DHF	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
THF	THF	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
THFGlu	THFGlu	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Gly	Gly	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Ser	Ser	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
myTHFGlu	myTHFGlu	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
MTHFGlu	MTHFGlu	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Hcy	Hcy	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Met	Met	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
dTMP	dTMP	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
dUMP	dUMP	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
meTHFGlu	meTHFGlu	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
fTHFGlu	fTHFGlu	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
fmrRNA	fmrRNA	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
mtRNA	mtRNA	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
COTwo	COTwo	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
ADP	ADP	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
ATP	ATP	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
NADP	NADP	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
NADPH	NADPH	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
AMP	AMP	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
DLp	DLp	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
SAmDLp	SAmDLp	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Lp	Lp	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
NAD	NAD	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
NADH	NADH	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
Ammonia	Ammonia	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	\square	\square
Formyl	Formyl	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	\square	\square
ffTHFGlu	ffTHFGlu	compartment	$\mu\text{mol} \cdot \text{l}^{-1}$	\square	\square

5 Function definitions

This is an overview of 24 function definitions.

5.1 Function definition `Henri_Michaelis_Menten_irreversible`

Name Henri-Michaelis-Menten (irreversible)

Arguments substrate, Km, V

Mathematical Expression

$$\frac{V \cdot \text{substrate}}{K_m + \text{substrate}} \quad (1)$$

5.2 Function definition `Rate_Law_for_R1`

Name Rate Law for R1

Notes Taken from DeLeo et al 1973, JBC 248, 2344-2353

Arguments v_{max}, [PEP], [EP], k_{pep}, k_{ep}

Mathematical Expression

$$\frac{v_{\max} \cdot [\text{EP}] \cdot [\text{PEP}]}{k_{\text{pep}} \cdot k_{\text{ep}} + k_{\text{pep}} \cdot [\text{EP}] + k_{\text{ep}} \cdot [\text{PEP}] + [\text{EP}] \cdot [\text{PEP}]} \quad (2)$$

5.3 Function definition `Rate_Law_for_R6`

Name Rate Law for R6

Arguments [PEP], v_{max}, [SKP], k_{pep}, k_{skp}

Mathematical Expression

$$\frac{v_{\max} \cdot [\text{PEP}] \cdot [\text{SKP}]}{k_{\text{pep}} \cdot k_{\text{skp}} + k_{\text{pep}} \cdot [\text{SKP}] + k_{\text{skp}} \cdot [\text{PEP}] + [\text{SKP}] \cdot [\text{PEP}]} \quad (3)$$

5.4 Function definition `Rate_Law_for_R8`

Name Rate Law for R8

Arguments v_{max}, [CM], [Gln], k_{cm}, k_{gln}

Mathematical Expression

$$\frac{v_{\max} \cdot [\text{CM}] \cdot [\text{Gln}]}{k_{\text{cm}} \cdot k_{\text{gln}} + k_{\text{cm}} \cdot [\text{Gln}] + k_{\text{gln}} \cdot [\text{CM}] + [\text{CM}] \cdot [\text{Gln}]} \quad (4)$$

5.5 Function definition [Rate_Law_for_R14](#)

Name Rate Law for R14

Arguments vmax, [DHP], [Glu], kdhp, kglu, [ATP], katp

Mathematical Expression

$$\frac{vmax \cdot [DHP] \cdot [Glu] \cdot [ATP]}{kdhp \cdot kglu \cdot katp + kdhp \cdot ([Glu] + [ATP]) + kglu \cdot ([DHP] + [ATP]) + katp \cdot ([Glu] + [ATP]) + [DHP] \cdot [Glu] \cdot [ATP]} \quad (5)$$

5.6 Function definition [Rate_Law_for_R16](#)

Name Rate Law for R16

Arguments vmax, [THF], [Glu], kthf, kglu, [ATP], katp, [DHF], kidhf

Mathematical Expression

$$\frac{vmax \cdot [THF] \cdot [Glu] \cdot [ATP]}{kthf \cdot \left(1 + \frac{[DHF]}{kidhf}\right) \cdot kglu \cdot katp + kthf \cdot ([Glu] + [ATP]) + kglu \cdot ([THF] + [ATP]) + katp \cdot ([THF] + [Glu]) + [THF] \cdot [Glu] \cdot [ATP]} \quad (6)$$

5.7 Function definition [Rate_Law_for_R17](#)

Name Rate Law for R17

Arguments vmax, [THFGlu], [Ser], kthfglu, kser, [THF], kithf

Mathematical Expression

$$\frac{vmax \cdot [THFGlu] \cdot [Ser]}{kthfglu \cdot \left(1 + \frac{[THF]}{kithf}\right) \cdot kser + kthfglu \cdot [Ser] + kser \cdot [THFGlu] + [THFGlu] \cdot [Ser]} \quad (7)$$

5.8 Function definition [Rate_Law_for_R18c](#)

Name Rate Law for R18c

Arguments vmax, [THFGlu], kthfglu, [SAmDLp], ksamdlp

Mathematical Expression

$$\frac{vmax \cdot [THFGlu] \cdot [SAmDLp]}{kthfglu \cdot ksamdlp + kthfglu \cdot [SAmDLp] + ksamdlp \cdot [THFGlu] + [THFGlu] \cdot [SAmDLp]} \quad (8)$$

5.9 Function definition `Rate_Law_for_R20`

Name Rate Law for R20

Arguments `vmax`, `[MTHFGlu]`, `[Hcy]`, `kmthfglu`, `khcy`

Mathematical Expression

$$\frac{vmax \cdot [MTHFGlu] \cdot [Hcy]}{kmthfglu \cdot khcy + kmthfglu \cdot [Hcy] + khcy \cdot [MTHFGlu] + [MTHFGlu] \cdot [Hcy]} \quad (9)$$

5.10 Function definition `Rate_Law_for_R21`

Name Rate Law for R21

Arguments `vmax`, `[myTHFGlu]`, `[dUMP]`, `kdump`, `kmythfglu`, `[DHF]`, `kidhf`

Mathematical Expression

$$\frac{vmax \cdot [myTHFGlu] \cdot [dUMP]}{kmythfglu \cdot \left(1 + \frac{[DHF]}{kidhf}\right) \cdot kdump + kmythfglu \cdot [dUMP] + kdump \cdot [myTHFGlu] + [myTHFGlu] \cdot [dUMP]} \quad (10)$$

5.11 Function definition `Rate_Law_for_R18b`

Name Rate Law for R18b

Arguments `vmax`, `[Gly]`, `[DLp]`, `kgly`, `kdlp`

Mathematical Expression

$$\frac{vmax \cdot [Gly] \cdot [DLp]}{kgly \cdot kdlp + kgly \cdot [DLp] + kdlp \cdot [Gly] + [Gly] \cdot [DLp]} \quad (11)$$

5.12 Function definition `Rate_Law_for_R18a`

Name Rate Law for R18a

Arguments `vmax`, `[NADH]`, `[Lp]`, `knadh`, `klp`

Mathematical Expression

$$\frac{vmax \cdot [NADH] \cdot [Lp]}{knadh \cdot klp + knadh \cdot [Lp] + klp \cdot [NADH] + [NADH] \cdot [Lp]} \quad (12)$$

5.13 Function definition `Rate_Law_for_R4`

Name Rate Law for R4

Arguments `vmax`, `[DHSK]`, `[NADPH]`, `kdhsk`, `knadph`

Mathematical Expression

$$\frac{vmax \cdot [DHSK] \cdot [NADPH]}{kdhsk \cdot knadph + kdhsk \cdot [NADPH] + knadph \cdot [DHSK] + [DHSK] \cdot [NADPH]} \quad (13)$$

5.14 Function definition `Rate_Law_for_R5`

Name Rate Law for R5

Arguments `vmax`, `[SK]`, `[ATP]`, `ksk`, `katp`

Mathematical Expression

$$\frac{vmax \cdot [SK] \cdot [ATP]}{ksk \cdot katp + ksk \cdot [ATP] + katp \cdot [SK] + [SK] \cdot [ATP]} \quad (14)$$

5.15 Function definition `Rate_Law_for_R12`

Name Rate Law for R12

Arguments `vmax`, `[ATP]`, `katp`, `[AHMDHP]`, `kahmdhp`

Mathematical Expression

$$\frac{vmax \cdot [AHMDHP] \cdot [ATP]}{kahmdhp \cdot katp + katp \cdot [AHMDHP] + kahmdhp \cdot [ATP] + [AHMDHP] \cdot [ATP]} \quad (15)$$

5.16 Function definition `Rate_Law_for_R15`

Name Rate Law for R15

Arguments `vmax`, `[DHF]`, `[NADPH]`, `kdhf`, `knadph`

Mathematical Expression

$$\frac{vmax \cdot [DHF] \cdot [NADPH]}{kdhf \cdot knadph + kdhf \cdot [NADPH] + knadph \cdot [DHF] + [DHF] \cdot [NADPH]} \quad (16)$$

5.17 Function definition `Rate_Law_for_R19`

Name Rate Law for R19

Arguments `vmax`, `[myTHFGlu]`, `[NADPH]`, `knadph`, `kmythfglu`, `[DHF]`, `kidhf`

Mathematical Expression

$$\frac{vmax \cdot [myTHFGlu] \cdot [NADPH]}{kmythfglu \cdot \left(1 + \frac{[DHF]}{kidhf}\right) \cdot knadph + kmythfglu \cdot [NADPH] + knadph \cdot [myTHFGlu] + [myTHFGlu] \cdot [NADPH]} \quad (17)$$

5.18 Function definition `Rate_Law_for_R22`

Name Rate Law for R22

Arguments `vmax`, `[myTHFGlu]`, `[NADP]`, `kmythfglu`, `knadp`, `[DHF]`, `kidhf`

Mathematical Expression

$$\frac{vmax \cdot [myTHFGlu] \cdot [NADP]}{kmythfglu \cdot \left(1 + \frac{[DHF]}{kidhf}\right) \cdot knadp + kmythfglu \cdot [NADP] + knadp \cdot [myTHFGlu] + [myTHFGlu] \cdot [NADP]} \quad (18)$$

5.19 Function definition `Rate_Law_for_R25`

Name Rate Law for R25

Arguments `vmax`, `[fTHFGlu]`, `[mtRNA]`, `kfthfglu`, `kmtrna`

Mathematical Expression

$$\frac{vmax \cdot [fTHFGlu] \cdot [mtRNA]}{kfthfglu \cdot kmtrna + kfthfglu \cdot [mtRNA] + kmtrna \cdot [fTHFGlu] + [fTHFGlu] \cdot [mtRNA]} \quad (19)$$

5.20 Function definition `Rate_Law_for_R26`

Name Rate Law for R26

Arguments `vmax`, `[fTHFGlu]`, `[NADP]`, `kfthfglu`, `knadp`

Mathematical Expression

$$\frac{vmax \cdot [fTHFGlu] \cdot [NADP]}{kfthfglu \cdot knadp + kfthfglu \cdot [NADP] + knadp \cdot [fTHFGlu] + [fTHFGlu] \cdot [NADP]} \quad (20)$$

5.21 Function definition `Rate_Law_for_R13`

Name Rate Law for R13

Arguments `vmax`, `kahmdpp`, `kpaba`, `[AHMDPP]`, `[pABA]`

Mathematical Expression

$$\frac{vmax \cdot [AHMDPP] \cdot [pABA]}{kahmdpp \cdot kpaba + kpaba \cdot [AHMDPP] + kahmdpp \cdot [pABA] + [AHMDPP] \cdot [pABA]} \quad (21)$$

5.22 Function definition `Rate_Law_for_R24`

Name Rate Law for R24

Arguments `vmax`, `kthfglu`, `kformyl`, `katp`, `[THFGlu]`, `[Formyl]`, `[ATP]`

Mathematical Expression

$$\frac{vmax \cdot [THFGlu] \cdot [Formyl] \cdot [ATP]}{kthfglu \cdot kformyl \cdot katp + kthfglu \cdot ([Formyl] + [ATP]) + kformyl \cdot ([THFGlu] + [ATP]) + katp \cdot ([Formyl] + [THFGlu])} \quad (22)$$

5.23 Function definition `Rate_Law_for_R10`

Name Rate Law for R10

Arguments `vmax`, `[GTP]`, `kgtp`, `[THF]`, `kiTHF`

Mathematical Expression

$$\frac{vmax \cdot [GTP]}{kgtp \cdot \left(1 + \frac{[THF]}{kiTHF}\right) + [GTP]} \quad (23)$$

5.24 Function definition `Rate_Law_for_R29`

Name Rate Law for R29

Arguments `vmax`, `[ATP]`, `[ffTHFGlu]`, `katp`, `kffthfglu`

Mathematical Expression

$$\frac{vmax \cdot [ATP] \cdot [ffTHFGlu]}{katp \cdot kffthfglu + katp \cdot [ffTHFGlu] + kffthfglu \cdot [ATP] + [ATP] \cdot [ffTHFGlu]} \quad (24)$$

6 Reactions

This model contains 31 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 4: Overview of all reactions

Nº	Id	Name	Reaction Equation	SBO
1	R1	R1	$\text{PEP} + \text{EP} \xrightarrow{\text{PEP, EP}} \text{DAHP} + \text{Pi}$	
2	R2	R2	$\text{DAHP} \xrightarrow{\text{DAHP}} \text{DHQ} + \text{Pi}$	
3	R3	R3	$\text{DHQ} \xrightarrow{\text{DHQ}} \text{DHSK}$	
4	R4	R4	$\text{DHSK} + \text{NADPH} \xrightarrow{\text{DHSK, NADPH}} \text{SK} + \text{NADP}$	
5	R5	R5	$\text{SK} + \text{ATP} \xrightarrow{\text{SK, ATP}} \text{SKP} + \text{ADP} + \text{Pi}$	
6	R6	R6	$\text{SKP} + \text{PEP} \xrightarrow{\text{SKP, PEP}} \text{CVPSK} + \text{Pi}$	
7	R7	R7	$\text{CVPSK} \xrightarrow{\text{CVPSK}} \text{CM} + \text{Pi}$	
8	R8	R8	$\text{CM} + \text{Gln} \xrightarrow{\text{CM, Gln}} \text{ADC} + \text{Glu}$	
9	R9	R9	$\text{ADC} \xrightarrow{\text{ADC}} \text{pABA} + \text{Pyr}$	
10	R10	R10	$\text{GTP} \xrightarrow{\text{THF, GTP, THF}} \text{DHNTP} + \text{Formyl}$	
11	R11	R11	$\text{DHNTP} \xrightarrow{\text{DHNTP}} \text{AHMDHP} + \text{HAD} + \text{Pi}$	
12	R27	R27	$\text{DHNTP} \xrightarrow{\text{DHNTP}} \text{PTHP} + \text{Pi}$	
13	R12	R12	$\text{AHMDHP} + \text{ATP} \xrightarrow{\text{AHMDHP, ATP}} \text{AHMDPP} + \text{AMP}$	
14	R14	R14	$\text{DHP} + \text{Glu} + \text{ATP} \xrightarrow{\text{DHP, Glu, ATP}} \text{DHF} + \text{ADP} + \text{Pi}$	
15	R15	R15	$\text{DHF} + \text{NADPH} \xrightarrow{\text{DHF, NADPH}} \text{THF} + \text{NADP}$	

Nº	Id	Name	Reaction Equation	SBO
16	R16	R16	$\text{THF} + \text{Glu} + \text{ATP} \xrightarrow{\text{DHF, THF, Glu, ATP, DHF}} \text{THFGlu} + \text{ADP} + \text{Pi}$	
17	R17	R17	$\text{THFGlu} + \text{Ser} \xrightleftharpoons{\text{THF, THFGlu, Ser, THF}} \text{myTHFGlu} + \text{Gly}$	
18	R18b	R18b	$\text{DLp} + \text{Gly} \xrightleftharpoons{\text{DLp, Gly}} \text{SAmDLp} + \text{COTwo}$	
19	R19	R19	$\text{myTHFGlu} + \text{NADPH} \xrightarrow{\text{DHF, myTHFGlu, NADPH, DHF}} \text{MTHFGlu} + \text{NADP}$	
20	R20	R20	$\text{MTHFGlu} + \text{Hcy} \xrightarrow{\text{MTHFGlu, Hcy}} \text{THFGlu} + \text{Met}$	
21	R21	R21	$\text{myTHFGlu} + \text{dUMP} \xrightarrow{\text{DHF, myTHFGlu, dUMP, DHF}} \text{dTMP} + \text{DHF}$	
22	R22	R22	$\text{myTHFGlu} + \text{NADP} \xrightleftharpoons{\text{DHF, myTHFGlu, NADP, DHF}} \text{meTHFGlu} + \text{NADPH}$	
23	R25	R25	$\text{fTHFGlu} + \text{mtRNA} \xrightleftharpoons{\text{fTHFGlu, mtRNA}} \text{fmtRNA} + \text{THFGlu}$	
24	R26	R26	$\text{fTHFGlu} + \text{NADP} \xrightleftharpoons{\text{fTHFGlu, NADP}} \text{THFGlu} + \text{COTwo} + \text{NADPH}$	
25	R18c	R18c	$\text{THFGlu} + \text{SAmDLp} \xrightleftharpoons{\text{THFGlu, SAmDLp}} \text{myTHFGlu} + \text{Lp} + \text{Ammonia}$	
26	R18a	R18a	$\text{Lp} + \text{NADH} \xrightleftharpoons{\text{NADH, Lp}} \text{DLp} + \text{NAD}$	
27	R13	R13	$\text{AHMDPP} + \text{pABA} \xrightarrow{\text{AHMDPP, pABA}} \text{DHP} + \text{Pi}$	
28	R24	R24	$\text{fTHFGlu} + \text{ADP} + \text{Pi} \xrightleftharpoons{\text{fTHFGlu, ADP, Pi}} \text{THFGlu} + \text{ATP} + \text{Formyl}$	

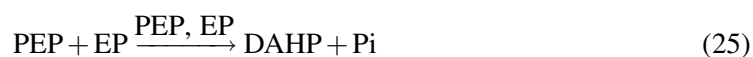
Nº	Id	Name	Reaction Equation	SBO
29	R23	R23	$\text{meTHFGlu} \xrightleftharpoons{\text{meTHFGlu, fTHFGlu}} \text{fTHFGlu}$	
30	R28	R28	$\text{meTHFGlu} \xrightarrow{\text{meTHFGlu}} \text{ffTHFGlu}$	
31	R29	R29	$\text{ATP} + \text{ffTHFGlu} \xrightarrow{\text{ATP, ffTHFGlu}} \text{ADP} + \text{Pi} + \text{meTHFGlu}$	

6.1 Reaction R1

This is an irreversible reaction of two reactants forming two products influenced by two modifiers.

Name R1

Reaction equation



Reactants

Table 5: Properties of each reactant.

Id	Name	SBO
PEP	PEP	
EP	EP	

Modifiers

Table 6: Properties of each modifier.

Id	Name	SBO
PEP	PEP	
EP	EP	

Products

Table 7: Properties of each product.

Id	Name	SBO
DAHP	DAHP	
Pi	Pi	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R1}(\text{vmax}, [\text{PEP}], [\text{EP}], \text{kpep}, \text{kep}) \quad (26)$$

$$\begin{aligned} &\text{Rate_Law_for_R1}(\text{vmax}, [\text{PEP}], [\text{EP}], \text{kpep}, \text{kep}) \\ &= \frac{\text{vmax} \cdot [\text{EP}] \cdot [\text{PEP}]}{\text{kpep} \cdot \text{kep} + \text{kpep} \cdot [\text{EP}] + \text{kep} \cdot [\text{PEP}] + [\text{EP}] \cdot [\text{PEP}]} \end{aligned} \quad (27)$$

$$\begin{aligned} &\text{Rate_Law_for_R1}(\text{vmax}, [\text{PEP}], [\text{EP}], \text{kpep}, \text{kep}) \\ &= \frac{\text{vmax} \cdot [\text{EP}] \cdot [\text{PEP}]}{\text{kpep} \cdot \text{kep} + \text{kpep} \cdot [\text{EP}] + \text{kep} \cdot [\text{PEP}] + [\text{EP}] \cdot [\text{PEP}]} \end{aligned} \quad (28)$$

Table 8: Properties of each parameter.

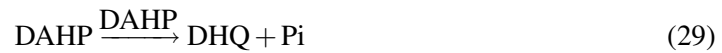
Id	Name	SBO	Value	Unit	Constant
vmax	vmax		578.76		<input checked="" type="checkbox"/>
kpep	kpep		36.00		<input checked="" type="checkbox"/>
kep	kep		285.00		<input checked="" type="checkbox"/>

6.2 Reaction R2

This is an irreversible reaction of one reactant forming two products influenced by one modifier.

Name R2

Reaction equation



Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
DAHP	DAHP	

Modifier

Table 10: Properties of each modifier.

Id	Name	SBO
DAHP	DAHP	

Products

Table 11: Properties of each product.

Id	Name	SBO
DHQ	DHQ	
Pi	Pi	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol}(\text{compartment}) \cdot \text{Henri_Michaelis_Menten_irreversible}([\text{DAHP}], \text{Km}, \text{V}) \quad (30)$$

$$\text{Henri_Michaelis_Menten_irreversible}(\text{substrate}, \text{Km}, \text{V}) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \quad (31)$$

$$\text{Henri_Michaelis_Menten_irreversible}(\text{substrate}, \text{Km}, \text{V}) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \quad (32)$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km	Km		4.700		<input checked="" type="checkbox"/>
V	V		7.462		<input checked="" type="checkbox"/>

6.3 Reaction R3

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

Name R3

Reaction equation



Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
DHQ	DHQ	

Modifier

Table 14: Properties of each modifier.

Id	Name	SBO
DHQ	DHQ	

Product

Table 15: Properties of each product.

Id	Name	SBO
DHSK	DHSK	

Kinetic Law**Derived unit** contains undeclared units

$$v_3 = \text{vol}(\text{compartment}) \cdot \text{Henri_Michaelis_Menten_irreversible}([\text{DHQ}], \text{Km}, \text{V}) \quad (34)$$

$$\text{Henri_Michaelis_Menten_irreversible}(\text{substrate}, \text{Km}, \text{V}) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \quad (35)$$

$$\text{Henri_Michaelis_Menten_irreversible}(\text{substrate}, \text{Km}, \text{V}) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \quad (36)$$

Table 16: Properties of each parameter.

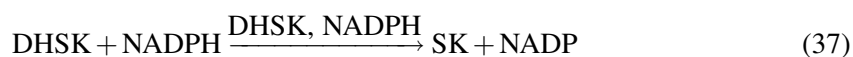
Id	Name	SBO	Value	Unit	Constant
Km	Km		58.00		<input checked="" type="checkbox"/>
V	V		116.48		<input checked="" type="checkbox"/>

6.4 Reaction R4

This is an irreversible reaction of two reactants forming two products influenced by two modifiers.

Name R4

Reaction equation



Reactants

Table 17: Properties of each reactant.

Id	Name	SBO
DHSK	DHSK	
NADPH	NADPH	

Modifiers

Table 18: Properties of each modifier.

Id	Name	SBO
DHSK	DHSK	
NADPH	NADPH	

Products

Table 19: Properties of each product.

Id	Name	SBO
SK	SK	
NADP	NADP	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R4}(v_{\max}, [\text{DHSK}], [\text{NADPH}], k_{\text{dhsk}}, k_{\text{nadph}}) \quad (38)$$

$$\begin{aligned} &\text{Rate_Law_for_R4}(v_{\max}, [\text{DHSK}], [\text{NADPH}], k_{\text{dhsK}}, k_{\text{nadph}}) \\ &= \frac{v_{\max} \cdot [\text{DHSK}] \cdot [\text{NADPH}]}{k_{\text{dhsK}} \cdot k_{\text{nadph}} + k_{\text{dhsK}} \cdot [\text{NADPH}] + k_{\text{nadph}} \cdot [\text{DHSK}] + [\text{DHSK}] \cdot [\text{NADPH}]} \end{aligned} \quad (39)$$

$$\begin{aligned} &\text{Rate_Law_for_R4}(v_{\max}, [\text{DHSK}], [\text{NADPH}], k_{\text{dhsK}}, k_{\text{nadph}}) \\ &= \frac{v_{\max} \cdot [\text{DHSK}] \cdot [\text{NADPH}]}{k_{\text{dhsK}} \cdot k_{\text{nadph}} + k_{\text{dhsK}} \cdot [\text{NADPH}] + k_{\text{nadph}} \cdot [\text{DHSK}] + [\text{DHSK}] \cdot [\text{NADPH}]} \end{aligned} \quad (40)$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vmax	vmax		17290.0		<input checked="" type="checkbox"/>
kdhsk	kdhsk		30.0		<input checked="" type="checkbox"/>
knadph	knadph		11.0		<input checked="" type="checkbox"/>

6.5 Reaction R5

This is an irreversible reaction of two reactants forming three products influenced by two modifiers.

Name R5

Reaction equation



Reactants

Table 21: Properties of each reactant.

Id	Name	SBO
SK	SK	
ATP	ATP	

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
SK	SK	
ATP	ATP	

Products

Table 23: Properties of each product.

Id	Name	SBO
SKP	SKP	
ADP	ADP	
Pi	Pi	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R5}(v_{\max}, [\text{SK}], [\text{ATP}], k_{\text{sk}}, k_{\text{atp}}) \quad (42)$$

$$\begin{aligned} & \text{Rate_Law_for_R5}(v_{\max}, [\text{SK}], [\text{ATP}], k_{\text{sk}}, k_{\text{atp}}) \\ &= \frac{v_{\max} \cdot [\text{SK}] \cdot [\text{ATP}]}{k_{\text{sk}} \cdot k_{\text{atp}} + k_{\text{sk}} \cdot [\text{ATP}] + k_{\text{atp}} \cdot [\text{SK}] + [\text{SK}] \cdot [\text{ATP}]} \end{aligned} \quad (43)$$

$$\begin{aligned} & \text{Rate_Law_for_R5}(v_{\max}, [\text{SK}], [\text{ATP}], k_{\text{sk}}, k_{\text{atp}}) \\ &= \frac{v_{\max} \cdot [\text{SK}] \cdot [\text{ATP}]}{k_{\text{sk}} \cdot k_{\text{atp}} + k_{\text{sk}} \cdot [\text{ATP}] + k_{\text{atp}} \cdot [\text{SK}] + [\text{SK}] \cdot [\text{ATP}]} \end{aligned} \quad (44)$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vmax	vmax		18200.0		✓
ksk	ksk		200.0		✓
katp	katp		151.5		✓

6.6 Reaction R6

This is an irreversible reaction of two reactants forming two products influenced by two modifiers.

Name R6

Reaction equation



Reactants

Table 25: Properties of each reactant.

Id	Name	SBO
SKP	SKP	
PEP	PEP	

Modifiers

Table 26: Properties of each modifier.

Id	Name	SBO
SKP	SKP	
PEP	PEP	

Products

Table 27: Properties of each product.

Id	Name	SBO
CVPSK	CVPSK	
Pi	Pi	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R6}([\text{SKP}], v_{\text{max}}, [\text{PEP}], k_{\text{pep}}, k_{\text{skp}}) \quad (46)$$

$$\begin{aligned} &\text{Rate_Law_for_R6}([PEP], v_{\max}, [SKP], k_{\text{pep}}, k_{\text{skp}}) \\ &= \frac{v_{\max} \cdot [PEP] \cdot [SKP]}{k_{\text{pep}} \cdot k_{\text{skp}} + k_{\text{pep}} \cdot [SKP] + k_{\text{skp}} \cdot [PEP] + [SKP] \cdot [PEP]} \end{aligned} \quad (47)$$

$$\begin{aligned} &\text{Rate_Law_for_R6}([PEP], v_{\max}, [SKP], k_{\text{pep}}, k_{\text{skp}}) \\ &= \frac{v_{\max} \cdot [PEP] \cdot [SKP]}{k_{\text{pep}} \cdot k_{\text{skp}} + k_{\text{pep}} \cdot [SKP] + k_{\text{skp}} \cdot [PEP] + [SKP] \cdot [PEP]} \end{aligned} \quad (48)$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vmax	vmax		1547.0		<input checked="" type="checkbox"/>
kpep	kpep		93.0		<input checked="" type="checkbox"/>
kskp	kskp		80.0		<input checked="" type="checkbox"/>

6.7 Reaction R7

This is an irreversible reaction of one reactant forming two products influenced by one modifier.

Name R7

Reaction equation



Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
CVPSK	CVPSK	

Modifier

Table 30: Properties of each modifier.

Id	Name	SBO
CVPSK	CVPSK	

Products

Table 31: Properties of each product.

Id	Name	SBO
CM	CM	
Pi	Pi	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{vol}(\text{compartment}) \cdot \text{Henri_Michaelis_Menten_irreversible}([\text{CVPSK}], \text{Km}, \text{V}) \quad (50)$$

$$\text{Henri_Michaelis_Menten_irreversible}(\text{substrate}, \text{Km}, \text{V}) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \quad (51)$$

$$\text{Henri_Michaelis_Menten_irreversible}(\text{substrate}, \text{Km}, \text{V}) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \quad (52)$$

Table 32: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km	Km		12.7		<input checked="" type="checkbox"/>
V	V		728.0		<input checked="" type="checkbox"/>

6.8 Reaction R8

This is an irreversible reaction of two reactants forming two products influenced by two modifiers.

Name R8

Reaction equation



Reactants

Table 33: Properties of each reactant.

Id	Name	SBO
CM	CM	
Gln	Gln	

Modifiers

Table 34: Properties of each modifier.

Id	Name	SBO
CM	CM	
Gln	Gln	

Products

Table 35: Properties of each product.

Id	Name	SBO
ADC	ADC	
Glu	Glu	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R8}(v_{\max}, [\text{CM}], [\text{Gln}], k_{\text{cm}}, k_{\text{gln}}) \quad (54)$$

$$\begin{aligned} & \text{Rate_Law_for_R8}(v_{\max}, [\text{CM}], [\text{Gln}], k_{\text{cm}}, k_{\text{gln}}) \\ &= \frac{v_{\max} \cdot [\text{CM}] \cdot [\text{Gln}]}{k_{\text{cm}} \cdot k_{\text{gln}} + k_{\text{cm}} \cdot [\text{Gln}] + k_{\text{gln}} \cdot [\text{CM}] + [\text{CM}] \cdot [\text{Gln}]} \end{aligned} \quad (55)$$

$$\begin{aligned} & \text{Rate_Law_for_R8}(v_{\max}, [\text{CM}], [\text{Gln}], k_{\text{cm}}, k_{\text{gln}}) \\ &= \frac{v_{\max} \cdot [\text{CM}] \cdot [\text{Gln}]}{k_{\text{cm}} \cdot k_{\text{gln}} + k_{\text{cm}} \cdot [\text{Gln}] + k_{\text{gln}} \cdot [\text{CM}] + [\text{CM}] \cdot [\text{Gln}]} \end{aligned} \quad (56)$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vmax	vmax		26.0		<input checked="" type="checkbox"/>
kcm	kcm		13.0		<input checked="" type="checkbox"/>
kgln	kgln		1100.0		<input checked="" type="checkbox"/>

6.9 Reaction R9

This is an irreversible reaction of one reactant forming two products influenced by one modifier.

Name R9

Reaction equation



Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
ADC	ADC	

Modifier

Table 38: Properties of each modifier.

Id	Name	SBO
ADC	ADC	

Products

Table 39: Properties of each product.

Id	Name	SBO
pABA	pABA	
Pyr	Pyr	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{vol}(\text{compartment}) \cdot \text{Henri_Michaelis_Menten_irreversible}([\text{ADC}], \text{Km}, \text{V}) \quad (58)$$

$$\text{Henri_Michaelis_Menten_irreversible}(\text{substrate}, \text{Km}, \text{V}) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \quad (59)$$

$$\text{Henri_Michaelis_Menten_irreversible}(\text{substrate}, \text{Km}, \text{V}) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \quad (60)$$

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km	Km		1.1		<input checked="" type="checkbox"/>
V	V		2.2		<input checked="" type="checkbox"/>

6.10 Reaction R10

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

Name R10

Reaction equation



Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
GTP	GTP	

Modifiers

Table 42: Properties of each modifier.

Id	Name	SBO
THF	THF	
GTP	GTP	
THF	THF	

Products

Table 43: Properties of each product.

Id	Name	SBO
DHNTp	DHNTp	
Formyl	Formyl	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R10}(v_{\max}, [\text{GTP}], k_{\text{gtp}}, [\text{THF}], k_{\text{iTHF}}) \quad (62)$$

$$\text{Rate_Law_for_R10}(v_{\max}, [\text{GTP}], k_{\text{gtp}}, [\text{THF}], k_{\text{iTHF}}) = \frac{v_{\max} \cdot [\text{GTP}]}{k_{\text{gtp}} \cdot \left(1 + \frac{[\text{THF}]}{k_{\text{iTHF}}}\right) + [\text{GTP}]} \quad (63)$$

$$\text{Rate_Law_for_R10}(v_{\max}, [\text{GTP}], k_{\text{gtp}}, [\text{THF}], k_{\text{iTHF}}) = \frac{v_{\max} \cdot [\text{GTP}]}{k_{\text{gtp}} \cdot \left(1 + \frac{[\text{THF}]}{k_{\text{iTHF}}}\right) + [\text{GTP}]} \quad (64)$$

Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vmax	vmax		1515.150		✓
kgtp	kgtp		17.600		✓
kiTHF	kiTHF		0.157		✓

6.11 Reaction R11

This is an irreversible reaction of one reactant forming three products influenced by one modifier.

Name R11

Reaction equation



Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
DHNTP	DHNTP	

Modifier

Table 46: Properties of each modifier.

Id	Name	SBO
DHNTP	DHNTP	

Products

Table 47: Properties of each product.

Id	Name	SBO
AHMDHP	AHMDHP	
HAD	HAD	
Pi	Pi	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \text{vol}(\text{compartment}) \cdot \text{Henri_Michaelis_Menten_irreversible}([\text{DHNTTP}], \text{Km}, \text{V}) \quad (66)$$

$$\text{Henri_Michaelis_Menten_irreversible}(\text{substrate}, \text{Km}, \text{V}) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \quad (67)$$

$$\text{Henri_Michaelis_Menten_irreversible}(\text{substrate}, \text{Km}, \text{V}) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \quad (68)$$

Table 48: Properties of each parameter.

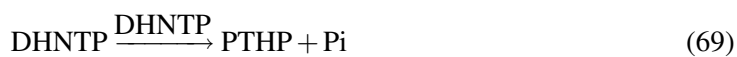
Id	Name	SBO	Value	Unit	Constant
Km	Km		7.400		<input checked="" type="checkbox"/>
V	V		792.064		<input checked="" type="checkbox"/>

6.12 Reaction R27

This is an irreversible reaction of one reactant forming two products influenced by one modifier.

Name R27

Reaction equation



Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
DHNTP	DHNTP	

Modifier

Table 50: Properties of each modifier.

Id	Name	SBO
DHNTP	DHNTP	

Products

Table 51: Properties of each product.

Id	Name	SBO
PTHP	PTHP	
Pi	Pi	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \text{vol}(\text{compartment}) \cdot \text{Henri_Michaelis_Menten_irreversible}([\text{DHNTP}], \text{Km}, \text{V}) \quad (70)$$

$$\text{Henri_Michaelis_Menten_irreversible}(\text{substrate}, \text{Km}, \text{V}) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \quad (71)$$

$$\text{Henri_Michaelis_Menten_irreversible}(\text{substrate}, \text{Km}, \text{V}) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \quad (72)$$

Table 52: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km	Km		10.000		<input checked="" type="checkbox"/>
V	V		22.659		<input checked="" type="checkbox"/>

6.13 Reaction R12

This is an irreversible reaction of two reactants forming two products influenced by two modifiers.

Name R12

Reaction equation



Reactants

Table 53: Properties of each reactant.

Id	Name	SBO
AHMDHP	AHMDHP	
ATP	ATP	

Modifiers

Table 54: Properties of each modifier.

Id	Name	SBO
AHMDHP	AHMDHP	
ATP	ATP	

Products

Table 55: Properties of each product.

Id	Name	SBO
AHMDPP	AHMDPP	
AMP	AMP	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R12}(v_{\max}, [\text{AHMDHP}], \text{katp}, [\text{ATP}], \text{kahmdhp}) \quad (74)$$

$$\begin{aligned} & \text{Rate_Law_for_R12}(v_{\max}, [\text{ATP}], \text{katp}, [\text{AHMDHP}], \text{kahmdhp}) \\ &= \frac{v_{\max} \cdot [\text{AHMDHP}] \cdot [\text{ATP}]}{\text{kahmdhp} \cdot \text{katp} + \text{katp} \cdot [\text{AHMDHP}] + \text{kahmdhp} \cdot [\text{ATP}] + [\text{AHMDHP}] \cdot [\text{ATP}]} \end{aligned} \quad (75)$$

$$\begin{aligned} & \text{Rate_Law_for_R12}(v_{\max}, [\text{ATP}], \text{katp}, [\text{AHMDHP}], \text{kahmdhp}) \\ &= \frac{v_{\max} \cdot [\text{AHMDHP}] \cdot [\text{ATP}]}{\text{kahmdhp} \cdot \text{katp} + \text{katp} \cdot [\text{AHMDHP}] + \text{kahmdhp} \cdot [\text{ATP}] + [\text{AHMDHP}] \cdot [\text{ATP}]} \end{aligned} \quad (76)$$

Table 56: Properties of each parameter.

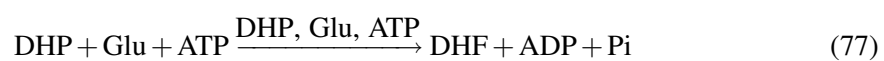
Id	Name	SBO	Value	Unit	Constant
vmax	vmax		382.2		<input checked="" type="checkbox"/>
katp	katp		15.0		<input checked="" type="checkbox"/>
kahmdhp	kahmdhp		3.6		<input checked="" type="checkbox"/>

6.14 Reaction R14

This is an irreversible reaction of three reactants forming three products influenced by three modifiers.

Name R14

Reaction equation



Reactants

Table 57: Properties of each reactant.

Id	Name	SBO
DHP	DHP	
Glu	Glu	
ATP	ATP	

Modifiers

Table 58: Properties of each modifier.

Id	Name	SBO
DHP	DHP	
Glu	Glu	
ATP	ATP	

Products

Table 59: Properties of each product.

Id	Name	SBO
DHF	DHF	
ADP	ADP	
Pi	Pi	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R14}(v_{\max}, [\text{DHP}], [\text{Glu}], k_{\text{dhp}}, k_{\text{glu}}, [\text{ATP}], k_{\text{atp}}) \quad (78)$$

$$\text{Rate_Law_for_R14}(v_{\max}, [\text{DHP}], [\text{Glu}], k_{\text{dhp}}, k_{\text{glu}}, [\text{ATP}], k_{\text{atp}}) \quad (79)$$

$$= \frac{v_{\max} \cdot [\text{DHP}] \cdot [\text{Glu}] \cdot [\text{ATP}]}{k_{\text{dhp}} \cdot k_{\text{glu}} \cdot k_{\text{atp}} + k_{\text{dhp}} \cdot ([\text{Glu}] + [\text{ATP}]) + k_{\text{glu}} \cdot ([\text{DHP}] + [\text{ATP}]) + k_{\text{atp}} \cdot ([\text{Glu}] + [\text{ATP}]) + [\text{DHP}] \cdot [\text{Glu}] \cdot [\text{ATP}]}$$

$$\text{Rate_Law_for_R14}(v_{\max}, [\text{DHP}], [\text{Glu}], k_{\text{dhp}}, k_{\text{glu}}, [\text{ATP}], k_{\text{atp}}) \quad (80)$$

$$= \frac{v_{\max} \cdot [\text{DHP}] \cdot [\text{Glu}] \cdot [\text{ATP}]}{k_{\text{dhp}} \cdot k_{\text{glu}} \cdot k_{\text{atp}} + k_{\text{dhp}} \cdot ([\text{Glu}] + [\text{ATP}]) + k_{\text{glu}} \cdot ([\text{DHP}] + [\text{ATP}]) + k_{\text{atp}} \cdot ([\text{Glu}] + [\text{ATP}]) + [\text{DHP}] \cdot [\text{Glu}] \cdot [\text{ATP}]}$$

Table 60: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vmax	vmax		2.821		<input checked="" type="checkbox"/>
kdhp	kdhp		1.000		<input checked="" type="checkbox"/>
kglu	kglu		1380.000		<input checked="" type="checkbox"/>
katp	katp		100.000		<input checked="" type="checkbox"/>

6.15 Reaction R15

This is an irreversible reaction of two reactants forming two products influenced by two modifiers.

Name R15

Reaction equation



Reactants

Table 61: Properties of each reactant.

Id	Name	SBO
DHF	DHF	
NADPH	NADPH	

Modifiers

Table 62: Properties of each modifier.

Id	Name	SBO
DHF	DHF	
NADPH	NADPH	

Products

Table 63: Properties of each product.

Id	Name	SBO
THF	THF	

Id	Name	SBO
NADP	NADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R15}(v_{\max}, [\text{DHF}], [\text{NADPH}], k_{\text{dhf}}, k_{\text{nadph}}) \quad (82)$$

$$\begin{aligned} & \text{Rate_Law_for_R15}(v_{\max}, [\text{DHF}], [\text{NADPH}], k_{\text{dhf}}, k_{\text{nadph}}) \\ &= \frac{v_{\max} \cdot [\text{DHF}] \cdot [\text{NADPH}]}{k_{\text{dhf}} \cdot k_{\text{nadph}} + k_{\text{dhf}} \cdot [\text{NADPH}] + k_{\text{nadph}} \cdot [\text{DHF}] + [\text{DHF}] \cdot [\text{NADPH}]} \end{aligned} \quad (83)$$

$$\begin{aligned} & \text{Rate_Law_for_R15}(v_{\max}, [\text{DHF}], [\text{NADPH}], k_{\text{dhf}}, k_{\text{nadph}}) \\ &= \frac{v_{\max} \cdot [\text{DHF}] \cdot [\text{NADPH}]}{k_{\text{dhf}} \cdot k_{\text{nadph}} + k_{\text{dhf}} \cdot [\text{NADPH}] + k_{\text{nadph}} \cdot [\text{DHF}] + [\text{DHF}] \cdot [\text{NADPH}]} \end{aligned} \quad (84)$$

Table 64: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vmax	vmax		3000.00		✓
kdhf	kdhf		3.00		✓
knadph	knadph		6.12		✓

6.16 Reaction R16

This is an irreversible reaction of three reactants forming three products influenced by five modifiers.

Name R16

Reaction equation



Reactants

Table 65: Properties of each reactant.

Id	Name	SBO
THF	THF	
Glu	Glu	
ATP	ATP	

Modifiers

Table 66: Properties of each modifier.

Id	Name	SBO
DHF	DHF	
THF	THF	
Glu	Glu	
ATP	ATP	
DHF	DHF	

Products

Table 67: Properties of each product.

Id	Name	SBO
THFGlu	THFGlu	
ADP	ADP	
Pi	Pi	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R16}(v_{\max}, [\text{THF}], [\text{Glu}], k_{\text{thf}}, k_{\text{glu}}, [\text{ATP}], k_{\text{atp}}, [\text{DHF}], k_{\text{idhf}}) \quad (86)$$

$$\text{Rate_Law_for_R16}(v_{\max}, [\text{THF}], [\text{Glu}], k_{\text{thf}}, k_{\text{glu}}, [\text{ATP}], k_{\text{atp}}, [\text{DHF}], k_{\text{idhf}}) = \frac{v_{\max} \cdot [\text{THF}] \cdot [\text{Glu}] \cdot [\text{ATP}]}{k_{\text{thf}} \cdot \left(1 + \frac{[\text{DHF}]}{k_{\text{idhf}}}\right) \cdot k_{\text{glu}} \cdot k_{\text{atp}} + k_{\text{thf}} \cdot ([\text{Glu}] + [\text{ATP}]) + k_{\text{glu}} \cdot ([\text{THF}] + [\text{ATP}]) + k_{\text{atp}} \cdot ([\text{THF}] + [\text{Glu}]) + [\text{THF}] \cdot [\text{Glu}] \cdot [\text{ATP}]} \quad (87)$$

$$\text{Rate_Law_for_R16}(v_{\max}, [\text{THF}], [\text{Glu}], k_{\text{thf}}, k_{\text{glu}}, [\text{ATP}], k_{\text{atp}}, [\text{DHF}], k_{\text{idhf}}) = \frac{v_{\max} \cdot [\text{THF}] \cdot [\text{Glu}] \cdot [\text{ATP}]}{k_{\text{thf}} \cdot \left(1 + \frac{[\text{DHF}]}{k_{\text{idhf}}}\right) \cdot k_{\text{glu}} \cdot k_{\text{atp}} + k_{\text{thf}} \cdot ([\text{Glu}] + [\text{ATP}]) + k_{\text{glu}} \cdot ([\text{THF}] + [\text{ATP}]) + k_{\text{atp}} \cdot ([\text{THF}] + [\text{Glu}]) + [\text{THF}] \cdot [\text{Glu}] \cdot [\text{ATP}]} \quad (88)$$

Table 68: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vmax	vmax		84.63		<input checked="" type="checkbox"/>
kthf	kthf		26.00		<input checked="" type="checkbox"/>
kglu	kglu		740.00		<input checked="" type="checkbox"/>
katp	katp		128.00		<input checked="" type="checkbox"/>
kidhf	kidhf		3.10		<input checked="" type="checkbox"/>

6.17 Reaction R17

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

Name R17

Reaction equation



Reactants

Table 69: Properties of each reactant.

Id	Name	SBO
THFGlu	THFGlu	
Ser	Ser	

Modifiers

Table 70: Properties of each modifier.

Id	Name	SBO
THF	THF	
THFGlu	THFGlu	
Ser	Ser	
THF	THF	

Products

Table 71: Properties of each product.

Id	Name	SBO
myTHFGlu	myTHFGlu	
Gly	Gly	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R17}(v_{\max}, [\text{THFGlu}], [\text{Ser}], k_{\text{thfglu}}, k_{\text{ser}}, [\text{THF}], k_{\text{ithf}}) \quad (90)$$

$$\begin{aligned} & \text{Rate_Law_for_R17}(v_{\max}, [\text{THFGlu}], [\text{Ser}], k_{\text{thfglu}}, k_{\text{ser}}, [\text{THF}], k_{\text{ithf}}) \\ &= \frac{v_{\max} \cdot [\text{THFGlu}] \cdot [\text{Ser}]}{k_{\text{thfglu}} \cdot \left(1 + \frac{[\text{THF}]}{k_{\text{ithf}}}\right) \cdot k_{\text{ser}} + k_{\text{thfglu}} \cdot [\text{Ser}] + k_{\text{ser}} \cdot [\text{THFGlu}] + [\text{THFGlu}] \cdot [\text{Ser}]} \end{aligned} \quad (91)$$

$$\begin{aligned} & \text{Rate_Law_for_R17}(v_{\max}, [\text{THFGlu}], [\text{Ser}], k_{\text{thfglu}}, k_{\text{ser}}, [\text{THF}], k_{\text{ithf}}) \\ &= \frac{v_{\max} \cdot [\text{THFGlu}] \cdot [\text{Ser}]}{k_{\text{thfglu}} \cdot \left(1 + \frac{[\text{THF}]}{k_{\text{ithf}}}\right) \cdot k_{\text{ser}} + k_{\text{thfglu}} \cdot [\text{Ser}] + k_{\text{ser}} \cdot [\text{THFGlu}] + [\text{THFGlu}] \cdot [\text{Ser}]} \end{aligned} \quad (92)$$

Table 72: Properties of each parameter.

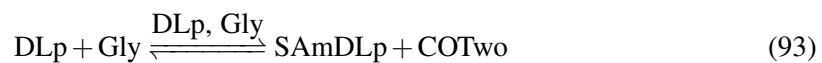
Id	Name	SBO	Value	Unit	Constant
vmax	vmax		682.500		✓
kthfglu	kthfglu		40.000		✓
kser	kser		700.000		✓
kithf	kithf		0.157		✓

6.18 Reaction R18b

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

Name R18b

Reaction equation



Reactants

Table 73: Properties of each reactant.

Id	Name	SBO
DLp	DLp	
Gly	Gly	

Modifiers

Table 74: Properties of each modifier.

Id	Name	SBO
DLp	DLp	
Gly	Gly	

Products

Table 75: Properties of each product.

Id	Name	SBO
SAmDLp	SAmDLp	
COTwo	COTwo	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R18b}(v_{\max}, [\text{DLp}], [\text{Gly}], \text{kgly}, \text{kdlp}) \quad (94)$$

$$\begin{aligned} & \text{Rate_Law_for_R18b}(v_{\max}, [\text{Gly}], [\text{DLp}], \text{kgly}, \text{kdlp}) \\ &= \frac{v_{\max} \cdot [\text{Gly}] \cdot [\text{DLp}]}{\text{kgly} \cdot \text{kdlp} + \text{kgly} \cdot [\text{DLp}] + \text{kdlp} \cdot [\text{Gly}] + [\text{Gly}] \cdot [\text{DLp}]} \end{aligned} \quad (95)$$

$$\begin{aligned} & \text{Rate_Law_for_R18b}(v_{\max}, [\text{Gly}], [\text{DLp}], \text{kgly}, \text{kdlp}) \\ &= \frac{v_{\max} \cdot [\text{Gly}] \cdot [\text{DLp}]}{\text{kgly} \cdot \text{kdlp} + \text{kgly} \cdot [\text{DLp}] + \text{kdlp} \cdot [\text{Gly}] + [\text{Gly}] \cdot [\text{DLp}]} \end{aligned} \quad (96)$$

Table 76: Properties of each parameter.

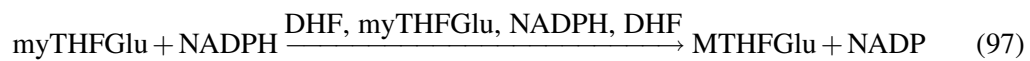
Id	Name	SBO	Value	Unit	Constant
vmax	vmax		751.66		<input checked="" type="checkbox"/>
kgly	kgly		4505.00		<input checked="" type="checkbox"/>
kdlp	kdlp		290.00		<input checked="" type="checkbox"/>

6.19 Reaction R19

This is an irreversible reaction of two reactants forming two products influenced by four modifiers.

Name R19

Reaction equation



Reactants

Table 77: Properties of each reactant.

Id	Name	SBO
myTHFGlu	myTHFGlu	
NADPH	NADPH	

Modifiers

Table 78: Properties of each modifier.

Id	Name	SBO
DHF	DHF	
myTHFGlu	myTHFGlu	
NADPH	NADPH	
DHF	DHF	

Products

Table 79: Properties of each product.

Id	Name	SBO
MTHFGlu	MTHFGlu	
NADP	NADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R19}(v_{\max}, [\text{myTHFGlu}], [\text{NADPH}], \text{knadph}, \text{kmythfglu}, [\text{DHF}], \text{kidhf}) \quad (98)$$

$$\begin{aligned} & \text{Rate_Law_for_R19}(v_{\max}, [\text{myTHFGlu}], [\text{NADPH}], \text{knadph}, \text{kmythfglu}, [\text{DHF}], \text{kidhf}) \quad (99) \\ &= \frac{v_{\max} \cdot [\text{myTHFGlu}] \cdot [\text{NADPH}]}{\text{kmythfglu} \cdot \left(1 + \frac{[\text{DHF}]}{\text{kidhf}}\right) \cdot \text{knadph} + \text{kmythfglu} \cdot [\text{NADPH}] + \text{knadph} \cdot [\text{myTHFGlu}] + [\text{myTHFGlu}] \cdot [\text{NADPH}]} \end{aligned}$$

$$\begin{aligned} & \text{Rate_Law_for_R19}(v_{\max}, [\text{myTHFGlu}], [\text{NADPH}], \text{knadph}, \text{kmythfglu}, [\text{DHF}], \text{kidhf}) \quad (100) \\ &= \frac{v_{\max} \cdot [\text{myTHFGlu}] \cdot [\text{NADPH}]}{\text{kmythfglu} \cdot \left(1 + \frac{[\text{DHF}]}{\text{kidhf}}\right) \cdot \text{knadph} + \text{kmythfglu} \cdot [\text{NADPH}] + \text{knadph} \cdot [\text{myTHFGlu}] + [\text{myTHFGlu}] \cdot [\text{NADPH}]} \end{aligned}$$

Table 80: Properties of each parameter.

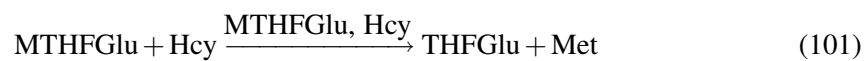
Id	Name	SBO	Value	Unit	Constant
vmax	vmax		738.920		✓
knadph	knadph		19.000		✓
kmythfglu	kmythfglu		33.000		✓
kidhf	kidhf		0.428		✓

6.20 Reaction R20

This is an irreversible reaction of two reactants forming two products influenced by two modifiers.

Name R20

Reaction equation



Reactants

Table 81: Properties of each reactant.

Id	Name	SBO
MTHFGlu	MTHFGlu	
Hcy	Hcy	

Modifiers

Table 82: Properties of each modifier.

Id	Name	SBO
MTHFGlu	MTHFGlu	
Hcy	Hcy	

Products

Table 83: Properties of each product.

Id	Name	SBO
THFGlu	THFGlu	
Met	Met	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R20}(v_{\max}, [\text{MTHFGlu}], [\text{Hcy}], \text{kmthfglu}, \text{khcy}) \quad (102)$$

$$\begin{aligned} & \text{Rate_Law_for_R20}(v_{\max}, [\text{MTHFGlu}], [\text{Hcy}], \text{kmthfglu}, \text{khcy}) \\ &= \frac{v_{\max} \cdot [\text{MTHFGlu}] \cdot [\text{Hcy}]}{\text{kmthfglu} \cdot \text{khcy} + \text{kmthfglu} \cdot [\text{Hcy}] + \text{khcy} \cdot [\text{MTHFGlu}] + [\text{MTHFGlu}] \cdot [\text{Hcy}]} \end{aligned} \quad (103)$$

$$\begin{aligned} & \text{Rate_Law_for_R20}(v_{\max}, [\text{MTHFGlu}], [\text{Hcy}], \text{kmthfglu}, \text{khcy}) \\ &= \frac{v_{\max} \cdot [\text{MTHFGlu}] \cdot [\text{Hcy}]}{\text{kmthfglu} \cdot \text{khcy} + \text{kmthfglu} \cdot [\text{Hcy}] + \text{khcy} \cdot [\text{MTHFGlu}] + [\text{MTHFGlu}] \cdot [\text{Hcy}]} \end{aligned} \quad (104)$$

Table 84: Properties of each parameter.

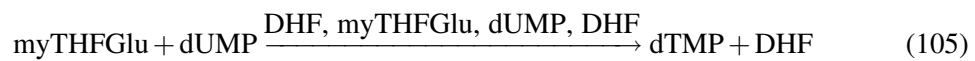
Id	Name	SBO	Value	Unit	Constant
vmax	vmax		379.925		<input checked="" type="checkbox"/>
kmthfglu	kmthfglu		30.000		<input checked="" type="checkbox"/>
khcy	khcy		17.000		<input checked="" type="checkbox"/>

6.21 Reaction R21

This is an irreversible reaction of two reactants forming two products influenced by four modifiers.

Name R21

Reaction equation



Reactants

Table 85: Properties of each reactant.

Id	Name	SBO
myTHFGlu	myTHFGlu	
dUMP	dUMP	

Modifiers

Table 86: Properties of each modifier.

Id	Name	SBO
DHF	DHF	
myTHFGlu	myTHFGlu	
dUMP	dUMP	
DHF	DHF	

Products

Table 87: Properties of each product.

Id	Name	SBO
dTMP	dTMP	
DHF	DHF	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R21} (v_{\max}, [\text{myTHFGlu}], [\text{dUMP}], k_{\text{dump}}, k_{\text{mythfglu}}, [\text{DHF}], k_{\text{dhf}}) \quad (106)$$

$$\begin{aligned} & \text{Rate_Law_for_R21} (v_{\max}, [\text{myTHFGlu}], [\text{dUMP}], k_{\text{dump}}, k_{\text{mythfglu}}, [\text{DHF}], k_{\text{dhf}}) \quad (107) \\ &= \frac{v_{\max} \cdot [\text{myTHFGlu}] \cdot [\text{dUMP}]}{k_{\text{mythfglu}} \cdot \left(1 + \frac{[\text{DHF}]}{k_{\text{dhf}}}\right) \cdot k_{\text{dump}} + k_{\text{mythfglu}} \cdot [\text{dUMP}] + k_{\text{dump}} \cdot [\text{myTHFGlu}] + [\text{myTHFGlu}] \cdot [\text{dUMP}]} \end{aligned}$$

$$\begin{aligned} & \text{Rate_Law_for_R21} (v_{\max}, [\text{myTHFGlu}], [\text{dUMP}], k_{\text{dump}}, k_{\text{mythfglu}}, [\text{DHF}], k_{\text{dhf}}) \quad (108) \\ &= \frac{v_{\max} \cdot [\text{myTHFGlu}] \cdot [\text{dUMP}]}{k_{\text{mythfglu}} \cdot \left(1 + \frac{[\text{DHF}]}{k_{\text{dhf}}}\right) \cdot k_{\text{dump}} + k_{\text{mythfglu}} \cdot [\text{dUMP}] + k_{\text{dump}} \cdot [\text{myTHFGlu}] + [\text{myTHFGlu}] \cdot [\text{dUMP}]} \end{aligned}$$

Table 88: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vmax	vmax		49.140		✓
kdump	kdump		5.400		✓
kmythfglu	kmythfglu		17.000		✓
kidhf	kidhf		0.428		✓

6.22 Reaction R22

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

Name R22

Reaction equation



Reactants

Table 89: Properties of each reactant.

Id	Name	SBO
myTHFGlu	myTHFGlu	
NADP	NADP	

Modifiers

Table 90: Properties of each modifier.

Id	Name	SBO
DHF	DHF	
myTHFGlu	myTHFGlu	
NADP	NADP	
DHF	DHF	

Products

Table 91: Properties of each product.

Id	Name	SBO
meTHFGlu	meTHFGlu	
NADPH	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R22}(v_{\max}, [\text{myTHFGlu}], [\text{NADP}], k_{\text{mythfglu}}, \text{knadp}, [\text{DHF}], k_{\text{idhf}}) \quad (110)$$

$$\text{Rate_Law_for_R22}(v_{\max}, [\text{myTHFGlu}], [\text{NADP}], k_{\text{mythfglu}}, \text{knadp}, [\text{DHF}], k_{\text{idhf}}) \quad (111)$$

$$= \frac{v_{\max} \cdot [\text{myTHFGlu}] \cdot [\text{NADP}]}{k_{\text{mythfglu}} \cdot \left(1 + \frac{[\text{DHF}]}{k_{\text{idhf}}}\right) \cdot \text{knadp} + k_{\text{mythfglu}} \cdot [\text{NADP}] + \text{knadp} \cdot [\text{myTHFGlu}] + [\text{myTHFGlu}] \cdot [\text{NADP}]}$$

$$\text{Rate_Law_for_R22}(v_{\max}, [\text{myTHFGlu}], [\text{NADP}], k_{\text{mythfglu}}, \text{knadp}, [\text{DHF}], k_{\text{idhf}}) \quad (112)$$

$$= \frac{v_{\max} \cdot [\text{myTHFGlu}] \cdot [\text{NADP}]}{k_{\text{mythfglu}} \cdot \left(1 + \frac{[\text{DHF}]}{k_{\text{idhf}}}\right) \cdot \text{knadp} + k_{\text{mythfglu}} \cdot [\text{NADP}] + \text{knadp} \cdot [\text{myTHFGlu}] + [\text{myTHFGlu}] \cdot [\text{NADP}]}$$

Table 92: Properties of each parameter.

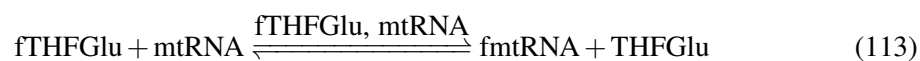
Id	Name	SBO	Value	Unit	Constant
vmax	vmax		1892.800		<input checked="" type="checkbox"/>
kmythfglu	kmythfglu		25.000		<input checked="" type="checkbox"/>
knadp	knadp		22.000		<input checked="" type="checkbox"/>
kidhf	kidhf		0.428		<input checked="" type="checkbox"/>

6.23 Reaction R25

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

Name R25

Reaction equation



Reactants

Table 93: Properties of each reactant.

Id	Name	SBO
fTHFGlu	fTHFGlu	
mtRNA	mtRNA	

Modifiers

Table 94: Properties of each modifier.

Id	Name	SBO
fTHFGlu	fTHFGlu	
mtRNA	mtRNA	

Products

Table 95: Properties of each product.

Id	Name	SBO
fmtRNA	fmtRNA	
THFGlu	THFGlu	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R25}(v_{\max}, [\text{fTHFGlu}], [\text{mtRNA}], k_{\text{fthfglu}}, k_{\text{mtrna}}) \quad (114)$$

$$\begin{aligned} & \text{Rate_Law_for_R25}(v_{\max}, [\text{fTHFGlu}], [\text{mtRNA}], k_{\text{fthfglu}}, k_{\text{mtrna}}) \\ &= \frac{v_{\max} \cdot [\text{fTHFGlu}] \cdot [\text{mtRNA}]}{k_{\text{fthfglu}} \cdot k_{\text{mtrna}} + k_{\text{fthfglu}} \cdot [\text{mtRNA}] + k_{\text{mtrna}} \cdot [\text{fTHFGlu}] + [\text{fTHFGlu}] \cdot [\text{mtRNA}]} \end{aligned} \quad (115)$$

$$\begin{aligned} & \text{Rate_Law_for_R25}(v_{\max}, [\text{fTHFGlu}], [\text{mtRNA}], k_{\text{fthfglu}}, k_{\text{mtrna}}) \\ &= \frac{v_{\max} \cdot [\text{fTHFGlu}] \cdot [\text{mtRNA}]}{k_{\text{fthfglu}} \cdot k_{\text{mtrna}} + k_{\text{fthfglu}} \cdot [\text{mtRNA}] + k_{\text{mtrna}} \cdot [\text{fTHFGlu}] + [\text{fTHFGlu}] \cdot [\text{mtRNA}]} \end{aligned} \quad (116)$$

Table 96: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vmax	vmax		116.48		✓
kfthfglu	kfthfglu		12.15		✓
kmtrna	kmtrna		1.07		✓

6.24 Reaction R26

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

Name R26

Reaction equation



Reactants

Table 97: Properties of each reactant.

Id	Name	SBO
fTHFGlu	fTHFGlu	
NADP	NADP	

Modifiers

Table 98: Properties of each modifier.

Id	Name	SBO
fTHFGlu	fTHFGlu	
NADP	NADP	

Products

Table 99: Properties of each product.

Id	Name	SBO
THFGlu	THFGlu	
COTwo	COTwo	
NADPH	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R26}(v_{\max}, [\text{fTHFGlu}], [\text{NADP}], k_{\text{fthfglu}}, k_{\text{nadp}}) \quad (118)$$

$$\begin{aligned} & \text{Rate_Law_for_R26}(v_{\max}, [\text{fTHFGlu}], [\text{NADP}], k_{\text{fthfglu}}, k_{\text{nadp}}) \\ &= \frac{v_{\max} \cdot [\text{fTHFGlu}] \cdot [\text{NADP}]}{k_{\text{fthfglu}} \cdot k_{\text{nadp}} + k_{\text{fthfglu}} \cdot [\text{NADP}] + k_{\text{nadp}} \cdot [\text{fTHFGlu}] + [\text{fTHFGlu}] \cdot [\text{NADP}]} \end{aligned} \quad (119)$$

$$\begin{aligned} & \text{Rate_Law_for_R26}(v_{\max}, [\text{fTHFGlu}], [\text{NADP}], k_{\text{fthfglu}}, k_{\text{nadp}}) \\ &= \frac{v_{\max} \cdot [\text{fTHFGlu}] \cdot [\text{NADP}]}{k_{\text{fthfglu}} \cdot k_{\text{nadp}} + k_{\text{fthfglu}} \cdot [\text{NADP}] + k_{\text{nadp}} \cdot [\text{fTHFGlu}] + [\text{fTHFGlu}] \cdot [\text{NADP}]} \end{aligned} \quad (120)$$

Table 100: Properties of each parameter.

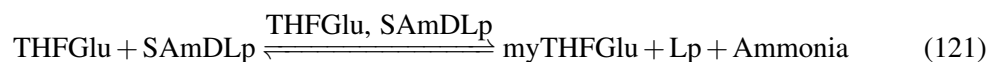
Id	Name	SBO	Value	Unit	Constant
vmax	vmax		59.332		✓
kfthfglu	kfthfglu		7.850		✓
knadp	knadp		0.900		✓

6.25 Reaction R18c

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

Name R18c

Reaction equation



Reactants

Table 101: Properties of each reactant.

Id	Name	SBO
THFGlu	THFGlu	
SAmDLp	SAmDLp	

Modifiers

Table 102: Properties of each modifier.

Id	Name	SBO
THFGlu	THFGlu	
SAmDLp	SAmDLp	

Products

Table 103: Properties of each product.

Id	Name	SBO
myTHFGlu	myTHFGlu	
Lp	Lp	
Ammonia	Ammonia	

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R18c}(v_{\text{max}}, [\text{THFGlu}], k_{\text{thfglu}}, [\text{SAmDLp}], k_{\text{samdlp}}) \quad (122)$$

$$\text{Rate_Law_for_R18c}(v_{\max}, [\text{THFGlu}], k_{\text{thfglu}}, [\text{SAmDLp}], k_{\text{samdlp}}) = \frac{v_{\max} \cdot [\text{THFGlu}] \cdot [\text{SAmDLp}]}{k_{\text{thfglu}} \cdot k_{\text{samdlp}} + k_{\text{thfglu}} \cdot [\text{SAmDLp}] + k_{\text{samdlp}} \cdot [\text{THFGlu}] + [\text{THFGlu}] \cdot [\text{SAmDLp}]} \quad (123)$$

$$\text{Rate_Law_for_R18c}(v_{\max}, [\text{THFGlu}], k_{\text{thfglu}}, [\text{SAmDLp}], k_{\text{samdlp}}) = \frac{v_{\max} \cdot [\text{THFGlu}] \cdot [\text{SAmDLp}]}{k_{\text{thfglu}} \cdot k_{\text{samdlp}} + k_{\text{thfglu}} \cdot [\text{SAmDLp}] + k_{\text{samdlp}} \cdot [\text{THFGlu}] + [\text{THFGlu}] \cdot [\text{SAmDLp}]} \quad (124)$$

Table 104: Properties of each parameter.

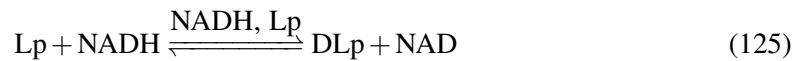
Id	Name	SBO	Value	Unit	Constant
vmax	vmax		196.56		<input checked="" type="checkbox"/>
kthfglu	kthfglu		67.70		<input checked="" type="checkbox"/>
ksamdlp	ksamdlp		290.00		<input checked="" type="checkbox"/>

6.26 Reaction R18a

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

Name R18a

Reaction equation



Reactants

Table 105: Properties of each reactant.

Id	Name	SBO
Lp	Lp	
NADH	NADH	

Modifiers

Table 106: Properties of each modifier.

Id	Name	SBO
NADH	NADH	

Id	Name	SBO
Lp	Lp	

Products

Table 107: Properties of each product.

Id	Name	SBO
DLp	DLp	
NAD	NAD	

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R18a}(v_{\max}, [\text{NADH}], [\text{Lp}], \text{knadh}, \text{klp}) \quad (126)$$

$$\begin{aligned} & \text{Rate_Law_for_R18a}(v_{\max}, [\text{NADH}], [\text{Lp}], \text{knadh}, \text{klp}) \\ &= \frac{v_{\max} \cdot [\text{NADH}] \cdot [\text{Lp}]}{\text{knadh} \cdot \text{klp} + \text{knadh} \cdot [\text{Lp}] + \text{klp} \cdot [\text{NADH}] + [\text{NADH}] \cdot [\text{Lp}]} \end{aligned} \quad (127)$$

$$\begin{aligned} & \text{Rate_Law_for_R18a}(v_{\max}, [\text{NADH}], [\text{Lp}], \text{knadh}, \text{klp}) \\ &= \frac{v_{\max} \cdot [\text{NADH}] \cdot [\text{Lp}]}{\text{knadh} \cdot \text{klp} + \text{knadh} \cdot [\text{Lp}] + \text{klp} \cdot [\text{NADH}] + [\text{NADH}] \cdot [\text{Lp}]} \end{aligned} \quad (128)$$

Table 108: Properties of each parameter.

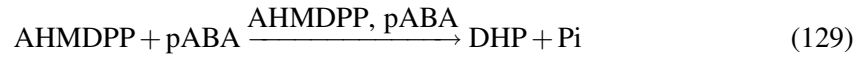
Id	Name	SBO	Value	Unit	Constant
vmax	vmax		5432.7		<input checked="" type="checkbox"/>
knadh	knadh		58.0		<input checked="" type="checkbox"/>
klp	klp		1280.0		<input checked="" type="checkbox"/>

6.27 Reaction R13

This is an irreversible reaction of two reactants forming two products influenced by two modifiers.

Name R13

Reaction equation



Reactants

Table 109: Properties of each reactant.

Id	Name	SBO
AHMDPP	AHMDPP	
pABA	pABA	

Modifiers

Table 110: Properties of each modifier.

Id	Name	SBO
AHMDPP	AHMDPP	
pABA	pABA	

Products

Table 111: Properties of each product.

Id	Name	SBO
DHP	DHP	
Pi	Pi	

Kinetic Law

Derived unit contains undeclared units

$$v_{27} = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R13}(\text{vmax}, \text{kahmdpp}, \text{kpaba}, [\text{AHMDPP}], [\text{pABA}]) \quad (130)$$

$$\begin{aligned} & \text{Rate_Law_for_R13}(\text{vmax}, \text{kahmdpp}, \text{kpaba}, [\text{AHMDPP}], [\text{pABA}]) \\ &= \frac{\text{vmax} \cdot [\text{AHMDPP}] \cdot [\text{pABA}]}{\text{kahmdpp} \cdot \text{kpaba} + \text{kpaba} \cdot [\text{AHMDPP}] + \text{kahmdpp} \cdot [\text{pABA}] + [\text{AHMDPP}] \cdot [\text{pABA}]} \end{aligned} \quad (131)$$

$$\begin{aligned} &\text{Rate_Law_for_R13}(\text{vmax}, \text{kahmdpp}, \text{kpaba}, [\text{AHMDPP}], [\text{pABA}]) \\ &= \frac{\text{vmax} \cdot [\text{AHMDPP}] \cdot [\text{pABA}]}{\text{kahmdpp} \cdot \text{kpaba} + \text{kpaba} \cdot [\text{AHMDPP}] + \text{kahmdpp} \cdot [\text{pABA}] + [\text{AHMDPP}] \cdot [\text{pABA}]} \end{aligned} \quad (132)$$

Table 112: Properties of each parameter.

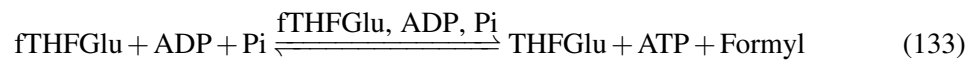
Id	Name	SBO	Value	Unit	Constant
vmax	vmax		105.014		✓
kahmdpp	kahmdpp		3.150		✓
kpaba	kpaba		2.600		✓

6.28 Reaction R24

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

Name R24

Reaction equation



Reactants

Table 113: Properties of each reactant.

Id	Name	SBO
fTHFGlu	fTHFGlu	
ADP	ADP	
Pi	Pi	

Modifiers

Table 114: Properties of each modifier.

Id	Name	SBO
fTHFGlu	fTHFGlu	
ADP	ADP	
Pi	Pi	

Products

Table 115: Properties of each product.

Id	Name	SBO
THFGlu	THFGlu	
ATP	ATP	
Formyl	Formyl	

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R24}(v_{\text{max}}, k_{\text{thfglu}}, k_{\text{formyl}}, k_{\text{atp}}, [\text{THFGlu}], [\text{ADP}], [\text{Pi}]) \quad (134)$$

$$\text{Rate_Law_for_R24}(v_{\text{max}}, k_{\text{thfglu}}, k_{\text{formyl}}, k_{\text{atp}}, [\text{THFGlu}], [\text{Formyl}], [\text{ATP}]) \quad (135)$$

$$= \frac{v_{\text{max}} \cdot [\text{THFGlu}] \cdot [\text{Formyl}] \cdot [\text{ATP}]}{k_{\text{thfglu}} \cdot k_{\text{formyl}} \cdot k_{\text{atp}} + k_{\text{thfglu}} \cdot ([\text{Formyl}] + [\text{ATP}]) + k_{\text{formyl}} \cdot ([\text{THFGlu}] + [\text{ATP}]) + k_{\text{atp}} \cdot ([\text{Formyl}] + [\text{THFGlu}])}$$

$$\text{Rate_Law_for_R24}(v_{\text{max}}, k_{\text{thfglu}}, k_{\text{formyl}}, k_{\text{atp}}, [\text{THFGlu}], [\text{Formyl}], [\text{ATP}]) \quad (136)$$

$$= \frac{v_{\text{max}} \cdot [\text{THFGlu}] \cdot [\text{Formyl}] \cdot [\text{ATP}]}{k_{\text{thfglu}} \cdot k_{\text{formyl}} \cdot k_{\text{atp}} + k_{\text{thfglu}} \cdot ([\text{Formyl}] + [\text{ATP}]) + k_{\text{formyl}} \cdot ([\text{THFGlu}] + [\text{ATP}]) + k_{\text{atp}} \cdot ([\text{Formyl}] + [\text{THFGlu}])}$$

Table 116: Properties of each parameter.

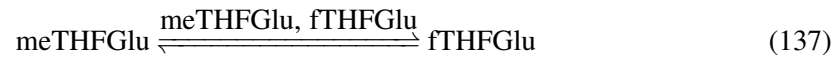
Id	Name	SBO	Value	Unit	Constant
vmax	vmax		15315.3		✓
kthfglu	kthfglu		134.0		✓
kformyl	kformyl		3190.0		✓
katp	katp		74.5		✓

6.29 Reaction R23

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

Name R23

Reaction equation



Reactant

Table 117: Properties of each reactant.

Id	Name	SBO
meTHFGlu	meTHFGlu	

Modifiers

Table 118: Properties of each modifier.

Id	Name	SBO
meTHFGlu	meTHFGlu	
fTHFGlu	fTHFGlu	

Product

Table 119: Properties of each product.

Id	Name	SBO
fTHFGlu	fTHFGlu	

Kinetic Law

Derived unit contains undeclared units

$$v_{29} = \text{vol}(\text{compartment}) \cdot (k_1 \cdot [\text{meTHFGlu}] - k_2 \cdot [\text{fTHFGlu}]) \quad (138)$$

Table 120: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.080		✓
k2	k2		0.031		✓

6.30 Reaction R28

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

Name R28

Reaction equation



Reactant

Table 121: Properties of each reactant.

Id	Name	SBO
meTHFGlu	meTHFGlu	

Modifier

Table 122: Properties of each modifier.

Id	Name	SBO
meTHFGlu	meTHFGlu	

Product

Table 123: Properties of each product.

Id	Name	SBO
ffTHFGlu	ffTHFGlu	

Kinetic Law

Derived unit contains undeclared units

$$v_{30} = \text{vol}(\text{compartment}) \cdot \text{Henri_Michaelis_Menten_irreversible}([\text{meTHFGlu}], \text{Km}, \text{V}) \quad (140)$$

$$\text{Henri_Michaelis_Menten_irreversible}(\text{substrate}, \text{Km}, \text{V}) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \quad (141)$$

$$\text{Henri_Michaelis_Menten_irreversible}(\text{substrate}, \text{Km}, \text{V}) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \quad (142)$$

Table 124: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km	Km		67.0		<input checked="" type="checkbox"/>
V	V		200.0		<input checked="" type="checkbox"/>

6.31 Reaction R29

This is an irreversible reaction of two reactants forming three products influenced by two modifiers.

Name R29

Reaction equation



Reactants

Table 125: Properties of each reactant.

Id	Name	SBO
ATP	ATP	
ffTHFGlu	ffTHFGlu	

Modifiers

Table 126: Properties of each modifier.

Id	Name	SBO
ATP	ATP	
ffTHFGlu	ffTHFGlu	

Products

Table 127: Properties of each product.

Id	Name	SBO
ADP	ADP	
Pi	Pi	
meTHFGlu	meTHFGlu	

Kinetic Law

Derived unit contains undeclared units

$$v_{31} = \text{vol}(\text{compartment}) \cdot \text{Rate_Law_for_R29}(v_{\max}, [\text{ATP}], [\text{ffTHFGlu}], \text{katp}, \text{kffthfglu}) \quad (144)$$

$$\begin{aligned} & \text{Rate_Law_for_R29}(v_{\max}, [\text{ATP}], [\text{ffTHFGlu}], \text{katp}, \text{kffthfglu}) \\ &= \frac{v_{\max} \cdot [\text{ATP}] \cdot [\text{ffTHFGlu}]}{\text{katp} \cdot \text{kffthfglu} + \text{katp} \cdot [\text{ffTHFGlu}] + \text{kffthfglu} \cdot [\text{ATP}] + [\text{ATP}] \cdot [\text{ffTHFGlu}]} \end{aligned} \quad (145)$$

$$\begin{aligned} & \text{Rate_Law_for_R29}(v_{\max}, [\text{ATP}], [\text{ffTHFGlu}], \text{katp}, \text{kffthfglu}) \\ &= \frac{v_{\max} \cdot [\text{ATP}] \cdot [\text{ffTHFGlu}]}{\text{katp} \cdot \text{kffthfglu} + \text{katp} \cdot [\text{ffTHFGlu}] + \text{kffthfglu} \cdot [\text{ATP}] + [\text{ATP}] \cdot [\text{ffTHFGlu}]} \end{aligned} \quad (146)$$

Table 128: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vmax	vmax		500.0		✓
katp	katp		50.0		✓
kffthfglu	kffthfglu		5.0		✓

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 DAHP

Name DAHP

Initial concentration $0.9796078511 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in R2 and as a product in R1 and as a modifier in R2).

$$\frac{d}{dt}\text{DAHP} = v_1 - v_2 \quad (147)$$

7.2 Species PEP

Name PEP

Initial concentration 16.01031821 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in R1, R6 and as a modifier in R1, R6), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{PEP} = 0 \quad (148)$$

7.3 Species Pi

Name Pi

Initial concentration 2.725541316 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in 13 reactions (as a reactant in R24 and as a product in R1, R2, R5, R6, R7, R11, R27, R14, R16, R13, R29 and as a modifier in R24).

$$\frac{d}{dt}\text{Pi} = v_1 + v_2 + v_5 + v_6 + v_7 + v_{11} + v_{12} + v_{14} + v_{16} + v_{27} + v_{31} - v_{28} \quad (149)$$

7.4 Species DHQ

Name DHQ

Initial concentration 0.9994087764 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in R3 and as a product in R2 and as a modifier in R3).

$$\frac{d}{dt}\text{DHQ} = v_2 - v_3 \quad (150)$$

7.5 Species EP

Name EP

Initial concentration 107.502052 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in R1 and as a modifier in R1), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{EP} = 0 \quad (151)$$

7.6 Species DHSK

Name DHSK

Initial concentration $1.92788104 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in R4 and as a product in R3 and as a modifier in R4).

$$\frac{d}{dt}\text{DHSK} = v_3 - v_4 \quad (152)$$

7.7 Species SK

Name SK

Initial concentration $5.06777189 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in R5 and as a product in R4 and as a modifier in R5).

$$\frac{d}{dt}\text{SK} = v_4 - v_5 \quad (153)$$

7.8 Species SKP

Name SKP

Initial concentration $2 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in R6 and as a product in R5 and as a modifier in R6).

$$\frac{d}{dt}\text{SKP} = v_5 - v_6 \quad (154)$$

7.9 Species CVPSK

Name CVPSK

Initial concentration $0.9174312684 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in R7 and as a product in R6 and as a modifier in R7).

$$\frac{d}{dt}\text{CVPSK} = v_6 - v_7 \quad (155)$$

7.10 Species CM

Name CM

Initial concentration 1.009195849 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in R8 and as a product in R7 and as a modifier in R8).

$$\frac{d}{dt}\text{CM} = v_7 - v_8 \quad (156)$$

7.11 Species Gln

Name Gln

Initial concentration 381.0009289 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in R8 and as a modifier in R8), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{Gln} = 0 \quad (157)$$

7.12 Species Glu

Name Glu

Initial concentration 959.9999225 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in R14, R16 and as a product in R8 and as a modifier in R14, R16).

$$\frac{d}{dt}\text{Glu} = v_8 - v_{14} - v_{16} \quad (158)$$

7.13 Species ADC

Name ADC

Initial concentration 0.9907047071 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in R9 and as a product in R8 and as a modifier in R9).

$$\frac{d}{dt}\text{ADC} = v_8 - v_9 \quad (159)$$

7.14 Species Pyr

Name Pyr

Initial concentration $1.000006539 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in [R9](#)).

$$\frac{d}{dt}\text{Pyr} = v_9 \quad (160)$$

7.15 Species pABA

Name pABA

Initial concentration $1.00378139 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in [R13](#) and as a product in [R9](#) and as a modifier in [R13](#)).

$$\frac{d}{dt}\text{pABA} = v_9 - v_{27} \quad (161)$$

7.16 Species DHNTP

Name DHNTP

Initial concentration $4 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in [R11](#), [R27](#) and as a product in [R10](#) and as a modifier in [R11](#), [R27](#)).

$$\frac{d}{dt}\text{DHNTP} = v_{10} - v_{11} - v_{12} \quad (162)$$

7.17 Species GTP

Name GTP

Initial concentration $487.4867469 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in [R10](#) and as a modifier in [R10](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{GTP} = 0 \quad (163)$$

7.18 Species AHMDHP

Name AHMDHP

Initial concentration $2.01877235 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in [R12](#) and as a product in [R11](#) and as a modifier in [R12](#)).

$$\frac{d}{dt}\text{AHMDHP} = v_{11} - v_{13} \quad (164)$$

7.19 Species HAD

Name HAD

Initial concentration $2.002305849 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in [R11](#)).

$$\frac{d}{dt}\text{HAD} = v_{11} \quad (165)$$

7.20 Species PTHP

Name PTHP

Initial concentration $1.002298517 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in [R27](#)).

$$\frac{d}{dt}\text{PTHP} = v_{12} \quad (166)$$

7.21 Species AHMDPP

Name AHMDPP

Initial concentration $0.9873083466 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in [R13](#) and as a product in [R12](#) and as a modifier in [R13](#)).

$$\frac{d}{dt}\text{AHMDPP} = v_{13} - v_{27} \quad (167)$$

7.22 Species DHP

Name DHP

Initial concentration $0.9963801483 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in R14 and as a product in R13 and as a modifier in R14).

$$\frac{d}{dt}\text{DHP} = v_{27} - v_{14} \quad (168)$$

7.23 Species DHF

Name DHF

Initial concentration $1.142744159 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in twelve reactions (as a reactant in R15 and as a product in R14, R21 and as a modifier in R15, R16, R16, R19, R19, R21, R21, R22, R22).

$$\frac{d}{dt}\text{DHF} = v_{14} + v_{21} - v_{15} \quad (169)$$

7.24 Species THF

Name THF

Initial concentration $8 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in seven reactions (as a reactant in R16 and as a product in R15 and as a modifier in R10, R10, R16, R17, R17).

$$\frac{d}{dt}\text{THF} = v_{15} - v_{16} \quad (170)$$

7.25 Species THFGlu

Name THFGlu

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

This species takes part in nine reactions (as a reactant in R17, R18c and as a product in R16, R20, R25, R26, R24 and as a modifier in R17, R18c).

$$\frac{d}{dt}\text{THFGlu} = v_{16} + v_{20} + v_{23} + v_{24} + v_{28} - v_{17} - v_{25} \quad (171)$$

7.26 Species Gly

Name Gly

Initial concentration 499.9974679 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in R18b and as a product in R17 and as a modifier in R18b), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{Gly} = 0 \quad (172)$$

7.27 Species Ser

Name Ser

Initial concentration 6.803576818 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in R17 and as a modifier in R17), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{Ser} = 0 \quad (173)$$

7.28 Species myTHFGlu

Name myTHFGlu

Initial concentration 1.04350884 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in eight reactions (as a reactant in R19, R21, R22 and as a product in R17, R18c and as a modifier in R19, R21, R22).

$$\frac{d}{dt}\text{myTHFGlu} = v_{17} + v_{25} - v_{19} - v_{21} - v_{22} \quad (174)$$

7.29 Species MTHFGlu

Name MTHFGlu

Initial concentration 1.000096392 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in R20 and as a product in R19 and as a modifier in R20).

$$\frac{d}{dt}\text{MTHFGlu} = v_{19} - v_{20} \quad (175)$$

7.30 Species Hcy

Name Hcy

Initial concentration $1.000182797 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in [R20](#) and as a modifier in [R20](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{Hcy} = 0 \quad (176)$$

7.31 Species Met

Name Met

Initial concentration $0.9998172031 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in [R20](#)).

$$\frac{d}{dt}\text{Met} = v_{20} \quad (177)$$

7.32 Species dTMP

Name dTMP

Initial concentration $0.9974700923 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in [R21](#)).

$$\frac{d}{dt}\text{dTMP} = v_{21} \quad (178)$$

7.33 Species dUMP

Name dUMP

Initial concentration $20.00252991 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in [R21](#) and as a modifier in [R21](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{dUMP} = 0 \quad (179)$$

7.34 Species meTHFGlu

Name meTHFGlu

Initial concentration $0.9082384182 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in [R23](#), [R28](#) and as a product in [R22](#), [R29](#) and as a modifier in [R23](#), [R28](#)).

$$\frac{d}{dt}\text{meTHFGlu} = v_{22} + v_{31} - v_{29} - v_{30} \quad (180)$$

7.35 Species fTHFGlu

Name fTHFGlu

Initial concentration $1.83347183 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in eight reactions (as a reactant in [R25](#), [R26](#), [R24](#) and as a product in [R23](#) and as a modifier in [R25](#), [R26](#), [R24](#), [R23](#)).

$$\frac{d}{dt}\text{fTHFGlu} = v_{29} - v_{23} - v_{24} - v_{28} \quad (181)$$

7.36 Species fmtRNA

Name fmtRNA

Initial concentration $0.9968760756 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in [R25](#)).

$$\frac{d}{dt}\text{fmtRNA} = v_{23} \quad (182)$$

7.37 Species mtRNA

Name mtRNA

Initial concentration $1.003123924 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in [R25](#) and as a modifier in [R25](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{mtRNA} = 0 \quad (183)$$

7.38 Species COTwo

Name COTwo

Initial concentration $0.988683328 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a product in [R18b](#), [R26](#)).

$$\frac{d}{dt}\text{COTwo} = v_{18} + v_{24} \quad (184)$$

7.39 Species ADP

Name ADP

Initial concentration $2.828115142 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in [R24](#) and as a product in [R5](#), [R14](#), [R16](#), [R29](#) and as a modifier in [R24](#)).

$$\frac{d}{dt}\text{ADP} = v_5 + v_{14} + v_{16} + v_{31} - v_{28} \quad (185)$$

7.40 Species ATP

Name ATP

Initial concentration $963.0188351 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in eleven reactions (as a reactant in [R5](#), [R12](#), [R14](#), [R16](#), [R29](#) and as a product in [R24](#) and as a modifier in [R5](#), [R12](#), [R14](#), [R16](#), [R29](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{ATP} = 0 \quad (186)$$

7.41 Species NADP

Name NADP

Initial concentration $2 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in seven reactions (as a reactant in [R22](#), [R26](#) and as a product in [R4](#), [R15](#), [R19](#) and as a modifier in [R22](#), [R26](#)).

$$\frac{d}{dt}\text{NADP} = v_4 + v_{15} + v_{19} - v_{22} - v_{24} \quad (187)$$

7.42 Species NADPH

Name NADPH

Initial concentration 12.19849409 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in eight reactions (as a reactant in [R4](#), [R15](#), [R19](#) and as a product in [R22](#), [R26](#) and as a modifier in [R4](#), [R15](#), [R19](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{NADPH} = 0 \quad (188)$$

7.43 Species AMP

Name AMP

Initial concentration 0.983533495 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in [R12](#)).

$$\frac{d}{dt}\text{AMP} = v_{13} \quad (189)$$

7.44 Species DLp

Name DLp

Initial concentration 0.7017503089 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in [R18b](#) and as a product in [R18a](#) and as a modifier in [R18b](#)).

$$\frac{d}{dt}\text{DLp} = v_{26} - v_{18} \quad (190)$$

7.45 Species SAmDLp

Name SAmDLp

Initial concentration 1.000015336 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in [R18c](#) and as a product in [R18b](#) and as a modifier in [R18c](#)).

$$\frac{d}{dt}\text{SAmDLp} = v_{18} - v_{25} \quad (191)$$

7.46 Species L_p

Name L_p

Initial concentration $1.298234355 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in [R18a](#) and as a product in [R18c](#) and as a modifier in [R18a](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}L_p = 0 \quad (192)$$

7.47 Species NAD

Name NAD

Initial concentration $0.7017656449 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in [R18a](#)).

$$\frac{d}{dt}NAD = v_{26} \quad (193)$$

7.48 Species $NADH$

Name $NADH$

Initial concentration $8.349823436 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in [R18a](#) and as a modifier in [R18a](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}NADH = 0 \quad (194)$$

7.49 Species $Ammonia$

Name $Ammonia$

Initial concentration $0.9895374253 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in [R18c](#)).

$$\frac{d}{dt}Ammonia = v_{25} \quad (195)$$

7.50 Species Formyl

Name Formyl

Initial concentration $8 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a product in R10, R24).

$$\frac{d}{dt}\text{Formyl} = v_{10} + v_{28} \quad (196)$$

7.51 Species ffTHFGlu

Name ffTHFGlu

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

This species takes part in three reactions (as a reactant in R29 and as a product in R28 and as a modifier in R29).

$$\frac{d}{dt}\text{ffTHFGlu} = v_{30} - v_{31} \quad (197)$$

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