SBML Model Report

Model name: “Reyes-Palomares2012 - a combined model hepatic polyamine and sulfur aminoacid metabolism - version1”

July 3, 2018

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Armando Reyes-Palomares[1] and Matthew Grant Roberts[2] at February 14th 2018 at 1:11 p. m. and last time modified at February 14th 2018 at 4:15 p. m. Table 1 provides 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	4
species types	0	species	53
events	0	constraints	0
reactions	73	function definitions	69
global parameters	177	unit definitions	2
rules	17	initial assignments	2

Model Notes

Reyes-Palomares2012 - a combined modelhepatic polyamine and sulfur aminoacid metabolism - version1

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Mammalian polyamine metabolism consists of a bi-cycle with two required entrances, omithine and S-adenosyl methionine (SAM), and several alternative exists. The relevant regulatory roles of the short half-life enzymes ornithine decarboxylase (ODC), S-adenosyl methione decarboxylase (SAMDC) and spermindine/spermine acetyl transferase (SSAT) in polyamine metabolism are well studied, and has been modelled here.

This model is described in the article:A combined model of hepatic polyamine and sulfur amino acid metabolism to analyze S-adenosyl methionine availability.Reyes-Palomares A, Montaez R, Snchez-Jimnez F, Medina MA.Amino Acids 2012 Feb; 42(2-3): 597-610

Abstract:

Many molecular details remain to be uncovered concerning the regulation of polyamine metabolism. A previous model of mammalian polyamine metabolism showed that S-adenosyl methionine availability could play a key role in polyamine homeostasis. To get a deeper insight in this prediction, we have built a combined model by integration of the previously published polyamine model and one-carbon and glutathione metabolism model, published by different research groups. The combined model is robust and it is able to achieve physiological steady-state values, as well as to reproduce the predictions of the individual models. Furthermore, a transition between two versions of our model with new regulatory factors added properly simulates the switch in methionine adenosyl transferase isozymes occurring when the liver enters in proliferative conditions. The combined model is useful to support the previous prediction on the role of S-adenosyl methionine availability in polyamine homeostasis. Furthermore, it could be easily adapted to get deeper insights on the connections of polyamines with energy metabolism.

Notes by the author:

This model combines BIOMD0000000190 and BIOMD0000000268 from BioModels Database, both models include corrections respect to their originals publications.

This model is hosted on BioModels Database and identified by: BIOMD0000000674.

To cite BioModels Database, please use: Chelliah V et al. BioModels: ten-year anniversary. Nucl. Acids Res. 2015, 43(Database issue):D542-8.

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 3600 s

2.2 Unit substance

Name substance

Definition µmol

2.3 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

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 Compartments

This model contains four compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
blood	blood		3	1	litre	☑	
cytosol	cytosol		3	1	litre	☑	
mito	mitochondrion		3	1	litre	☑	
cell	cell		3	1	litre	☑	

3.1 Compartment blood

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

Name blood

3.2 Compartment `cytosol`

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

Name cytosol

3.3 Compartment `mito`

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

Name mitochondrion

3.4 Compartment `cell`

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

Name cell

4 Species

This model contains 53 species. The boundary condition of eleven of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 10 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
b_met	b_Methionine	blood	$\mu mol \cdot l^{-1}$	☐	☑
b_ser	b_Serine	blood	$\mu mol \cdot l^{-1}$	☐	☑
b_gly	b_Glycine	blood	$\mu mol \cdot l^{-1}$	☐	☐
b_glu	b_Glutamate	blood	$\mu mol \cdot l^{-1}$	☐	☐
b_cys	b_Cysteine	blood	$\mu mol \cdot l^{-1}$	☐	☐
b_gsg	b_GSSG	blood	$\mu mol \cdot l^{-1}$	☐	☐
b_gsh	b_GSH	blood	$\mu mol \cdot l^{-1}$	☐	☐
GAR	GAR	cytosol	$\mu mol \cdot l^{-1}$	☑	☑
NADPH	NADPH	cytosol	$\mu mol \cdot l^{-1}$	☑	☑
BET	Betaine	cytosol	$\mu mol \cdot l^{-1}$	☑	☑
DUMP	dUMP	cytosol	$\mu mol \cdot l^{-1}$	☑	☑
H2O2	H2O2	cytosol	$\mu mol \cdot l^{-1}$	☑	☑
c_thf	c_THF	cytosol	$\mu mol \cdot l^{-1}$	☐	☐
c_5mf	c_5-methyl-THF	cytosol	$\mu mol \cdot l^{-1}$	☐	☐
c_2cf	c_5-10-methylene-THF	cytosol	$\mu mol \cdot l^{-1}$	☐	☐
c_1cf	c_5-10-methenyl-THF	cytosol	$\mu mol \cdot l^{-1}$	☐	☐
c_10f	c_10-formyl-THF	cytosol	$\mu mol \cdot l^{-1}$	☐	☐
c_dhf	c_DHF	cytosol	$\mu mol \cdot l^{-1}$	☐	☐
aic	AICAR	cytosol	$\mu mol \cdot l^{-1}$	☐	☐
c_glu	c_Glutamate	cytosol	$\mu mol \cdot l^{-1}$	☐	☐

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
c_cys	c_Cysteine	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
glc	Glutamyl-Cysteine	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
c_gly	c_Glycine	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
c_gsg	c_GSSG	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
c_gsh	c_GSH	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
cyt	Cystathionine	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
hcy	Homocysteine	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
c_ser	c_Serine	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
sah	SAH	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
sam	SAM	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
met	c_Methionine	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
c_coo	c_Formate	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
species_1	dcSAM	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
species_2	Putrescine	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
species_3	Spermine	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
species_4	Spermidine	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
species_5	Acetylspermine	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
species_6	Acetylspermidine	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
species_7	Ornithine	cytosol	$\mu mol \cdot l^{-1}$	☑	☑
species_8	Acetyl-CoA	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
species_9	CoA	cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
CO	CO2	mito	$\mu mol \cdot l^{-1}$	☑	☑
m_thf	m_THF	mito	$\mu mol \cdot l^{-1}$	⊟	⊟
m_2cf	m_5-10-methylene-THF	mito	$\mu mol \cdot l^{-1}$	⊟	⊟
m_1cf	m_5-10-methenyl-THF	mito	$\mu mol \cdot l^{-1}$	⊟	⊟
m_10f	m_10-formyl-THF	mito	$\mu mol \cdot l^{-1}$	⊟	⊟
m_ser	m_Serine	mito	$\mu mol \cdot l^{-1}$	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
m_gly	m_Glycine	mito	$\mu mol \cdot l^{-1}$	☐	☐
m_coo	m_Formate	mito	$\mu mol \cdot l^{-1}$	☐	☐
Fol	Folate	cell	$\mu mol \cdot l^{-1}$	☑	☑
HCHO	Formaldehyde	cell	$\mu mol \cdot l^{-1}$	☑	☑
src	Sarcosine	cell	$\mu mol \cdot l^{-1}$	☐	☐
dmg	Dimethylglycine	cell	$\mu mol \cdot l^{-1}$	☐	☐

5 Parameters

This model contains 177 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
tot_cfol	tot_cfol		13.400		☐
tot_mfol	tot_mfol		40.200		☐
V_oCys_b	V_oCys_b		17.500		☐
V_oGly_b	V_oGly_b		157.500		☐
V_oGlu_b	V_oGlu_b		68.250		☐
V_gshHb	V_gshHb		150.000		☑
K_gshHb	K_gshHb		150.000		☑
V_gshLb	V_gshLb		1100.000		☑
h_gshLb	h_gshLb		3.000		☑
K_gshLb	K_gshLb		3000.000		☑
V_gsgHb	V_gsgHb		40.000		☑
K_gsgHb	K_gsgHb		1250.000		☑
V_gsgLb	V_gsgLb		4025.000		☑
K_gsgLb	K_gsgLb		7100.000		☑
V_bcysc	V_bcysc		14950.000		☑
K_bcysc	K_bcysc		2100.000		☑
V_bglutc	V_bglutc		28000.000		☑
K_bglutc	K_bglutc		300.000		☑
k_out_glu	k_out_glu		1.000		☑
V_bglyc	V_bglyc		4600.000		☑
K_bglyc	K_bglyc		150.000		☑
k_out_gly	k_out_gly		1.000		☑
V_bserc	V_bserc		2700.000		☑
K_bserc	K_bserc		150.000		☑
k_out_ser	k_out_ser		1.000		☑
V_bmetc	V_bmetc		913.400		☑
K_bmetc	K_bmetc		150.000		☑
k_out_met	k_out_met		1.000		☑
Vm_mFTD	Vm_mFTD		1050.000		☑
K_10f_FTD	K_10f_FTD		20.000		☑
Vf_mSHMT	Vf_mSHMT		11440.000		☑
K_thf_SHMT	K_thf_SHMT		50.000		☑
K_ser_SHMT	K_ser_SHMT		600.000		☑
Vr_mSHMT	Vr_mSHMT		$3 \cdot 10^7$		☑
K_gly_SHMT	K_gly_SHMT		10000.000		☑
K_2cf_SHMT	K_2cf_SHMT		3200.000		☑

Id	Name	SBO	Value	Unit	Constant
Vf_mFTS	Vf_mFTS		2000.000		☑
K_thf_mFTS	K_thf_mFTS		3.000		☑
K_coo_mFTS	K_coo_mFTS		43.000		☑
Vr_mFTS	Vr_mFTS		6300.000		☑
K_10f_mFTS	K_10f_mFTS		22.000		☑
k1_mNE	k1_mNE		0.030		☑
k2_mNE	k2_mNE		20.000		☑
Vm_GDC	Vm_GDC		15000.000		☑
K_thf_GDC	K_thf_GDC		50.000		☑
K_gly_GDC	K_gly_GDC		3400.000		☑
Vm_SDH	Vm_SDH		15000.000		☑
K_thf_SDH	K_thf_SDH		50.000		☑
K_src_SDH	K_src_SDH		320.000		☑
Vm_DMGD	Vm_DMGD		15000.000		☑
K_thf_DMGD	K_thf_DMGD		50.000		☑
K_dmg_DMGD	K_dmg_DMGD		50.000		☑
Vf_mMTD	Vf_mMTD		180000.000		☑
K_2cf_MTD	K_2cf_MTD		2.000		☑
Vr_MTD	Vr_MTD		594000.000		☑
K_1cf_MTD	K_1cf_MTD		10.000		☑
Vf_mMTCH	Vf_mMTCH		790000.000		☑
K_1cf_MTCH	K_1cf_MTCH		250.000		☑
Vr_MTCH	Vr_MTCH		20000.000		☑
K_10f_MTCH	K_10f_MTCH		100.000		☑
V_mser	V_mser		10000.000		☑
K_mser	K_mser		5700.000		☑
V_cser	V_cser		10000.000		☑
K_cser	K_cser		5700.000		☑
k_in_coo	k_in_coo		100.000		☑
k_out_coo	k_out_coo		100.000		☑
V_mgly	V_mgly		10000.000		☑
K_mgly	K_mgly		5700.000		☑
V_cgly	V_cgly		10000.000		☑
K_cgly	K_cgly		5700.000		☑
Vm_MS	Vm_MS		500.000		☑
K_5mf_MS	K_5mf_MS		25.000		☑
K_hcy_MS	K_hcy_MS		1.000		☑
ssH2O2	ssH2O2		0.010		☑
Ki_MS	Ki_MS		0.010		☑
Vm_DHFR	Vm_DHFR		2000.000		☑
K_dhf_DHFR	K_dhf_DHFR		0.500		☑
K_NADPH_DHFR	K_NADPH_DHFR		4.000		☑

Id	Name	SBO	Value	Unit	Constant
Vm_cFTD	Vm_cFTD		500.000		☑
Vm_PGT	Vm_PGT		24300.000		☑
K_10f_PGT	K_10f_PGT		4.900		☑
K_GAR_PGT	K_GAR_PGT		520.000		☑
Vm_cFTS	Vm_cFTS		3900.000		☑
K_thf_cFTS	K_thf_cFTS		3.000		☑
K_coo_cFTS	K_coo_cFTS		43.000		☑
Vf_cSHMT	Vf_cSHMT		5200.000		☑
Vr_cSHMT	Vr_cSHMT		$1.5 \cdot 10^7$		☑
k1_cNE	k1_cNE		0.030		☑
k2_cNE	k2_cNE		22.000		☑
Vm_TS	Vm_TS		5000.000		☑
K_DUMP_TS	K_DUMP_TS		6.300		☑
K_2cf_TS	K_2cf_TS		14.000		☑
Vm_MTHFR	Vm_MTHFR		5300.000		☑
K_2cf_MTHFR	K_2cf_MTHFR		50.000		☑
K_NADPH-_MTHFR	K_NADPH-_MTHFR		16.000		☑
Vf_cMTD	Vf_cMTD		80000.000		☑
Vr_cMTD	Vr_cMTD		600000.000		☑
Vf_cMTCH	Vf_cMTCH		500000.000		☑
Vm_ART	Vm_ART		55000.000		☑
K_10f_ART	K_10f_ART		5.900		☑
K_aic_ART	K_aic_ART		100.000		☑
Vm_BHMT	Vm_BHMT		2160.000		☑
K_hcy_BHMT	K_hcy_BHMT		12.000		☑
K_bet_BHMT	K_bet_BHMT		100.000		☑
Ki_BHMT	Ki_BHMT		0.010		☑
Vm_MAT1	Vm_MAT1		260.000		☑
Km_MAT1	Km_MAT1		41.000		☑
Ki_MAT1	Ki_MAT1		2140.000		☑
Vm_MAT3	Vm_MAT3		220.000		☑
Km_MAT3	Km_MAT3		300.000		☑
Ka_MAT3	Ka_MAT3		360.000		☑
Ki_MAT3	Ki_MAT3		4030.000		☑
Vm_GNMT	Vm_GNMT		260.000		☑
K_sam_GNMT	K_sam_GNMT		63.000		☑
K_gly_GNMT	K_gly_GNMT		130.000		☑
Ki_GNMT	Ki_GNMT		18.000		☑
Vm_DNMT	Vm_DNMT		180.000		☑
Km_DNMT	Km_DNMT		1.400		☑
Ki_DNMT	Ki_DNMT		1.400		☑

Id	Name	SBO	Value	Unit	Constant
Vf_SAHH	Vf_SAHH		320.000		☑
K_sah_SAHH	K_sah_SAHH		6.500		☑
Vr_SAHH	Vr_SAHH		4530.000		☑
K_hcy_SAHH	K_hcy_SAHH		150.000		☑
Vm_CBS	Vm_CBS		420000.000		☑
K_hcy_CBS	K_hcy_CBS		1000.000		☑
K_ser_CBS	K_ser_CBS		2000.000		☑
Ka_CBS	Ka_CBS		0.035		☑
Vm_CTGL	Vm_CTGL		1500.000		☑
K_cyt_CTGL	K_cyt_CTGL		500.000		☑
Vm_GCS	Vm_GCS		3600.000		☑
Ke_GCS	Ke_GCS		5597.000		☑
K_cys_GCS	K_cys_GCS		100.000		☑
K_glu_GCS	K_glu_GCS		1900.000		☑
Ki_GCS	Ki_GCS		8200.000		☑
Kp_GCS	Kp_GCS		300.000		☑
Ka_GCS	Ka_GCS		0.010		☑
Vm_GS	Vm_GS		5400.000		☑
Ke_GS	Ke_GS		5600.000		☑
K_gly_GS	K_gly_GS		300.000		☑
K_glc_GS	K_glc_GS		22.000		☑
Kp_GS	Kp_GS		30.000		☑
Vm_GPX	Vm_GPX		4500.000		☑
K_gsh_GPX	K_gsh_GPX		1330.000		☑
K_H2O2_GPX	K_H2O2_GPX		0.090		☑
Vm_GR	Vm_GR		892.500		☑
K_gsg_GR	K_gsg_GR		107.000		☑
K_NADPH_GR	K_NADPH_GR		10.400		☑
dinner	dinner		3.250		☑
lunch	lunch		1.750		☑
breakfast	breakfast		1.750		☑
fasting	fasting		0.250		☑
daytime	daytime		0.000		☐
aa_input	Aminoacid_input		0.250		☐
b_met_basal	b_met_basal		30.000		☑
b_ser_basal	b_ser_basal		150.000		☑
V_oGly_b_basal	V_oGly_b_basal		630.000		☑
V_oGlu_b_basal	V_oGlu_b_basal		273.000		☑
V_oCys_b_basal	V_oCys_b_basal		70.000		☑

Id	Name	SBO	Value	Unit	Constant
k_out_cys	k_out_cys		1.000		☑
parameter_1	Vm_ODC		72.256		⊟
parameter_2	Vm_SSAT		42.285		⊟
parameter_3	Vm_SAMDC		21.134		⊟
parameter_4	ANTZ		0.585		⊟
parameter_5	Ke_POL		1.000		☑
parameter_6	Kd_ODC		3.000		☑
parameter_7	Ks_ODC		300.000		☑
parameter_8	Kd_SSAT		12.000		☑
parameter_9	Ks_SSAT		0.060		☑
parameter_10	Kd_SAMDC		1.200		☑
parameter_11	Ks_SAMDC		60.000		☑
parameter_12	Kd_ANTZ		0.020		☑
parameter_13	Ks_ANTZ		0.020		☑
parameter_14	K_accoa		0.240		⊟
parameter_15	K_coa		0.720		⊟
parameter_16	R		0.240		☑
parameter_17	S+D		140.951		⊟
parameter_18	R_percent		100.000		⊟

6 Initialassignments

This is an overview of two initialassignments.

6.1 Initialassignment c_thf

Derived unit contains undeclared units

Math $\frac{[\mathrm{Fol}]}{\frac{2 \cdot 3}{4}} - ([\mathrm{c\_5mf}] + [\mathrm{c\_2cf}] + [\mathrm{c\_1cf}] + [\mathrm{c\_10f}] + [\mathrm{c\_dhf}])$

6.2 Initialassignment m_thf

Derived unit contains undeclared units

Math $\frac{[\mathrm{Fol}]}{\frac{2 \cdot 1}{4}} - ([\mathrm{m\_2cf}] + [\mathrm{m\_1cf}] + [\mathrm{m\_10f}])$

7 Function definitions

This is an overview of 69 function definitions.

7.1 Function definition Constant_flux__reversible

Name Constant flux (reversible)

Argument v

Mathematical Expression

$$\mathrm{v} \tag{1}$$

7.2 Function definition function_4_VmNE_1

Name function_4_VmNE_1

Arguments [HCHO], k1_mNE, k2_mNE, [m_2cf], [m_thf], vol (mito)

Mathematical Expression

$$\mathrm{vol}\,(\mathrm{mito}) \cdot (\mathrm{k1\_mNE} \cdot [\mathrm{m\_thf}] \cdot [\mathrm{HCHO}] - \mathrm{k2\_mNE} \cdot [\mathrm{m\_2cf}]) \tag{2}$$

7.3 Function definition function_4_b_cys_loss_1

Name function_4_b_cys_loss_1

Argument [b_cys]

Mathematical Expression

$$0.1 \cdot [\mathrm{b\_cys}] \tag{3}$$

7.4 Function definition function_4_V_ODC_1

Name function_4_V_ODC_1

Arguments Kipodc, Kmodc, parameter_1, [species_2], [species_7]

Mathematical Expression

$$\frac{\mathrm{parameter\_1} \cdot [\mathrm{species\_7}]}{\mathrm{Kmodc} \cdot \left(1 + \frac{[\mathrm{species\_2}]}{\mathrm{Kipodc}}\right) + [\mathrm{species\_7}]} \tag{4}$$

7.5 Function definition function_4_V_PAO_AS_1

Name function_4_V_PAO_AS_1

Arguments Kmadpao, Kmaspao, Kmdpao, Kmspao, Vmpao, [species_3], [species_4], [species_5], [species_6]

Mathematical Expression

$$\frac{\mathrm{Vmpao} \cdot [\mathrm{species\_5}]}{\mathrm{Kmaspao} \cdot \left(1 + \frac{[\mathrm{species\_6}]}{\mathrm{Kmadpao}} + \frac{[\mathrm{species\_5}]}{\mathrm{Kmaspao}} + \frac{[\mathrm{species\_4}]}{\mathrm{Kmdpao}} + \frac{[\mathrm{species\_3}]}{\mathrm{Kmspao}}\right)} \tag{5}$$

7.6 Function definition function_4_gluconeogenesis_ser_1

Name function_4_gluconeogenesis_ser_1

Argument [c_ser]

Mathematical Expression

$$1.2 \cdot [\text{c\_ser}] \tag{6}$$

7.7 Function definition function_4_V_CTGL_1

Name function_4_V_CTGL_1

Arguments K_cyt_CTGL, Vm_CTGL, [cyt]

Mathematical Expression

$$\frac{\text{Vm\_CTGL} \cdot [\text{cyt}]}{\text{K\_cyt\_CTGL} + [\text{cyt}]} \tag{7}$$

7.8 Function definition function_4_V_GR_1

Name function_4_V_GR_1

Arguments K_NADPH_GR, K_gsg_GR, [NADPH], Vm_GR, [c_gsg]

Mathematical Expression

$$\frac{\text{Vm\_GR} \cdot [\text{c\_gsg}] \cdot [\text{NADPH}]}{(\text{K\_gsg\_GR} + [\text{c\_gsg}]) \cdot (\text{K\_NADPH\_GR} + [\text{NADPH}])} \tag{8}$$

7.9 Function definition function_4_V_GCS_1

Name function_4_V_GCS_1

Arguments [H2O2], K_cys_GCS, K_glu_GCS, Ka_GCS, Ke_GCS, Ki_GCS, Kp_GCS, Vm_GCS, [c_cys], [c_glu], [c_gsh], [glc], ssH2O2

Mathematical Expression

$$\frac{\text{Vm\_GCS} \cdot \left([\text{c\_cys}] \cdot [\text{c\_glu}] - \frac{[\text{glc}]}{\text{Ke\_GCS}}\right)}{\text{K\_cys\_GCS} \cdot \text{K\_glu\_GCS} + [\text{c\_glu}] \cdot \text{K\_cys\_GCS} + [\text{c\_cys}] \cdot \left(\text{K\_glu\_GCS} \cdot \left(1 + \frac{[\text{c\_gsh}]}{\text{Ki\_GCS}}\right) + [\text{c\_glu}]\right) + \frac{[\text{glc}]}{\text{Kp\_GCS}} + \frac{[}{\text{K}}} \cdot \frac{[\text{H2O2}] + \text{Ka\_GCS}}{\text{ssH2O2} + \text{Ka\_GCS}} \tag{9}$$

7.10 Function definition function_4_b_glu_loss_1

Name function_4_b_glu_loss_1

Argument [b_glu]

Mathematical Expression

$$0.1 \cdot [\text{b\_glu}] \tag{10}$$

7.11 Function definition function_4_V_GS_1

Name function_4_V_GS_1

Arguments K_glc_GS, K_gly_GS, Ke_GS, Kp_GS, Vm_GS, [c_gly], [c_gsh], [glc]

Mathematical Expression

$$\frac{\text{Vm\_GS} \cdot \left([\text{c\_gly}] \cdot [\text{glc}] - \frac{[\text{c\_gsh}]}{\text{Ke\_GS}}\right)}{\text{K\_gly\_GS} \cdot \text{K\_glc\_GS} + [\text{glc}] \cdot \text{K\_gly\_GS} + [\text{c\_gly}] \cdot (\text{K\_glc\_GS} + [\text{glc}]) + \frac{[\text{c\_gsh}]}{\text{Kp\_GS}}} \tag{11}$$

7.12 Function definition function_4_V_DNMT_1

Name function_4_V_DNMT_1

Arguments Ki_DNMT, Km_DNMT, Vm_DNMT, [sah], [sam]

Mathematical Expression

$$\text{Vm\_DNMT} \cdot \frac{[\text{sam}]}{\text{Km\_DNMT} \cdot \left(1 + \frac{[\text{sah}]}{\text{Ki\_DNMT}}\right) + [\text{sam}]} \tag{12}$$

7.13 Function definition function_4_V_ART_1

Name function_4_V_ART_1

Arguments K_10f_ART, K_aic_ART, Vm_ART, [aic], [c_10f]

Mathematical Expression

$$\frac{\text{Vm\_ART} \cdot [\text{c\_10f}] \cdot [\text{aic}]}{(\text{K\_10f\_ART} + [\text{c\_10f}]) \cdot (\text{K\_aic\_ART} + [\text{aic}])} \tag{13}$$

7.14 Function definition function_4_b_gsg_loss_1

Name function_4_b_gsg_loss_1

Argument [b_gsg]

Mathematical Expression

$$7.5 \cdot [\text{b\_gsg}] \tag{14}$$

7.15 Function definition function_4_VcFTD_1

Name function_4_VcFTD_1

Arguments K_10f_FTD, Vm_cFTD, [c_10f]

Mathematical Expression

$$\frac{\text{Vm\_cFTD} \cdot [\text{c\_10f}]}{\text{K\_10f\_FTD} + [\text{c\_10f}]} \tag{15}$$

7.16 Function definition function_4_V_MATI_1

Name function_4_V_MATI_1

Arguments Ki_MAT1, Km_MAT1, Vm_MAT1, [c_gsg], [met], [sam]

Mathematical Expression

$$\text{Vm\_MAT1} \cdot \frac{[\text{met}]}{\text{Km\_MAT1} + [\text{met}]} \cdot (0.23 + 0.8 \cdot \exp(0.0026 \cdot [\text{sam}])) \cdot \frac{\text{Ki\_MAT1} + 66.71}{\text{Ki\_MAT1} + [\text{c\_gsg}]} \tag{16}$$

7.17 Function definition function_4_V_SAMDC_1

Name function_4_V_SAMDC_1

Arguments Kapsamdc, Kiasamdc, Kissamdc, Kmsamdc, parameter_3, [sam], [species_1], [species_2], [species_3]

Mathematical Expression

$$\frac{\frac{\text{parameter\_3}}{1 + \frac{[\text{species\_3}]}{\text{Kissamdc}}} \cdot [\text{sam}]}{\text{Kmsamdc} \cdot \left(1 + \frac{\text{Kapsamdc}}{[\text{species\_2}]} + \frac{[\text{species\_1}]}{\text{Kiasamdc}}\right) + [\text{sam}]} \tag{17}$$

7.18 Function definition function_4_V_GDC_1

Name function_4_V_GDC_1

Arguments K_gly_GDC, K_thf_GDC, Vm_GDC, [m_gly], [m_thf]

Mathematical Expression

$$\frac{\text{Vm\_GDC} \cdot [\text{m\_thf}] \cdot [\text{m\_gly}]}{(\text{K\_thf\_GDC} + [\text{m\_thf}]) \cdot (\text{K\_gly\_GDC} + [\text{m\_gly}])} \tag{18}$$

7.19 Function definition function_4_cys_usage_1

Name function_4_cys_usage_1

Argument [c_cys]

Mathematical Expression

$$\frac{0.35 \cdot [\text{c\_cys}]^2}{200} \tag{19}$$

7.20 Function definition function_4_c_glu_usage_1

Name function_4_c_glu_usage_1

Argument [c_glu]

Mathematical Expression

$$0.07 \cdot [\text{c\_glu}] \tag{20}$$

7.21 Function definition function_4_V_DHFR_1

Name function_4_V_DHFR_1

Arguments K_NADPH_DHFR, K_dhf_DHFR, [NADPH], Vm_DHFR, [c_dhf]

Mathematical Expression

$$\frac{\text{Vm\_DHFR} \cdot [\text{c\_dhf}] \cdot [\text{NADPH}]}{(\text{K\_dhf\_DHFR} + [\text{c\_dhf}]) \cdot (\text{K\_NADPH\_DHFR} + [\text{NADPH}])} \tag{21}$$

7.22 Function definition function_4_V_MATIII_1

Name function_4_V_MATIII_1

Arguments Ka_MAT3, Ki_MAT3, Km_MAT3, Vm_MAT3, [c_gsg], [met], [sam]

Mathematical Expression

$$\text{Vm\_MAT3} \cdot \frac{[\text{met}]^{1.21}}{\text{Km\_MAT3} + [\text{met}]^{1.21}} \cdot \left(1 + \frac{7.2 \cdot [\text{sam}]^2}{\text{Ka\_MAT3}^2 + [\text{sam}]^2}\right) \cdot \frac{\text{Ki\_MAT3} + 66.71}{\text{Ki\_MAT3} + [\text{c\_gsg}]} \tag{22}$$

7.23 Function definition function_4_b_cys_cystine_conv_1

Name function_4_b_cys_cystine_conv_1

Argument [b_cys]

Mathematical Expression

$$0.25 \cdot [\text{b\_cys}] \tag{23}$$

7.24 Function definition function_4_V_GPX_1

Name function_4_V_GPX_1

Arguments [H2O2], K_H2O2_GPX, K_gsh_GPX, Vm_GPX, [c_gsh]

Mathematical Expression

$$\text{Vm\_GPX} \cdot \left(\frac{[\text{c\_gsh}]}{\text{K\_gsh\_GPX} + [\text{c\_gsh}]}\right)^2 \cdot \frac{[\text{H2O2}]}{\text{K\_H2O2\_GPX} + [\text{H2O2}]} \tag{24}$$

7.25 Function definition function_4_b_gsh_loss_1

Name function_4_b_gsh_loss_1

Argument [b_gsh]

Mathematical Expression

$$0.7 \cdot [\text{b\_gsh}] \tag{25}$$

7.26 Function definition function_4_V_SSAT_S_1

Name function_4_V_SSAT_S_1

Arguments C, Kmaccoassat, Kmcoassat, Kmdssat, Kmsssat, parameter_2, [species_3], [species_4], [species_8], [species_9]

Mathematical Expression

$$\frac{\frac{1}{C} \cdot \text{parameter\_2} \cdot [\text{species\_3}] \cdot [\text{species\_8}]}{\text{Kmsssat} \cdot \left(1 + \frac{[\text{species\_4}]}{\text{Kmdssat}}\right) \cdot \text{Kmaccoassat} \cdot \left(1 + \frac{[\text{species\_9}]}{\text{Kmcoassat}}\right) + \text{Kmaccoassat} \cdot \left(1 + \frac{[\text{species\_9}]}{\text{Kmcoassat}}\right) \cdot [\text{species\_3}] + \text{Kmsssa} \quad (26)$$

7.27 Function definition function_4_b_gsg_decomp_1

Name function_4_b_gsg_decomp_1

Argument [b_gsg]

Mathematical Expression

$$67.5 \cdot [\text{b\_gsg}] \quad (27)$$

7.28 Function definition function_4_b_gly_loss_1

Name function_4_b_gly_loss_1

Argument [b_gly]

Mathematical Expression

$$0.1 \cdot [\text{b\_gly}] \quad (28)$$

7.29 Function definition function_4_VmFTD_1

Name function_4_VmFTD_1

Arguments K_10f_FTD, Vm_mFTD, [m_10f]

Mathematical Expression

$$\frac{\text{Vm\_mFTD} \cdot [\text{m\_10f}]}{\text{K\_10f\_FTD} + [\text{m\_10f}]} \quad (29)$$

7.30 Function definition function_4_b_gsh_decomp_1

Name function_4_b_gsh_decomp_1

Argument [b_gsh]

Mathematical Expression

$$90 \cdot [\text{b\_gsh}] \quad (30)$$

7.31 Function definition function_4_V_TS_1

Name function_4_V_TS_1

Arguments [DUMP], K_2cf_TS, K_DUMP_TS, Vm_TS, [c_2cf]

Mathematical Expression

$$\frac{\text{Vm\_TS} \cdot [\text{DUMP}] \cdot [\text{c\_2cf}]}{(\text{K\_DUMP\_TS} + [\text{DUMP}]) \cdot (\text{K\_2cf\_TS} + [\text{c\_2cf}])} \tag{31}$$

7.32 Function definition function_4_V_PGT_1

Name function_4_V_PGT_1

Arguments [GAR], K_10f_PGT, K_GAR_PGT, Vm_PGT, [c_10f]

Mathematical Expression

$$\frac{\text{Vm\_PGT} \cdot [\text{c\_10f}] \cdot [\text{GAR}]}{(\text{K\_10f\_PGT} + [\text{c\_10f}]) \cdot (\text{K\_GAR\_PGT} + [\text{GAR}])} \tag{32}$$

7.33 Function definition function_4_VcNE_1

Name function_4_VcNE_1

Arguments [HCHO], [c_2cf], [c_thf], vol (cytosol), k1_cNE, k2_cNE

Mathematical Expression

$$\text{vol}\,(\text{cytosol}) \cdot (\text{k1\_cNE} \cdot [\text{c\_thf}] \cdot [\text{HCHO}] - \text{k2\_cNE} \cdot [\text{c\_2cf}]) \tag{33}$$

7.34 Function definition function_4_VmHCOOHc_1

Name function_4_VmHCOOHc_1

Arguments [c_coo], vol (cytosol), k_in_coo, k_out_coo, [m_coo], vol (mito)

Mathematical Expression

$$\frac{\text{k\_in\_coo} \cdot [\text{m\_coo}] \cdot \text{vol}\,(\text{mito})}{3} - \text{k\_out\_coo} \cdot [\text{c\_coo}] \cdot \text{vol}\,(\text{cytosol}) \tag{34}$$

7.35 Function definition function_4_c_gsg_degr_1

Name function_4_c_gsg_degr_1

Argument [c_gsg]

Mathematical Expression

$$0.1 \cdot [\text{c\_gsg}] \tag{35}$$

7.36 Function definition function_4_c_gsh_degr_1

Name function_4_c_gsh_degr_1

Argument [c_gsh]

Mathematical Expression

$$0.0020 \cdot [\text{c\_gsh}] \tag{36}$$

7.37 Function definition function_4_V_SSAT_D_1

Name function_4_V_SSAT_D_1

Arguments Kmaccoassat, Kmcoassat, Kmdssat, Kmsssat, parameter_2, [species_3], [species_4], [species_8], [species_9]

Mathematical Expression

$$\frac{\text{parameter\_2} \cdot [\text{species\_4}] \cdot [\text{species\_8}]}{\text{Kmdssat} \cdot \left(1 + \frac{[\text{species\_3}]}{\text{Kmsssat}}\right) \cdot \text{Kmaccoassat} \cdot \left(1 + \frac{[\text{species\_9}]}{\text{Kmcoassat}}\right) + \text{Kmaccoassat} \cdot \left(1 + \frac{[\text{species\_9}]}{\text{Kmcoassat}}\right) \cdot [\text{species\_4}] + \text{Kmdssa}} \tag{37}$$

7.38 Function definition function_4_VcFTS_1

Name function_4_VcFTS_1

Arguments K_coo_cFTS, K_thf_cFTS, Vm_cFTS, [c_coo], [c_thf]

Mathematical Expression

$$\frac{\text{Vm\_cFTS} \cdot [\text{c\_thf}] \cdot [\text{c\_coo}]}{(\text{K\_thf\_cFTS} + [\text{c\_thf}]) \cdot (\text{K\_coo\_cFTS} + [\text{c\_coo}])} \tag{38}$$

7.39 Function definition function_4_V_c_gshLb_1

Name function_4_V_c_gshLb_1

Arguments K_gshLb, V_gshLb, [c_gsh], vol (cytosol), h_gshLb

Mathematical Expression

$$\frac{\text{vol}\,(\text{cytosol}) \cdot \text{V\_gshLb} \cdot [\text{c\_gsh}]^{\text{h\_gshLb}}}{\text{K\_gshLb}^{\text{h\_gshLb}} + [\text{c\_gsh}]^{\text{h\_gshLb}}} \tag{39}$$

7.40 Function definition function_4_V_PAO_AD_1

Name function_4_V_PAO_AD_1

Arguments Kmadpao, Kmaspao, Kmdpao, Kmspao, Vmpao, [species_3], [species_4], [species_5], [species_6]

Mathematical Expression

$$\frac{\text{Vmpao} \cdot [\text{species\_6}]}{\text{Kmadpao} \cdot \left(1 + \frac{[\text{species\_6}]}{\text{Kmadpao}} + \frac{[\text{species\_5}]}{\text{Kmaspao}} + \frac{[\text{species\_4}]}{\text{Kmdpao}} + \frac{[\text{species\_3}]}{\text{Kmspao}}\right)} \tag{40}$$

7.41 Function definition function_4_V_SPDS_1

Name function_4_V_SPDS_1

Arguments KaSpds, Kiaspds, Kidspds, Kpspds, Vmspds, [species_1], [species_2], [species_4]

Mathematical Expression

$$\frac{\text{Vmspds} \cdot [\text{species\_1}] \cdot [\text{species\_2}]}{\text{Kiaspds} \cdot \text{Kpspds} \cdot \left(1 + \frac{[\text{species\_4}]}{\text{Kidspds}}\right) + \text{Kpspds} \cdot [\text{species\_1}] + \text{KaSpds} \cdot \left(1 + \frac{[\text{species\_4}]}{\text{Kidspds}}\right) \cdot [\text{species\_2}] + [\text{species\_1}] \cdot [\text{s}} \tag{41}$$

7.42 Function definition function_4_V_SPMS_1

Name function_4_V_SPMS_1

Arguments Kaspms, Kdspms, Kiaspms, Kisspms, Vmspms, [species_1], [species_3], [species_4]

Mathematical Expression

$$\frac{\text{Vmspms} \cdot [\text{species\_1}] \cdot [\text{species\_4}]}{\text{Kiaspms} \cdot \text{Kdspms} \cdot \left(1 + \frac{[\text{species\_3}]}{\text{Kisspms}}\right) + \text{Kdspms} \cdot [\text{species\_1}] + \text{Kaspms} \cdot \left(1 + \frac{[\text{species\_3}]}{\text{Kisspms}}\right) \cdot [\text{species\_4}] + [\text{species\_1}]} \tag{42}$$

7.43 Function definition MM

Name MM

Arguments Vmax, Km, S

Mathematical Expression

$$\frac{\text{Vmax} \cdot \text{S}}{\text{Km} + \text{S}} \tag{43}$$

7.44 Function definition MM_twosubst

Name MM_twosubst

Arguments Vmax, Km1, Km2, S1, S2

Mathematical Expression

$$\frac{\mathrm{Vmax} \cdot \mathrm{S1} \cdot \mathrm{S2}}{(\mathrm{Km1} + \mathrm{S1}) \cdot (\mathrm{Km2} + \mathrm{S2})} \tag{44}$$

7.45 Function definition function_4_V_b_MET_c_1

Name function_4_V_b_MET_c_1

Arguments K_bmetc, V_bmetc, [b_met], vol (cytosol), k_out_met, [met]

Mathematical Expression

$$\mathrm{vol}\,(\mathrm{cytosol}) \cdot (\mathrm{MM}\,(\mathrm{V\_bmetc}, \mathrm{K\_bmetc}, [\mathrm{b\_met}]) - \mathrm{k\_out\_met} \cdot [\mathrm{met}]) \tag{45}$$

7.46 Function definition function_4_VmMTCH_1

Name function_4_VmMTCH_1

Arguments K_10f_MTCH, K_1cf_MTCH, Vf_mMTCH, Vr_MTCH, [m_10f], [m_1cf]

Mathematical Expression

$$\mathrm{MM}\,(\mathrm{Vf\_mMTCH}, \mathrm{K\_1cf\_MTCH}, [\mathrm{m\_1cf}]) - \mathrm{MM}\,(\mathrm{Vr\_MTCH}, \mathrm{K\_10f\_MTCH}, [\mathrm{m\_10f}]) \tag{46}$$

7.47 Function definition function_4_VmFTS_1

Name function_4_VmFTS_1

Arguments K_10f_mFTS, K_coo_mFTS, K_thf_mFTS, Vf_mFTS, Vr_mFTS, [m_10f], [m_coo], [m_thf]

Mathematical Expression

$$\mathrm{MM\_twosubst}\,(\mathrm{Vf\_mFTS}, \mathrm{K\_thf\_mFTS}, \mathrm{K\_coo\_mFTS}, [\mathrm{m\_thf}], [\mathrm{m\_coo}]) - \mathrm{MM}\,(\mathrm{Vr\_mFTS}, \mathrm{K\_10f\_mFTS}, [\mathrm{m\_10f}]) \tag{47}$$

7.48 Function definition function_4_VmSERc_1

Name function_4_VmSERc_1

Arguments K_cser, K_mser, V_cser, V_mser, [c_ser], vol (cytosol), [m_ser], vol (mito)

Mathematical Expression

$$\left(\frac{\mathrm{MM}\left(\mathrm{V\_mser}, \mathrm{K\_mser}, [\mathrm{m\_ser}]\right) \cdot \mathrm{vol}\left(\mathrm{mito}\right)}{3} - \mathrm{MM}\left(\mathrm{V\_cser}, \mathrm{K\_cser}, [\mathrm{c\_ser}]\right)\right) \cdot \mathrm{vol}\left(\mathrm{cytosol}\right) \tag{48}$$

7.49 Function definition function_4_V_DMGD_1

Name function_4_V_DMGD_1

Arguments K_dmg_DMGD, K_thf_DMGD, Vm_DMGD, [dmg], [m_thf], vol (mito)

Mathematical Expression

$$\mathrm{vol}\left(\mathrm{mito}\right) \cdot \mathrm{MM\_twosubst}\left(\mathrm{Vm\_DMGD}, \mathrm{K\_thf\_DMGD}, \mathrm{K\_dmg\_DMGD}, [\mathrm{m\_thf}], [\mathrm{dmg}]\right) \tag{49}$$

7.50 Function definition function_4_V_MTHFR_1

Name function_4_V_MTHFR_1

Arguments K_2cf_MTHFR, K_NADPH_MTHFR, [NADPH], Vm_MTHFR, [c_2cf], [sah], [sam]

Mathematical Expression

$$\frac{\mathrm{MM\_twosubst}\left(\mathrm{Vm\_MTHFR}, \mathrm{K\_2cf\_MTHFR}, \mathrm{K\_NADPH\_MTHFR}, [\mathrm{c\_2cf}], [\mathrm{NADPH}]\right) \cdot 72}{10 + [\mathrm{sam}] - [\mathrm{sah}]} \tag{50}$$

7.51 Function definition function_4_V_SAHH_1

Name function_4_V_SAHH_1

Arguments K_hcy_SAHH, K_sah_SAHH, Vf_SAHH, Vr_SAHH, [hcy], [sah]

Mathematical Expression

$$\mathrm{MM}\left(\mathrm{Vf\_SAHH}, \mathrm{K\_sah\_SAHH}, [\mathrm{sah}]\right) - \mathrm{MM}\left(\mathrm{Vr\_SAHH}, \mathrm{K\_hcy\_SAHH}, [\mathrm{hcy}]\right) \tag{51}$$

7.52 Function definition function_4_V_c_gsgHb_1

Name function_4_V_c_gsgHb_1

Arguments K_gsgHb, V_gsgHb, [c_gsg], vol (cytosol)

Mathematical Expression

$$\text{vol}\,(\text{cytosol}) \cdot \text{MM}\,(\text{V\_gsgHb}, \text{K\_gsgHb}, [\text{c\_gsg}]) \tag{52}$$

7.53 Function definition function_4_VmGLYc_1

Name function_4_VmGLYc_1

Arguments K_cgly, K_mgly, V_cgly, V_mgly, [c_gly], vol (cytosol), [m_gly], vol (mito)

Mathematical Expression

$$\begin{aligned} &\text{MM}\,(\text{V\_mgly}, \text{K\_mgly}, [\text{m\_gly}]) \cdot \text{vol}\,(\text{mito}) \cdot \frac{1}{3} \\ &- \text{MM}\,(\text{V\_cgly}, \text{K\_cgly}, [\text{c\_gly}]) \cdot \text{vol}\,(\text{cytosol}) \end{aligned} \tag{53}$$

7.54 Function definition function_4_VcSHMT_1

Name function_4_VcSHMT_1

Arguments K_2cf_SHMT, K_gly_SHMT, K_ser_SHMT, K_thf_SHMT, Vf_cSHMT, Vr_cSHMT, [c_2cf], [c_gly], [c_ser], [c_thf]

Mathematical Expression

$$\begin{aligned} &\text{MM\_twosubst}\,(\text{Vf\_cSHMT}, \text{K\_thf\_SHMT}, \text{K\_ser\_SHMT}, \\ &[\text{c\_thf}], [\text{c\_ser}]) - \text{MM\_twosubst}\,(\text{Vr\_cSHMT}, \\ &\text{K\_gly\_SHMT}, \text{K\_2cf\_SHMT}, [\text{c\_gly}], [\text{c\_2cf}]) \end{aligned} \tag{54}$$

7.55 Function definition function_4_V_BHMT_1

Name function_4_V_BHMT_1

Arguments [BET], [H2O2], K_bet_BHMT, K_hcy_BHMT, Ki_BHMT, Vm_BHMT, vol (cytosol), [hcy], [sah], [sam], ssH2O2

Mathematical Expression

$$\begin{aligned} &\text{vol}\,(\text{cytosol}) \cdot \exp\,(0.0021 \cdot ([\text{sam}] + [\text{sah}])) \cdot \exp\,(0.0021 \cdot 102.6) \\ &\cdot \text{MM\_twosubst}\,(\text{Vm\_BHMT}, \text{K\_hcy\_BHMT}, \\ &\text{K\_bet\_BHMT}, [\text{hcy}], [\text{BET}]) \cdot \frac{\text{ssH2O2} + \text{Ki\_BHMT}}{[\text{H2O2}] + \text{Ki\_BHMT}} \end{aligned} \tag{55}$$

7.56 Function definition function_4_V_CBS_1

Name function_4_V_CBS_1

Arguments [H2O2], K_hcy_CBS, K_ser_CBS, Ka_CBS, Vm_CBS, [c_ser], [hcy], [sah], [sam], ssH2O2

Mathematical Expression

$$\begin{aligned}&\mathrm{MM\_twosubst}\left(\mathrm{Vm\_CBS}, \mathrm{K\_hcy\_CBS}, \mathrm{K\_ser\_CBS}, [\mathrm{hcy}], [\mathrm{c\_ser}]\right)\\ &\cdot \frac{\left(\frac{30}{102.59}\right)^2 + 1}{\left(\frac{30}{[\mathrm{sam}]+[\mathrm{sah}]}\right)^2 + 1} \cdot \frac{[\mathrm{H2O2}] + \mathrm{Ka\_CBS}}{\mathrm{ssH2O2} + \mathrm{Ka\_CBS}}\end{aligned} \tag{56}$$

7.57 Function definition function_4_V_c_gshHb_1

Name function_4_V_c_gshHb_1

Arguments K_gshHb, V_gshHb, [c_gsh], vol (cytosol)

Mathematical Expression

$$\mathrm{vol}\left(\mathrm{cytosol}\right) \cdot \mathrm{MM}\left(\mathrm{V\_gshHb}, \mathrm{K\_gshHb}, [\mathrm{c\_gsh}]\right) \tag{57}$$

7.58 Function definition function_4_V_b_SER_c_1

Name function_4_V_b_SER_c_1

Arguments K_bserc, V_bserc, [b_ser], [c_ser], vol (cytosol), k_out_ser

Mathematical Expression

$$\mathrm{vol}\left(\mathrm{cytosol}\right) \cdot \left(\mathrm{MM}\left(\mathrm{V\_bserc}, \mathrm{K\_bserc}, [\mathrm{b\_ser}]\right) - \mathrm{k\_out\_ser} \cdot [\mathrm{c\_ser}]\right) \tag{58}$$

7.59 Function definition function_4_V_b_GLY_c_1

Name function_4_V_b_GLY_c_1

Arguments K_bglyc, V_bglyc, [b_gly], [c_gly], vol (cytosol), k_out_gly

Mathematical Expression

$$\mathrm{vol}\left(\mathrm{cytosol}\right) \cdot \left(\mathrm{MM}\left(\mathrm{V\_bglyc}, \mathrm{K\_bglyc}, [\mathrm{b\_gly}]\right) - \mathrm{k\_out\_gly} \cdot [\mathrm{c\_gly}]\right) \tag{59}$$

7.60 Function definition function_4_VmMTD_1

Name function_4_VmMTD_1

Arguments K_1cf_MTD, K_2cf_MTD, Vf_mMTD, Vr_MTD, [m_1cf], [m_2cf]

Mathematical Expression

$$\mathrm{MM}(\mathrm{Vf\_mMTD}, \mathrm{K\_2cf\_MTD}, [\mathrm{m\_2cf}]) - \mathrm{MM}(\mathrm{Vr\_MTD}, \mathrm{K\_1cf\_MTD}, [\mathrm{m\_1cf}]) \quad (60)$$

7.61 Function definition function_4_VmSHMT_1

Name function_4_VmSHMT_1

Arguments K_2cf_SHMT, K_gly_SHMT, K_ser_SHMT, K_thf_SHMT, Vf_mSHMT, Vr_mSHMT, [m_2cf], [m_gly], [m_ser], [m_thf]

Mathematical Expression

$$\mathrm{MM\_twosubst}(\mathrm{Vf\_mSHMT}, \mathrm{K\_thf\_SHMT}, \mathrm{K\_ser\_SHMT}, [\mathrm{m\_thf}], [\mathrm{m\_ser}]) - \mathrm{MM\_twosubst}(\mathrm{Vr\_mSHMT}, \mathrm{K\_gly\_SHMT}, \mathrm{K\_2cf\_SHMT}, [\mathrm{m\_gly}], [\mathrm{m\_2cf}]) \quad (61)$$

7.62 Function definition function_4_V_b_GLU_c_1

Name function_4_V_b_GLU_c_1

Arguments K_bglutc, V_bglutc, [b_glu], [c_glu], vol (cytosol), k_out_glu

Mathematical Expression

$$\mathrm{vol}(\mathrm{cytosol}) \cdot (\mathrm{MM}(\mathrm{V\_bglutc}, \mathrm{K\_bglutc}, [\mathrm{b\_glu}]) - \mathrm{k\_out\_glu} \cdot [\mathrm{c\_glu}]) \quad (62)$$

7.63 Function definition function_4_VcMTD_1

Name function_4_VcMTD_1

Arguments K_1cf_MTD, K_2cf_MTD, Vf_cMTD, Vr_cMTD, [c_1cf], [c_2cf]

Mathematical Expression

$$\mathrm{MM}(\mathrm{Vf\_cMTD}, \mathrm{K\_2cf\_MTD}, [\mathrm{c\_2cf}]) - \mathrm{MM}(\mathrm{Vr\_cMTD}, \mathrm{K\_1cf\_MTD}, [\mathrm{c\_1cf}]) \quad (63)$$

7.64 Function definition function_4_V_b_CYS_c_1

Name function_4_V_b_CYS_c_1

Arguments K_bcysc, V_bcysc, [b_cys], vol (cytosol)

Mathematical Expression

$$\text{vol}\,(\text{cytosol}) \cdot \text{MM}\,(\text{V\_bcysc}, \text{K\_bcysc}, [\text{b\_cys}]) \tag{64}$$

7.65 Function definition function_4_VcMTCH_1

Name function_4_VcMTCH_1

Arguments K_10f_MTCH, K_1cf_MTCH, Vf_cMTCH, Vr_MTCH, [c_10f], [c_1cf]

Mathematical Expression

$$\text{MM}\,(\text{Vf\_cMTCH}, \text{K\_1cf\_MTCH}, [\text{c\_1cf}]) - \text{MM}\,(\text{Vr\_MTCH}, \text{K\_10f\_MTCH}, [\text{c\_10f}]) \tag{65}$$

7.66 Function definition function_4_V_c_gsgLb_1

Name function_4_V_c_gsgLb_1

Arguments K_gsgLb, V_gsgLb, [c_gsg], vol (cytosol)

Mathematical Expression

$$\text{vol}\,(\text{cytosol}) \cdot \text{MM}\,(\text{V\_gsgLb}, \text{K\_gsgLb}, [\text{c\_gsg}]) \tag{66}$$

7.67 Function definition function_4_V_GNMT_1

Name function_4_V_GNMT_1

Arguments K_gly_GNMT, K_sam_GNMT, Ki_GNMT, Vm_GNMT, [c_5mf], [c_gly], vol (cytosol), [sah], [sam]

Mathematical Expression

$$\begin{aligned} &\text{vol}\,(\text{cytosol}) \\ &\quad \cdot \text{MM\_twosubst}\,(\text{Vm\_GNMT}, \text{K\_sam\_GNMT}, \text{K\_gly\_GNMT}, [\text{sam}], [\text{c\_gly}]) \\ &\quad \cdot \frac{1}{1 + \frac{[\text{sah}]}{\text{Ki\_GNMT}}} \cdot \frac{4.8}{0.35 + [\text{c\_5mf}]} \end{aligned} \tag{67}$$

7.68 Function definition function_4_V_MS_1

Name function_4_V_MS_1

Arguments [H2O2], K_5mf_MS, K_hcy_MS, Ki_MS, Vm_MS, [c_5mf], [hcy], ssH2O2

Mathematical Expression

$$\frac{\text{MM\_twosubst}\left(\text{Vm\_MS}, \text{K\_5mf\_MS}, \text{K\_hcy\_MS}, [\text{c\_5mf}], [\text{hcy}]\right) \cdot (\text{ssH2O2} + \text{Ki\_MS})}{[\text{H2O2}] + \text{Ki\_MS}} \tag{68}$$

7.69 Function definition function_4_V_SDH_1

Name function_4_V_SDH_1

Arguments K_src_SDH, K_thf_SDH, Vm_SDH, [m_thf], vol (mito), [src]

Mathematical Expression

$$\text{vol}\left(\text{mito}\right) \cdot \text{MM\_twosubst}\left(\text{Vm\_SDH}, \text{K\_thf\_SDH}, \text{K\_src\_SDH}, [\text{m\_thf}], [\text{src}]\right) \tag{69}$$

8 Rules

This is an overview of 17 rules.

8.1 Rule tot_cfol

Rule tot_cfol is an assignment rule for parameter tot_cfol:

$$\text{tot\_cfol} = [\text{c\_5mf}] + [\text{c\_2cf}] + [\text{c\_1cf}] + [\text{c\_10f}] + [\text{c\_dhf}] + [\text{c\_thf}] \tag{70}$$

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

8.2 Rule tot_mfol

Rule tot_mfol is an assignment rule for parameter tot_mfol:

$$\text{tot\_mfol} = [\text{m\_thf}] + [\text{m\_2cf}] + [\text{m\_1cf}] + [\text{m\_10f}] \tag{71}$$

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

8.3 Rule daytime

Rule daytime is an assignment rule for parameter daytime:

$$\text{daytime} = \text{time} - 24 \cdot \left\lfloor \frac{\text{time}}{24} \right\rfloor \tag{72}$$

8.4 Rule aa_input

Rule aa_input is an assignment rule for parameter aa_input:

$$\text{aa\_input} = \begin{cases} \text{breakfast} & \text{if } (7 \leq \text{daytime}) \wedge \\ \begin{cases} \text{lunch} & \text{if } (12 \leq \text{daytime}) \wedge (\text{daytime} \leq 15) \\ \begin{cases} \text{dinner} & \text{if } (18 \leq \text{daytime}) \wedge (\text{daytime} \leq 21) \\ \text{fasting} & \text{otherwise} \end{cases} & \text{otherwise} \end{cases} & \text{otherwise} \end{cases} \tag{73}$$

8.5 Rule b_met

Rule b_met is an assignment rule for species b_met:

$$\text{b\_met} = \text{aa\_input} \cdot \text{b\_met\_basal} \tag{74}$$

8.6 Rule b_ser

Rule b_ser is an assignment rule for species b_ser:

$$\text{b\_ser} = \text{aa\_input} \cdot \text{b\_ser\_basal} \tag{75}$$

8.7 Rule V_oGly_b

Rule V_oGly_b is an assignment rule for parameter V_oGly_b:

$$\text{V\_oGly\_b} = \text{aa\_input} \cdot \text{V\_oGly\_b\_basal} \tag{76}$$

8.8 Rule V_oCys_b

Rule V_oCys_b is an assignment rule for parameter V_oCys_b:

$$\text{V\_oCys\_b} = \text{aa\_input} \cdot \text{V\_oCys\_b\_basal} \tag{77}$$

8.9 Rule V_oGlu_b

Rule V_oGlu_b is an assignment rule for parameter V_oGlu_b:

$$\text{V\_oGlu\_b} = \text{aa\_input} \cdot \text{V\_oGlu\_b\_basal} \tag{78}$$

8.10 Rule parameter_14

Rule parameter_14 is an assignment rule for parameter parameter_14:

$$\text{parameter\_14} = \text{parameter\_16} \tag{79}$$

8.11 Rule parameter_15

Rule parameter_15 is an assignment rule for parameter parameter_15:

$$\text{parameter\_15} = 3 \cdot \text{parameter\_16} \tag{80}$$

8.12 Rule parameter_17

Rule parameter_17 is an assignment rule for parameter parameter_17:

$$\text{parameter\_17} = [\text{species\_3}] + [\text{species\_4}] \tag{81}$$

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

8.13 Rule parameter_18

Rule parameter_18 is an assignment rule for parameter parameter_18:

$$\text{parameter\_18} = 100 \cdot \frac{\text{parameter\_16}}{0.24} \tag{82}$$

8.14 Rule parameter_1

Rule parameter_1 is a rate rule for parameter parameter_1:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\text{parameter\_1} = {} & 60 \cdot \text{parameter\_7} \cdot \frac{1}{1 + \text{parameter\_5} \cdot ([\text{species\_4}] + [\text{species\_3}])} \\ & - \text{parameter\_6} \cdot \text{parameter\_4} \cdot \text{parameter\_1}\end{aligned} \tag{83}$$

8.15 Rule parameter_2

Rule parameter_2 is a rate rule for parameter parameter_2:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\text{parameter\_2} = {} & 60 \cdot \text{parameter\_9} \cdot \left(1 - \frac{1}{1 + \text{parameter\_5} \cdot ([\text{species\_4}] + [\text{species\_3}])}\right) \\ & - \text{parameter\_8} \cdot \frac{1}{1 + \text{parameter\_5} \cdot ([\text{species\_4}] + [\text{species\_3}])} \cdot \text{parameter\_2}\end{aligned} \tag{84}$$

8.16 Rule parameter_3

Rule parameter_3 is a rate rule for parameter parameter_3:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\text{parameter\_3} = {} & 60 \cdot \text{parameter\_11} \cdot \frac{1}{1 + \text{parameter\_5} \cdot ([\text{species\_4}] + [\text{species\_3}])} \\ & - \text{parameter\_10} \cdot \text{parameter\_3}\end{aligned} \tag{85}$$

8.17 Rule parameter_4

Rule parameter_4 is a rate rule for parameter parameter_4:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{parameter\_4} = 1 \cdot \mathrm{parameter\_13} \cdot \left(1 - \frac{1}{1 + \mathrm{parameter\_5} \cdot 0.01 \cdot (\mathrm{[species\_4]} + \mathrm{[species\_3]})}\right) - \mathrm{parameter\_12} \cdot \mathrm{parameter\_4} \tag{86}$$

9 Reactions

This model contains 73 reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 5: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	b_gsh_decomp	b_gsh_decomp	$\mathrm{b\_gsh} \xrightleftharpoons{\mathrm{b\_gsh}} \mathrm{b\_cys} + \mathrm{b\_gly} + \mathrm{b\_glu}$	
2	b_gsg_decomp	b_gsg_decomp	$\mathrm{b\_gsg} \xrightleftharpoons{\mathrm{b\_gsg}} 2\,\mathrm{b\_cys} + 2\,\mathrm{b\_gly} + 2\,\mathrm{b\_glu}$	
3	b_cys_cystine-_conv	b_cys_cystine_conv	$\mathrm{b\_cys} \xrightleftharpoons{\mathrm{b\_cys}} \emptyset$	
4	b_cys_loss	b_cys_loss	$\mathrm{b\_cys} \xrightleftharpoons{\mathrm{b\_cys}} \emptyset$	
5	b_glu_loss	b_glu_loss	$\mathrm{b\_glu} \xrightleftharpoons{\mathrm{b\_glu}} \emptyset$	
6	b_gly_loss	b_gly_loss	$\mathrm{b\_gly} \xrightleftharpoons{\mathrm{b\_gly}} \emptyset$	
7	b_gsh_loss	b_gsh_loss	$\mathrm{b\_gsh} \xrightleftharpoons{\mathrm{b\_gsh}} \emptyset$	
8	b_gsg_loss	b_gsg_loss	$\mathrm{b\_gsg} \xrightleftharpoons{\mathrm{b\_gsg}} \emptyset$	
9	b_cys_import	b_cys_import	$\emptyset \rightleftharpoons \mathrm{b\_cys}$	
10	b_gly_import	b_gly_import	$\emptyset \rightleftharpoons \mathrm{b\_gly}$	
11	b_glu_import	b_glu_import	$\emptyset \rightleftharpoons \mathrm{b\_glu}$	
12	V_c_gshHb	V_c_gshHb	$\mathrm{c\_gsh} \xrightleftharpoons{\mathrm{c\_gsh}} \mathrm{b\_gsh}$	
13	V_c_gshLb	V_c_gshLb	$\mathrm{c\_gsh} \xrightleftharpoons{\mathrm{c\_gsh}} \mathrm{b\_gsh}$	
14	V_c_gsgHb	V_c_gsgHb	$\mathrm{c\_gsg} \xrightleftharpoons{\mathrm{c\_gsg}} \mathrm{b\_gsg}$	
15	V_c_gsgLb	V_c_gsgLb	$\mathrm{c\_gsg} \xrightleftharpoons{\mathrm{c\_gsg}} \mathrm{b\_gsg}$	

№	Id	Name	Reaction Equation	SBO
16	V_b_CYS_c	V_b_CYS_c	$\mathrm{b\_cys} \overset{\mathrm{b\_cys}}{\rightleftharpoons} \mathrm{c\_cys}$	
17	V_b_GLU_c	V_b_GLU_c	$\mathrm{b\_glu} \overset{\mathrm{b\_glu,\ c\_glu}}{\rightleftharpoons} \mathrm{c\_glu}$	
18	V_b_GLY_c	V_b_GLY_c	$\mathrm{b\_gly} \overset{\mathrm{b\_gly,\ c\_gly}}{\rightleftharpoons} \mathrm{c\_gly}$	
19	V_b_SER_c	V_b_SER_c	$\mathrm{b\_ser} \overset{\mathrm{b\_ser,\ c\_ser}}{\rightleftharpoons} \mathrm{c\_ser}$	
20	V_b_MET_c	V_b_MET_c	$\mathrm{b\_met} \overset{\mathrm{b\_met,\ met}}{\rightleftharpoons} \mathrm{met}$	
21	VmFTD	VmFTD	$\mathrm{m\_10f} \overset{\mathrm{m\_10f}}{\rightleftharpoons} \mathrm{m\_thf}$	
22	VmSHMT	VmSHMT	$\mathrm{m\_thf} + \mathrm{m\_ser} \overset{\mathrm{m\_2cf,\ m\_gly,\ m\_ser,\ m\_thf}}{\rightleftharpoons} \mathrm{m\_gly} + \mathrm{m\_2cf}$	
23	VmFTS	VmFTS	$\mathrm{m\_thf} + \mathrm{m\_coo} \overset{\mathrm{m\_10f,\ m\_coo,\ m\_thf}}{\rightleftharpoons} \mathrm{m\_10f}$	
24	VmNE	VmNE	$\mathrm{m\_thf} + \mathrm{HCHO} \overset{\mathrm{HCHO,\ m\_2cf,\ m\_thf}}{\rightleftharpoons} \mathrm{m\_2cf}$	
25	V_GDC	V_GDC	$\mathrm{m\_thf} + \mathrm{m\_gly} \overset{\mathrm{m\_gly,\ m\_thf}}{\rightleftharpoons} \mathrm{m\_2cf} + \mathrm{CO}$	
26	V_SDH	V_SDH	$\mathrm{m\_thf} + \mathrm{src} \overset{\mathrm{m\_thf,\ src}}{\rightleftharpoons} \mathrm{m\_2cf} + \mathrm{m\_gly}$	
27	V_DMGD	V_DMGD	$\mathrm{m\_thf} + \mathrm{dmg} \overset{\mathrm{dmg,\ m\_thf}}{\rightleftharpoons} \mathrm{m\_2cf} + \mathrm{src}$	
28	VmMTD	VmMTD	$\mathrm{m\_2cf} \overset{\mathrm{m\_1cf,\ m\_2cf}}{\rightleftharpoons} \mathrm{m\_1cf}$	
29	VmMTCH	VmMTCH	$\mathrm{m\_1cf} \overset{\mathrm{m\_10f,\ m\_1cf}}{\rightleftharpoons} \mathrm{m\_10f}$	
30	VmSERc	VmSERc	$3\,\mathrm{m\_ser} \overset{\mathrm{c\_ser,\ m\_ser}}{\rightleftharpoons} \mathrm{c\_ser}$	
31	VmHCOOHc	VmHCOOHc	$3\,\mathrm{m\_coo} \overset{\mathrm{c\_coo,\ m\_coo}}{\rightleftharpoons} \mathrm{c\_coo}$	
32	VmGLYc	VmGLYc	$3\,\mathrm{m\_gly} \overset{\mathrm{c\_gly,\ m\_gly}}{\rightleftharpoons} \mathrm{c\_gly}$	
33	V_MS	V_MS	$\mathrm{c\_5mf} + \mathrm{hcy} \overset{\mathrm{H2O2,\ c\_5mf,\ hcy}}{\rightleftharpoons} \mathrm{c\_thf} + \mathrm{met}$	

№	Id	Name	Reaction Equation	SBO
34	V_DHFR	V_DHFR	$\text{c\_dhf} + \text{NADPH} \overset{\text{NADPH, c\_dhf}}{\rightleftharpoons} \text{c\_thf}$	
35	VcFTD	VcFTD	$\text{c\_10f} \overset{\text{c\_10f}}{\rightleftharpoons} \text{c\_thf}$	
36	V_PGT	V_PGT	$\text{c\_10f} + \text{GAR} \overset{\text{GAR, c\_10f}}{\rightleftharpoons} \text{aic} + \text{c\_thf}$	
37	VcFTS	VcFTS	$\text{c\_thf} + \text{c\_coo} \overset{\text{c\_coo, c\_thf}}{\rightleftharpoons} \text{c\_10f}$	
38	VcSHMT	VcSHMT	$\text{c\_ser} + \text{c\_thf} \overset{\text{c\_2cf, c\_gly, c\_ser, c\_thf}}{\rightleftharpoons} \text{c\_gly} + \text{c\_2cf}$	
39	VcNE	VcNE	$\text{c\_thf} + \text{HCHO} \overset{\text{HCHO, c\_2cf, c\_thf}}{\rightleftharpoons} \text{c\_2cf}$	
40	V_TS	V_TS	$\text{DUMP} + \text{c\_2cf} \overset{\text{DUMP, c\_2cf}}{\rightleftharpoons} \text{c\_dhf}$	
41	V_MTHFR	V_MTHFR	$\text{c\_2cf} + \text{NADPH} \overset{\text{sah, sam, NADPH, c\_2cf}}{\rightleftharpoons} \text{c\_5mf}$	
42	VcMTD	VcMTD	$\text{c\_2cf} \overset{\text{c\_1cf, c\_2cf}}{\rightleftharpoons} \text{c\_1cf} + \text{NADPH}$	
43	VcMTCH	VcMTCH	$\text{c\_1cf} \overset{\text{c\_10f, c\_1cf}}{\rightleftharpoons} \text{c\_10f}$	
44	V_ART	V_ART	$\text{c\_10f} + \text{aic} \overset{\text{aic, c\_10f}}{\rightleftharpoons} \text{c\_thf}$	
45	V_BHMT	V_BHMT	$\text{hcy} + \text{BET} \overset{\text{H2O2, sah, sam, BET, hcy}}{\rightleftharpoons} \text{met} + \text{dmg}$	
46	V_MATI	V_MATI	$\text{met} \overset{\text{c\_gsg, met, sam}}{\rightleftharpoons} \text{sam}$	
47	V_MATIII	V_MATIII	$\text{met} \overset{\text{c\_gsg, met, sam}}{\rightleftharpoons} \text{sam}$	
48	V_GNMT	V_GNMT	$\text{sam} + \text{c\_gly} \overset{\text{c\_5mf, c\_gly, sah, sam}}{\rightleftharpoons} \text{sah} + \text{src}$	
49	V_DNMT	V_DNMT	$\text{sam} \overset{\text{sah, sam}}{\rightleftharpoons} \text{sah}$	
50	V_SAHH	V_SAHH	$\text{sah} \overset{\text{hcy, sah}}{\rightleftharpoons} \text{hcy}$	
51	gluconeogenesis_ser	gluconeogenesis_ser	$\text{c\_ser} \overset{\text{c\_ser}}{\rightleftharpoons} \emptyset$	

№	Id	Name	Reaction Equation	SBO
52	V_CBS	V_CBS	$\mathrm{hcy} + \mathrm{c\_ser} \xrightleftharpoons{\mathrm{H2O2,\ sah,\ sam,\ c\_ser,\ hcy}} \mathrm{cyt}$	
53	V_CTGL	V_CTGL	$\mathrm{cyt} \xrightleftharpoons{\mathrm{cyt}} \mathrm{c\_cys}$	
54	V_GCS	V_GCS	$\mathrm{c\_cys} + \mathrm{c\_glu} \xrightleftharpoons{\mathrm{H2O2,\ c\_gsh,\ c\_cys,\ c\_glu,\ glc}} \mathrm{glc}$	
55	cys_usage	cys_usage	$\mathrm{c\_cys} \xrightleftharpoons{\mathrm{c\_cys}} \emptyset$	
56	c_glu_usage	c_glu_usage	$\mathrm{c\_glu} \xrightleftharpoons{\mathrm{c\_glu}} \emptyset$	
57	V_GS	V_GS	$\mathrm{glc} + \mathrm{c\_gly} \xrightleftharpoons{\mathrm{c\_gly,\ c\_gsh,\ glc}} \mathrm{c\_gsh}$	
58	V_GPX	V_GPX	$2\,\mathrm{c\_gsh} + \mathrm{H2O2} \xrightleftharpoons{\mathrm{H2O2,\ c\_gsh}} \mathrm{c\_gsg}$	
59	V_GR	V_GR	$\mathrm{c\_gsg} + \mathrm{NADPH} \xrightleftharpoons{\mathrm{NADPH,\ c\_gsg}} 2\,\mathrm{c\_gsh}$	
60	c_gsh_degr	c_gsh_degr	$\mathrm{c\_gsh} \xrightleftharpoons{\mathrm{c\_gsh}} \emptyset$	
61	c_gsg_degr	c_gsg_degr	$\mathrm{c\_gsg} \xrightleftharpoons{\mathrm{c\_gsg}} \emptyset$	
62	reaction_1	V_ODC	$\mathrm{species\_7} \xrightleftharpoons{\mathrm{species\_2,\ species\_7}} \mathrm{species\_2}$	
63	reaction_2	V_SAMDC	$\mathrm{sam} \xrightleftharpoons{\mathrm{species\_3,\ species\_2,\ sam,\ species\_1}} \mathrm{species\_1}$	
64	reaction_3	V_SSAT_S	$\mathrm{species\_3} + \mathrm{species\_8} \xrightleftharpoons{\mathrm{species\_4,\ species\_3,\ species\_8,\ species\_9}} \mathrm{species\_5} + \mathrm{species\_9}$	
65	reaction_4	V_SSAT_D	$\mathrm{species\_4} + \mathrm{species\_8} \xrightleftharpoons{\mathrm{species\_3,\ species\_4,\ species\_8,\ species\_9}} \mathrm{species\_6} + \mathrm{species\_9}$	
66	reaction_5	V_PAO_AD	$\mathrm{species\_6} \xrightleftharpoons{\mathrm{species\_5,\ species\_4,\ species\_3,\ species\_6}} \mathrm{species\_2}$	
67	reaction_6	V_PAO_AS	$\mathrm{species\_5} \xrightleftharpoons{\mathrm{species\_6,\ species\_3,\ species\_4,\ species\_5}} \mathrm{species\_4}$	
68	reaction_7	V_SPDS	$\mathrm{species\_1} + \mathrm{species\_2} \xrightleftharpoons{\mathrm{species\_1,\ species\_2,\ species\_4}} \mathrm{species\_4}$	

№	Id	Name	Reaction Equation	SBO
69	reaction_8	V_SPMS	$\text{species\_1} + \text{species\_4} \xrightleftharpoons{\text{species\_1, species\_3, species\_4}} \text{species\_3}$	
70	reaction_9	V_COA	$\text{species\_8} \xrightarrow{\text{species\_8}} \text{species\_9}$	
71	reaction_10	V_ACCOA	$\text{species\_9} \xrightarrow{\text{species\_9}} \text{species\_8}$	
72	reaction_11	V_PUT_efflux	$\text{species\_2} \xrightarrow{\text{species\_2}} \emptyset$	
73	reaction_12	V_AD_efflux	$\text{species\_6} \xrightarrow{\text{species\_6}} \emptyset$	

9.1 Reaction b_gsh_decomp

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

Name b_gsh_decomp

Reaction equation

$$\text{b\_gsh} \overset{\text{b\_gsh}}{\rightleftharpoons} \text{b\_cys} + \text{b\_gly} + \text{b\_glu} \tag{87}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
b_gsh	b_GSH	

Modifier

Table 7: Properties of each modifier.

Id	Name	SBO
b_gsh	b_GSH	

Products

Table 8: Properties of each product.

Id	Name	SBO
b_cys	b_Cysteine	
b_gly	b_Glycine	
b_glu	b_Glutamate	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}(\text{blood}) \cdot \text{function\_4\_b\_gsh\_decomp\_1}([\text{b\_gsh}]) \tag{88}$$

$$\text{function\_4\_b\_gsh\_decomp\_1}([\text{b\_gsh}]) = 90 \cdot [\text{b\_gsh}] \tag{89}$$

$$\text{function\_4\_b\_gsh\_decomp\_1}\left([\text{b\_gsh}]\right) = 90 \cdot [\text{b\_gsh}] \tag{90}$$

9.2 Reaction b_gsg_decomp

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

Name b_gsg_decomp

Reaction equation

$$\text{b\_gsg} \overset{\text{b\_gsg}}{\rightleftharpoons} 2\,\text{b\_cys} + 2\,\text{b\_gly} + 2\,\text{b\_glu} \tag{91}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
b_gsg	b_GSSG	

Modifier

Table 10: Properties of each modifier.

Id	Name	SBO
b_gsg	b_GSSG	

Products

Table 11: Properties of each product.

Id	Name	SBO
b_cys	b_Cysteine	
b_gly	b_Glycine	
b_glu	b_Glutamate	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol}\left(\text{blood}\right) \cdot \text{function\_4\_b\_gsg\_decomp\_1}\left([\text{b\_gsg}]\right) \tag{92}$$

$$\text{function\_4\_b\_gsg\_decomp\_1}([\text{b\_gsg}]) = 67.5 \cdot [\text{b\_gsg}] \tag{93}$$

$$\text{function\_4\_b\_gsg\_decomp\_1}([\text{b\_gsg}]) = 67.5 \cdot [\text{b\_gsg}] \tag{94}$$

9.3 Reaction b_cys_cystine_conv

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

Name b_cys_cystine_conv

Reaction equation

$$\text{b\_cys} \overset{\text{b\_cys}}{\rightleftharpoons} \emptyset \tag{95}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
b_cys	b_Cysteine	

Modifier

Table 13: Properties of each modifier.

Id	Name	SBO
b_cys	b_Cysteine	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}(\text{blood}) \cdot \text{function\_4\_b\_cys\_cystine\_conv\_1}([\text{b\_cys}]) \tag{96}$$

$$\text{function\_4\_b\_cys\_cystine\_conv\_1}([\text{b\_cys}]) = 0.25 \cdot [\text{b\_cys}] \tag{97}$$

$$\text{function\_4\_b\_cys\_cystine\_conv\_1}([\text{b\_cys}]) = 0.25 \cdot [\text{b\_cys}] \tag{98}$$

9.4 Reaction b_cys_loss

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

Name b_cys_loss

Reaction equation

$$\text{b\_cys} \underset{}{\overset{\text{b\_cys}}{\rightleftharpoons}} \emptyset \tag{99}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
b_cys	b_Cysteine	

Modifier

Table 15: Properties of each modifier.

Id	Name	SBO
b_cys	b_Cysteine	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{vol}\,(\text{blood}) \cdot \text{function\_4\_b\_cys\_loss\_1}\,([\text{b\_cys}]) \tag{100}$$

$$\text{function\_4\_b\_cys\_loss\_1}\,([\text{b\_cys}]) = 0.1 \cdot [\text{b\_cys}] \tag{101}$$

$$\text{function\_4\_b\_cys\_loss\_1}\,([\text{b\_cys}]) = 0.1 \cdot [\text{b\_cys}] \tag{102}$$

9.5 Reaction b_glu_loss

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

Name b_glu_loss

Reaction equation

$$\text{b\_glu} \underset{}{\overset{\text{b\_glu}}{\rightleftharpoons}} \emptyset \tag{103}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
b_glu	b_Glutamate	

Modifier

Table 17: Properties of each modifier.

Id	Name	SBO
b_glu	b_Glutamate	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\left(\mathrm{blood}\right) \cdot \mathrm{function\_4\_b\_glu\_loss\_1}\left(\left[\mathrm{b\_glu}\right]\right) \tag{104}$$

$$\mathrm{function\_4\_b\_glu\_loss\_1}\left(\left[\mathrm{b\_glu}\right]\right) = 0.1 \cdot \left[\mathrm{b\_glu}\right] \tag{105}$$

$$\mathrm{function\_4\_b\_glu\_loss\_1}\left(\left[\mathrm{b\_glu}\right]\right) = 0.1 \cdot \left[\mathrm{b\_glu}\right] \tag{106}$$

9.6 Reaction b_gly_loss

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

Name b_gly_loss

Reaction equation

$$\mathrm{b\_gly} \underset{}{\overset{\mathrm{b\_gly}}{\rightleftharpoons}} \emptyset \tag{107}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
b_gly	b_Glycine	

Modifier

Table 19: Properties of each modifier.

Id	Name	SBO
b_gly	b_Glycine	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{vol}(\text{blood}) \cdot \text{function\_4\_b\_gly\_loss\_1}([\text{b\_gly}]) \tag{108}$$

$$\text{function\_4\_b\_gly\_loss\_1}([\text{b\_gly}]) = 0.1 \cdot [\text{b\_gly}] \tag{109}$$

$$\text{function\_4\_b\_gly\_loss\_1}([\text{b\_gly}]) = 0.1 \cdot [\text{b\_gly}] \tag{110}$$

9.7 Reaction b_gsh_loss

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

Name b_gsh_loss

Reaction equation

$$\text{b\_gsh} \overset{\text{b\_gsh}}{\rightleftharpoons} \emptyset \tag{111}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
b_gsh	b_GSH	

Modifier

Table 21: Properties of each modifier.

Id	Name	SBO
b_gsh	b_GSH	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{blood}) \cdot \mathrm{function\_4\_b\_gsh\_loss\_1}\,([\mathrm{b\_gsh}]) \tag{112}$$

$$\mathrm{function\_4\_b\_gsh\_loss\_1}\,([\mathrm{b\_gsh}]) = 0.7 \cdot [\mathrm{b\_gsh}] \tag{113}$$

$$\mathrm{function\_4\_b\_gsh\_loss\_1}\,([\mathrm{b\_gsh}]) = 0.7 \cdot [\mathrm{b\_gsh}] \tag{114}$$

9.8 Reaction b_gsg_loss

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

Name b_gsg_loss

Reaction equation

$$\mathrm{b\_gsg} \underset{}{\overset{\mathrm{b\_gsg}}{\rightleftharpoons}} \emptyset \tag{115}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
b_gsg	b_GSSG	

Modifier

Table 23: Properties of each modifier.

Id	Name	SBO
b_gsg	b_GSSG	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\left(\mathrm{blood}\right) \cdot \mathrm{function\_4\_b\_gsg\_loss\_1}\left(\left[\mathrm{b\_gsg}\right]\right) \tag{116}$$

$$\mathrm{function\_4\_b\_gsg\_loss\_1}\left(\left[\mathrm{b\_gsg}\right]\right) = 7.5 \cdot \left[\mathrm{b\_gsg}\right] \tag{117}$$

$$\mathrm{function\_4\_b\_gsg\_loss\_1}\left(\left[\mathrm{b\_gsg}\right]\right) = 7.5 \cdot \left[\mathrm{b\_gsg}\right] \tag{118}$$

9.9 Reaction `b_cys_import`

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

Name b_cys_import

Reaction equation

$$\emptyset \rightleftharpoons \mathrm{b\_cys} \tag{119}$$

Product

Table 24: Properties of each product.

Id	Name	SBO
`b_cys`	b_Cysteine	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\left(\mathrm{blood}\right) \cdot \mathrm{Constant\_flux\_\_reversible}\left(\mathrm{V\_oCys\_b}\right) \tag{120}$$

$$\mathrm{Constant\_flux\_\_reversible}\left(\mathrm{v}\right) = \mathrm{v} \tag{121}$$

$$\mathrm{Constant\_flux\_\_reversible}\left(\mathrm{v}\right) = \mathrm{v} \tag{122}$$

9.10 Reaction `b_gly_import`

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

Name b_gly_import

Reaction equation

$$\emptyset \rightleftharpoons \text{b\_gly} \tag{123}$$

Product

Table 25: Properties of each product.

Id	Name	SBO
b_gly	b_Glycine	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{vol}\left(\text{blood}\right) \cdot \text{Constant\_flux\_\_reversible}\left(\text{V\_oGly\_b}\right) \tag{124}$$

$$\text{Constant\_flux\_\_reversible}\left(\text{v}\right) = \text{v} \tag{125}$$

$$\text{Constant\_flux\_\_reversible}\left(\text{v}\right) = \text{v} \tag{126}$$

9.11 Reaction b_glu_import

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

Name b_glu_import

Reaction equation

$$\emptyset \rightleftharpoons \text{b\_glu} \tag{127}$$

Product

Table 26: Properties of each product.

Id	Name	SBO
b_glu	b_Glutamate	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{blood}) \cdot \mathrm{Constant\_flux\_\_reversible}\,(\mathrm{V\_oGlu\_b}) \tag{128}$$

$$\mathrm{Constant\_flux\_\_reversible}\,(\mathrm{v}) = \mathrm{v} \tag{129}$$

$$\mathrm{Constant\_flux\_\_reversible}\,(\mathrm{v}) = \mathrm{v} \tag{130}$$

9.12 Reaction V_c_gshHb

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

Name V_c_gshHb

Reaction equation

$$\mathrm{c\_gsh} \overset{\mathrm{c\_gsh}}{\rightleftharpoons} \mathrm{b\_gsh} \tag{131}$$

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
c_gsh	c_GSH	

Modifier

Table 28: Properties of each modifier.

Id	Name	SBO
c_gsh	c_GSH	

Product

Table 29: Properties of each product.

Id	Name	SBO
b_gsh	b_GSH	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \text{function\_4\_V\_c\_gshHb\_1}\left(\text{K\_gshHb}, \text{V\_gshHb}, [\text{c\_gsh}], \text{vol}\left(\text{cytosol}\right)\right) \tag{132}$$

$$\begin{aligned}&\text{function\_4\_V\_c\_gshHb\_1}\left(\text{K\_gshHb}, \text{V\_gshHb}, [\text{c\_gsh}], \text{vol}\left(\text{cytosol}\right)\right)\\ &= \text{vol}\left(\text{cytosol}\right) \cdot \text{MM}\left(\text{V\_gshHb}, \text{K\_gshHb}, [\text{c\_gsh}]\right)\end{aligned} \tag{133}$$

9.13 Reaction V_c_gshLb

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

Name V_c_gshLb

Reaction equation

$$\text{c\_gsh} \overset{\text{c\_gsh}}{\rightleftharpoons} \text{b\_gsh} \tag{134}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
c_gsh	c_GSH	

Modifier

Table 31: Properties of each modifier.

Id	Name	SBO
c_gsh	c_GSH	

Product

Table 32: Properties of each product.

Id	Name	SBO
b_gsh	b_GSH	

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \text{function\_4\_V\_c\_gshLb\_1}\left(\text{K\_gshLb}, \text{V\_gshLb}, [\text{c\_gsh}], \text{vol}\left(\text{cytosol}\right), \text{h\_gshLb}\right) \quad (135)$$

$$\begin{aligned} &\text{function\_4\_V\_c\_gshLb\_1}\left(\text{K\_gshLb}, \text{V\_gshLb}, [\text{c\_gsh}], \text{vol}\left(\text{cytosol}\right), \text{h\_gshLb}\right) \\ &= \frac{\text{vol}\left(\text{cytosol}\right) \cdot \text{V\_gshLb} \cdot [\text{c\_gsh}]^{\text{h\_gshLb}}}{\text{K\_gshLb}^{\text{h\_gshLb}} + [\text{c\_gsh}]^{\text{h\_gshLb}}} \end{aligned} \quad (136)$$

9.14 Reaction V_c_gsgHb

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

Name V_c_gsgHb

Reaction equation

$$\text{c\_gsg} \overset{\text{c\_gsg}}{\rightleftharpoons} \text{b\_gsg} \quad (137)$$

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
c_gsg	c_GSSG	

Modifier

Table 34: Properties of each modifier.

Id	Name	SBO
c_gsg	c_GSSG	

Product

Table 35: Properties of each product.

Id	Name	SBO
b_gsg	b_GSSG	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \text{function\_4\_V\_c\_gsgHb\_1}\left(\text{K\_gsgHb}, \text{V\_gsgHb}, [\text{c\_gsg}], \text{vol}\left(\text{cytosol}\right)\right) \tag{138}$$

$$\begin{aligned} &\text{function\_4\_V\_c\_gsgHb\_1}\left(\text{K\_gsgHb}, \text{V\_gsgHb}, [\text{c\_gsg}], \text{vol}\left(\text{cytosol}\right)\right) \\ &= \text{vol}\left(\text{cytosol}\right) \cdot \text{MM}\left(\text{V\_gsgHb}, \text{K\_gsgHb}, [\text{c\_gsg}]\right) \end{aligned} \tag{139}$$

9.15 Reaction V_c_gsgLb

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

Name V_c_gsgLb

Reaction equation

$$\text{c\_gsg} \overset{\text{c\_gsg}}{\rightleftharpoons} \text{b\_gsg} \tag{140}$$

Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
c_gsg	c_GSSG	

Modifier

Table 37: Properties of each modifier.

Id	Name	SBO
c_gsg	c_GSSG	

Product

Table 38: Properties of each product.

Id	Name	SBO
b_gsg	b_GSSG	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{function\_4\_V\_c\_gsgLb\_1}\left(\text{K\_gsgLb}, \text{V\_gsgLb}, [\text{c\_gsg}], \text{vol}\left(\text{cytosol}\right)\right) \tag{141}$$

$$\begin{aligned} &\text{function\_4\_V\_c\_gsgLb\_1}\left(\text{K\_gsgLb}, \text{V\_gsgLb}, [\text{c\_gsg}], \text{vol}\left(\text{cytosol}\right)\right) \\ &= \text{vol}\left(\text{cytosol}\right) \cdot \text{MM}\left(\text{V\_gsgLb}, \text{K\_gsgLb}, [\text{c\_gsg}]\right) \end{aligned} \tag{142}$$

9.16 Reaction V_b_CYS_c

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

Name V_b_CYS_c

Reaction equation

$$\text{b\_cys} \underset{}{\overset{\text{b\_cys}}{\rightleftharpoons}} \text{c\_cys} \tag{143}$$

Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
b_cys	b_Cysteine	

Modifier

Table 40: Properties of each modifier.

Id	Name	SBO
b_cys	b_Cysteine	

Id	Name	SBO

Product

Table 41: Properties of each product.

Id	Name	SBO
c_cys	c_Cysteine	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \text{function\_4\_V\_b\_CYS\_c\_1}\left(\text{K\_bcysc}, \text{V\_bcysc}, [\text{b\_cys}], \text{vol}\left(\text{cytosol}\right)\right) \tag{144}$$

$$\begin{aligned} &\text{function\_4\_V\_b\_CYS\_c\_1}\left(\text{K\_bcysc}, \text{V\_bcysc}, [\text{b\_cys}], \text{vol}\left(\text{cytosol}\right)\right) \\ &= \text{vol}\left(\text{cytosol}\right) \cdot \text{MM}\left(\text{V\_bcysc}, \text{K\_bcysc}, [\text{b\_cys}]\right) \end{aligned} \tag{145}$$

9.17 Reaction V_b_GLU_c

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

Name V_b_GLU_c

Reaction equation

$$\text{b\_glu} \xrightleftharpoons{\text{b\_glu, c\_glu}} \text{c\_glu} \tag{146}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
b_glu	b_Glutamate	

Modifiers

Table 43: Properties of each modifier.

Id	Name	SBO
b_glu	b_Glutamate	
c_glu	c_Glutamate	

Product

Table 44: Properties of each product.

Id	Name	SBO
c_glu	c_Glutamate	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \text{function\_4\_V\_b\_GLU\_c\_1}\left(\text{K\_bglutc}, \text{V\_bglutc}, [\text{b\_glu}], [\text{c\_glu}], \text{vol}\left(\text{cytosol}\right), \text{k\_out\_glu}\right) \tag{147}$$

$$\begin{aligned}&\text{function\_4\_V\_b\_GLU\_c\_1}\left(\text{K\_bglutc}, \text{V\_bglutc}, [\text{b\_glu}], [\text{c\_glu}], \text{vol}\left(\text{cytosol}\right), \text{k\_out\_glu}\right)\\ &\quad = \text{vol}\left(\text{cytosol}\right) \cdot \left(\text{MM}\left(\text{V\_bglutc}, \text{K\_bglutc}, [\text{b\_glu}]\right) - \text{k\_out\_glu} \cdot [\text{c\_glu}]\right)\end{aligned} \tag{148}$$

9.18 Reaction V_b_GLY_c

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

Name V_b_GLY_c

Reaction equation

$$\text{b\_gly} \overset{\text{b\_gly, c\_gly}}{\rightleftharpoons} \text{c\_gly} \tag{149}$$

Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
b_gly	b_Glycine	

Modifiers

Table 46: Properties of each modifier.

Id	Name	SBO
b_gly	b_Glycine	
c_gly	c_Glycine	

Product

Table 47: Properties of each product.

Id	Name	SBO
c_gly	c_Glycine	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \text{function\_4\_V\_b\_GLY\_c\_1}\left(\text{K\_bglyc}, \text{V\_bglyc}, [\text{b\_gly}], [\text{c\_gly}], \text{vol}\left(\text{cytosol}\right), \text{k\_out\_gly}\right) \tag{150}$$

$$\begin{aligned} &\text{function\_4\_V\_b\_GLY\_c\_1}\left(\text{K\_bglyc}, \text{V\_bglyc}, [\text{b\_gly}], [\text{c\_gly}], \text{vol}\left(\text{cytosol}\right), \text{k\_out\_gly}\right) \\ &= \text{vol}\left(\text{cytosol}\right) \cdot \left(\text{MM}\left(\text{V\_bglyc}, \text{K\_bglyc}, [\text{b\_gly}]\right) - \text{k\_out\_gly} \cdot [\text{c\_gly}]\right) \end{aligned} \tag{151}$$

9.19 Reaction V_b_SER_c

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

Name V_b_SER_c

Reaction equation

$$\text{b\_ser} \underset{}{\overset{\text{b\_ser, c\_ser}}{\rightleftharpoons}} \text{c\_ser} \tag{152}$$

Reactant

Table 48: Properties of each reactant.

Id	Name	SBO
b_ser	b_Serine	

Modifiers

Table 49: Properties of each modifier.

Id	Name	SBO
b_ser	b_Serine	
c_ser	c_Serine	

Product

Table 50: Properties of each product.

Id	Name	SBO
c_ser	c_Serine	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \text{function\_4\_V\_b\_SER\_c\_1}\left(\text{K\_bserc}, \text{V\_bserc}, [\text{b\_ser}], [\text{c\_ser}], \text{vol}\left(\text{cytosol}\right), \text{k\_out\_ser}\right) \tag{153}$$

$$\begin{aligned}&\text{function\_4\_V\_b\_SER\_c\_1}\left(\text{K\_bserc}, \text{V\_bserc}, [\text{b\_ser}], [\text{c\_ser}], \text{vol}\left(\text{cytosol}\right), \text{k\_out\_ser}\right)\\ &= \text{vol}\left(\text{cytosol}\right) \cdot \left(\text{MM}\left(\text{V\_bserc}, \text{K\_bserc}, [\text{b\_ser}]\right) - \text{k\_out\_ser} \cdot [\text{c\_ser}]\right)\end{aligned} \tag{154}$$

9.20 Reaction V_b_MET_c

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

Name V_b_MET_c

Reaction equation

$$\text{b\_met} \overset{\text{b\_met, met}}{\rightleftharpoons} \text{met} \tag{155}$$

Reactant

Table 51: Properties of each reactant.

Id	Name	SBO
b_met	b_Methionine	

Modifiers

Table 52: Properties of each modifier.

Id	Name	SBO
b_met	b_Methionine	
met	c_Methionine	

Product

Table 53: Properties of each product.

Id	Name	SBO
met	c_Methionine	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \text{function\_4\_V\_b\_MET\_c\_1}\left(\text{K\_bmetc}, \text{V\_bmetc}, [\text{b\_met}], \text{vol}\left(\text{cytosol}\right), \text{k\_out\_met}, [\text{met}]\right) \tag{156}$$

$$\begin{aligned}&\text{function\_4\_V\_b\_MET\_c\_1}\left(\text{K\_bmetc}, \text{V\_bmetc}, [\text{b\_met}], \text{vol}\left(\text{cytosol}\right), \text{k\_out\_met}, [\text{met}]\right)\\ &= \text{vol}\left(\text{cytosol}\right) \cdot \left(\text{MM}\left(\text{V\_bmetc}, \text{K\_bmetc}, [\text{b\_met}]\right) - \text{k\_out\_met} \cdot [\text{met}]\right)\end{aligned} \tag{157}$$

9.21 Reaction VmFTD

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

Name VmFTD

Reaction equation

$$\mathrm{m\_10f} \underset{}{\overset{\mathrm{m\_10f}}{\rightleftharpoons}} \mathrm{m\_thf} \tag{158}$$

Reactant

Table 54: Properties of each reactant.

Id	Name	SBO
`m_10f`	m_10-formyl-THF	

Modifier

Table 55: Properties of each modifier.

Id	Name	SBO
`m_10f`	m_10-formyl-THF	

Product

Table 56: Properties of each product.

Id	Name	SBO
`m_thf`	m_THF	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \mathrm{vol}\left(\mathrm{mito}\right) \cdot \mathrm{function\_4\_VmFTD\_1}\left(\mathrm{K\_10f\_FTD}, \mathrm{Vm\_mFTD}, \left[\mathrm{m\_10f}\right]\right) \tag{159}$$

$$\mathrm{function\_4\_VmFTD\_1}\left(\mathrm{K\_10f\_FTD}, \mathrm{Vm\_mFTD}, \left[\mathrm{m\_10f}\right]\right) = \frac{\mathrm{Vm\_mFTD} \cdot \left[\mathrm{m\_10f}\right]}{\mathrm{K\_10f\_FTD} + \left[\mathrm{m\_10f}\right]} \tag{160}$$

$$\mathrm{function\_4\_VmFTD\_1}\left(\mathrm{K\_10f\_FTD}, \mathrm{Vm\_mFTD}, \left[\mathrm{m\_10f}\right]\right) = \frac{\mathrm{Vm\_mFTD} \cdot \left[\mathrm{m\_10f}\right]}{\mathrm{K\_10f\_FTD} + \left[\mathrm{m\_10f}\right]} \tag{161}$$

9.22 Reaction VmSHMT

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

Name VmSHMT

Reaction equation

$$\mathrm{m\_thf} + \mathrm{m\_ser} \xrightleftharpoons{\mathrm{m\_2cf},\ \mathrm{m\_gly},\ \mathrm{m\_ser},\ \mathrm{m\_thf}} \mathrm{m\_gly} + \mathrm{m\_2cf} \tag{162}$$

Reactants

Table 57: Properties of each reactant.

Id	Name	SBO
m_thf	m_THF	
m_ser	m_Serine	

Modifiers

Table 58: Properties of each modifier.

Id	Name	SBO
m_2cf	m_5-10-methylene-THF	
m_gly	m_Glycine	
m_ser	m_Serine	
m_thf	m_THF	

Products

Table 59: Properties of each product.

Id	Name	SBO
m_gly	m_Glycine	
m_2cf	m_5-10-methylene-THF	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \mathrm{vol}\,(\mathrm{mito}) \cdot \mathrm{function\_4\_VmSHMT\_1}\,(\mathrm{K\_2cf\_SHMT}, \mathrm{K\_gly\_SHMT}, \mathrm{K\_ser\_SHMT}, \mathrm{K\_thf\_SHMT}, \mathrm{Vf\_mSHMT}, \mathrm{Vr\_mSHMT}, [\mathrm{m\_2cf}], [\mathrm{m\_gly}], [\mathrm{m\_ser}], [\mathrm{m\_thf}]) \tag{163}$$

$$\mathrm{function\_4\_VmSHMT\_1}\,(\mathrm{K\_2cf\_SHMT}, \mathrm{K\_gly\_SHMT}, \mathrm{K\_ser\_SHMT}, \mathrm{K\_thf\_SHMT}, \mathrm{Vf\_mSHMT}, \mathrm{Vr\_mSHMT}, [\mathrm{m\_2cf}], [\mathrm{m\_gly}], [\mathrm{m\_ser}], [\mathrm{m\_thf}]) = \mathrm{MM\_twosubst}\,(\mathrm{Vf\_mSHMT}, \mathrm{K\_thf\_SHMT}, \mathrm{K\_ser\_SHMT}, [\mathrm{m\_thf}], [\mathrm{m\_ser}]) - \mathrm{MM\_twosubst}\,(\mathrm{Vr\_mSHMT}, \mathrm{K\_gly\_SHMT}, \mathrm{K\_2cf\_SHMT}, [\mathrm{m\_gly}], [\mathrm{m\_2cf}]) \tag{164}$$

$$\mathrm{function\_4\_VmSHMT\_1}\,(\mathrm{K\_2cf\_SHMT}, \mathrm{K\_gly\_SHMT}, \mathrm{K\_ser\_SHMT}, \mathrm{K\_thf\_SHMT}, \mathrm{Vf\_mSHMT}, \mathrm{Vr\_mSHMT}, [\mathrm{m\_2cf}], [\mathrm{m\_gly}], [\mathrm{m\_ser}], [\mathrm{m\_thf}]) = \mathrm{MM\_twosubst}\,(\mathrm{Vf\_mSHMT}, \mathrm{K\_thf\_SHMT}, \mathrm{K\_ser\_SHMT}, [\mathrm{m\_thf}], [\mathrm{m\_ser}]) - \mathrm{MM\_twosubst}\,(\mathrm{Vr\_mSHMT}, \mathrm{K\_gly\_SHMT}, \mathrm{K\_2cf\_SHMT}, [\mathrm{m\_gly}], [\mathrm{m\_2cf}]) \tag{165}$$

9.23 Reaction `VmFTS`

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

Name VmFTS

Reaction equation

$$\mathrm{m\_thf} + \mathrm{m\_coo} \xrightleftharpoons{\mathrm{m\_10f,\ m\_coo,\ m\_thf}} \mathrm{m\_10f} \tag{166}$$

Reactants

Table 60: Properties of each reactant.

Id	Name	SBO
`m_thf`	m_THF	
`m_coo`	m_Formate	

Modifiers

Table 61: Properties of each modifier.

Id	Name	SBO
`m_10f`	m_10-formyl-THF	

Id	Name	SBO
m_coo	m_Formate	
m_thf	m_THF	

Product

Table 62: Properties of each product.

Id	Name	SBO
m_10f	m_10-formyl-THF	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \mathrm{vol}\,(\mathrm{mito}) \cdot \mathrm{function\_4\_VmFTS\_1}\,(\mathrm{K\_10f\_mFTS}, \mathrm{K\_coo\_mFTS}, \mathrm{K\_thf\_mFTS}, \mathrm{Vf\_mFTS}, \mathrm{Vr\_mFTS}, [\mathrm{m\_10f}], [\mathrm{m\_coo}], [\mathrm{m\_thf}]) \tag{167}$$

$$\mathrm{function\_4\_VmFTS\_1}\,(\mathrm{K\_10f\_mFTS}, \mathrm{K\_coo\_mFTS}, \mathrm{K\_thf\_mFTS}, \mathrm{Vf\_mFTS}, \mathrm{Vr\_mFTS}, [\mathrm{m\_10f}], [\mathrm{m\_coo}], [\mathrm{m\_thf}]) = \mathrm{MM\_twosubst}\,(\mathrm{Vf\_mFTS}, \mathrm{K\_thf\_mFTS}, \mathrm{K\_coo\_mFTS}, [\mathrm{m\_thf}], [\mathrm{m\_coo}]) - \mathrm{MM}\,(\mathrm{Vr\_mFTS}, \mathrm{K\_10f\_mFTS}, [\mathrm{m\_10f}]) \tag{168}$$

$$\mathrm{function\_4\_VmFTS\_1}\,(\mathrm{K\_10f\_mFTS}, \mathrm{K\_coo\_mFTS}, \mathrm{K\_thf\_mFTS}, \mathrm{Vf\_mFTS}, \mathrm{Vr\_mFTS}, [\mathrm{m\_10f}], [\mathrm{m\_coo}], [\mathrm{m\_thf}]) = \mathrm{MM\_twosubst}\,(\mathrm{Vf\_mFTS}, \mathrm{K\_thf\_mFTS}, \mathrm{K\_coo\_mFTS}, [\mathrm{m\_thf}], [\mathrm{m\_coo}]) - \mathrm{MM}\,(\mathrm{Vr\_mFTS}, \mathrm{K\_10f\_mFTS}, [\mathrm{m\_10f}]) \tag{169}$$

9.24 Reaction VmNE

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

Name VmNE

Reaction equation

$$\mathrm{m\_thf} + \mathrm{HCHO} \underset{}{\overset{\mathrm{HCHO,\ m\_2cf,\ m\_thf}}{\rightleftharpoons}} \mathrm{m\_2cf} \tag{170}$$

Reactants

Table 63: Properties of each reactant.

Id	Name	SBO
m_thf	m_THF	
HCHO	Formaldehyde	

Modifiers

Table 64: Properties of each modifier.

Id	Name	SBO
HCHO	Formaldehyde	
m_2cf	m_5-10-methylene-THF	
m_thf	m_THF	

Product

Table 65: Properties of each product.

Id	Name	SBO
m_2cf	m_5-10-methylene-THF	

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \text{function\_4\_VmNE\_1}\left([\text{HCHO}], \text{k1\_mNE}, \text{k2\_mNE}, [\text{m\_2cf}], [\text{m\_thf}], \text{vol}\left(\text{mito}\right)\right) \quad (171)$$

$$\begin{aligned} &\text{function\_4\_VmNE\_1}\left([\text{HCHO}], \text{k1\_mNE}, \text{k2\_mNE}, [\text{m\_2cf}], [\text{m\_thf}], \text{vol}\left(\text{mito}\right)\right) \\ &\quad = \text{vol}\left(\text{mito}\right) \cdot \left(\text{k1\_mNE} \cdot [\text{m\_thf}] \cdot [\text{HCHO}] - \text{k2\_mNE} \cdot [\text{m\_2cf}]\right) \end{aligned} \quad (172)$$

9.25 Reaction V_GDC

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

Name V_GDC

Reaction equation

$$\text{m\_thf} + \text{m\_gly} \overset{\text{m\_gly, m\_thf}}{\rightleftharpoons} \text{m\_2cf} + \text{CO} \quad (173)$$

Reactants

Table 66: Properties of each reactant.

Id	Name	SBO
m_thf	m_THF	
m_gly	m_Glycine	

Modifiers

Table 67: Properties of each modifier.

Id	Name	SBO
m_gly	m_Glycine	
m_thf	m_THF	

Products

Table 68: Properties of each product.

Id	Name	SBO
m_2cf	m_5-10-methylene-THF	
CO	CO2	

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \mathrm{vol}\,(\mathrm{mito}) \cdot \mathrm{function\_4\_V\_GDC\_1}\,(\mathrm{K\_gly\_GDC}, \mathrm{K\_thf\_GDC}, \mathrm{Vm\_GDC}, [\mathrm{m\_gly}], [\mathrm{m\_thf}]) \tag{174}$$

$$\mathrm{function\_4\_V\_GDC\_1}\,(\mathrm{K\_gly\_GDC}, \mathrm{K\_thf\_GDC}, \mathrm{Vm\_GDC}, [\mathrm{m\_gly}], [\mathrm{m\_thf}]) = \frac{\mathrm{Vm\_GDC} \cdot [\mathrm{m\_thf}] \cdot [\mathrm{m\_gly}]}{(\mathrm{K\_thf\_GDC} + [\mathrm{m\_thf}]) \cdot (\mathrm{K\_gly\_GDC} + [\mathrm{m\_gly}])} \tag{175}$$

$$\mathrm{function\_4\_V\_GDC\_1}\,(\mathrm{K\_gly\_GDC}, \mathrm{K\_thf\_GDC}, \mathrm{Vm\_GDC}, [\mathrm{m\_gly}], [\mathrm{m\_thf}]) = \frac{\mathrm{Vm\_GDC} \cdot [\mathrm{m\_thf}] \cdot [\mathrm{m\_gly}]}{(\mathrm{K\_thf\_GDC} + [\mathrm{m\_thf}]) \cdot (\mathrm{K\_gly\_GDC} + [\mathrm{m\_gly}])} \tag{176}$$

9.26 Reaction V_SDH

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

Name V_SDH

Reaction equation

$$\mathrm{m\_thf} + \mathrm{src} \overset{\mathrm{m\_thf,\ src}}{\rightleftharpoons} \mathrm{m\_2cf} + \mathrm{m\_gly} \tag{177}$$

Reactants

Table 69: Properties of each reactant.

Id	Name	SBO
m_thf	m_THF	
src	Sarcosine	

Modifiers

Table 70: Properties of each modifier.

Id	Name	SBO
m_thf	m_THF	
src	Sarcosine	

Products

Table 71: Properties of each product.

Id	Name	SBO
m_2cf	m_5-10-methylene-THF	
m_gly	m_Glycine	

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = \mathrm{function\_4\_V\_SDH\_1}\left(\mathrm{K\_src\_SDH}, \mathrm{K\_thf\_SDH}, \mathrm{Vm\_SDH}, [\mathrm{m\_thf}], \mathrm{vol}\left(\mathrm{mito}\right), [\mathrm{src}]\right) \tag{178}$$

$$\begin{aligned}&\text{function\_4\_V\_SDH\_1}\left(\text{K\_src\_SDH}, \text{K\_thf\_SDH}, \text{Vm\_SDH}, [\text{m\_thf}], \text{vol}\left(\text{mito}\right), [\text{src}]\right)\\ &= \text{vol}\left(\text{mito}\right) \cdot \text{MM\_twosubst}\left(\text{Vm\_SDH}, \text{K\_thf\_SDH}, \text{K\_src\_SDH}, [\text{m\_thf}], [\text{src}]\right)\end{aligned} \tag{179}$$

9.27 Reaction V_DMGD

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

Name V_DMGD

Reaction equation

$$\text{m\_thf} + \text{dmg} \overset{\text{dmg, m\_thf}}{\rightleftharpoons} \text{m\_2cf} + \text{src} \tag{180}$$

Reactants

Table 72: Properties of each reactant.

Id	Name	SBO
m_thf	m_THF	
dmg	Dimethylglycine	

Modifiers

Table 73: Properties of each modifier.

Id	Name	SBO
dmg	Dimethylglycine	
m_thf	m_THF	

Products

Table 74: Properties of each product.

Id	Name	SBO
m_2cf	m_5-10-methylene-THF	
src	Sarcosine	

Kinetic Law

Derived unit contains undeclared units

$$v_{27} = \text{function\_4\_V\_DMGD\_1}\,(\text{K\_dmg\_DMGD}, \text{K\_thf\_DMGD}, \text{Vm\_DMGD}, [\text{dmg}], [\text{m\_thf}], \text{vol}\,(\text{mito})) \tag{181}$$

$$\begin{aligned}\text{function\_4\_V\_DMGD\_1}\,(&\text{K\_dmg\_DMGD}, \text{K\_thf\_DMGD},\\ &\text{Vm\_DMGD}, [\text{dmg}], [\text{m\_thf}], \text{vol}\,(\text{mito})) = \text{vol}\,(\text{mito})\\ &\cdot \text{MM\_twosubst}\,(\text{Vm\_DMGD}, \text{K\_thf\_DMGD}, \text{K\_dmg\_DMGD}, [\text{m\_thf}], [\text{dmg}])\end{aligned} \tag{182}$$

9.28 Reaction VmMTD

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

Name VmMTD

Reaction equation

$$\text{m\_2cf} \underset{}{\overset{\text{m\_1cf, m\_2cf}}{\rightleftharpoons}} \text{m\_1cf} \tag{183}$$

Reactant

Table 75: Properties of each reactant.

Id	Name	SBO
m_2cf	m_5-10-methylene-THF	

Modifiers

Table 76: Properties of each modifier.

Id	Name	SBO
m_1cf	m_5-10-methenyl-THF	
m_2cf	m_5-10-methylene-THF	

Product

Table 77: Properties of each product.

Id	Name	SBO
m_1cf	m_5-10-methenyl-THF	

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \mathrm{vol}(\mathrm{mito}) \cdot \mathrm{function\_4\_VmMTD\_1}(\mathrm{K\_1cf\_MTD}, \mathrm{K\_2cf\_MTD}, \mathrm{Vf\_mMTD}, \mathrm{Vr\_MTD}, [\mathrm{m\_1cf}], [\mathrm{m\_2cf}]) \tag{184}$$

$$\mathrm{function\_4\_VmMTD\_1}(\mathrm{K\_1cf\_MTD}, \mathrm{K\_2cf\_MTD}, \mathrm{Vf\_mMTD}, \mathrm{Vr\_MTD}, [\mathrm{m\_1cf}], [\mathrm{m\_2cf}]) = \mathrm{MM}(\mathrm{Vf\_mMTD}, \mathrm{K\_2cf\_MTD}, [\mathrm{m\_2cf}]) - \mathrm{MM}(\mathrm{Vr\_MTD}, \mathrm{K\_1cf\_MTD}, [\mathrm{m\_1cf}]) \tag{185}$$

$$\mathrm{function\_4\_VmMTD\_1}(\mathrm{K\_1cf\_MTD}, \mathrm{K\_2cf\_MTD}, \mathrm{Vf\_mMTD}, \mathrm{Vr\_MTD}, [\mathrm{m\_1cf}], [\mathrm{m\_2cf}]) = \mathrm{MM}(\mathrm{Vf\_mMTD}, \mathrm{K\_2cf\_MTD}, [\mathrm{m\_2cf}]) - \mathrm{MM}(\mathrm{Vr\_MTD}, \mathrm{K\_1cf\_MTD}, [\mathrm{m\_1cf}]) \tag{186}$$

9.29 Reaction VmMTCH

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

Name VmMTCH

Reaction equation

$$\mathrm{m\_1cf} \xrightleftharpoons{\mathrm{m\_10f},\ \mathrm{m\_1cf}} \mathrm{m\_10f} \tag{187}$$

Reactant

Table 78: Properties of each reactant.

Id	Name	SBO
m_1cf	m_5-10-methenyl-THF	

Modifiers

Table 79: Properties of each modifier.

Id	Name	SBO
m_10f	m_10-formyl-THF	
m_1cf	m_5-10-methenyl-THF	

Product

Table 80: Properties of each product.

Id	Name	SBO
m_10f	m_10-formyl-THF	

Kinetic Law

Derived unit contains undeclared units

$$v_{29} = \mathrm{vol}\,(\mathrm{mito}) \cdot \mathrm{function\_4\_VmMTCH\_1}\,(\mathrm{K\_10f\_MTCH}, \mathrm{K\_1cf\_MTCH}, \mathrm{Vf\_mMTCH}, \mathrm{Vr\_MTCH}, [\mathrm{m\_10f}], [\mathrm{m\_1cf}]) \tag{188}$$

$$\begin{aligned}\mathrm{function\_4\_VmMTCH\_1}\,(\mathrm{K\_10f\_MTCH}, \mathrm{K\_1cf\_MTCH}, \mathrm{Vf\_mMTCH},\\ \mathrm{Vr\_MTCH}, [\mathrm{m\_10f}], [\mathrm{m\_1cf}]) = \mathrm{MM}\,(\mathrm{Vf\_mMTCH}, \mathrm{K\_1cf\_MTCH}, [\mathrm{m\_1cf}])\\ - \mathrm{MM}\,(\mathrm{Vr\_MTCH}, \mathrm{K\_10f\_MTCH}, [\mathrm{m\_10f}])\end{aligned} \tag{189}$$

$$\begin{aligned}\mathrm{function\_4\_VmMTCH\_1}\,(\mathrm{K\_10f\_MTCH}, \mathrm{K\_1cf\_MTCH}, \mathrm{Vf\_mMTCH},\\ \mathrm{Vr\_MTCH}, [\mathrm{m\_10f}], [\mathrm{m\_1cf}]) = \mathrm{MM}\,(\mathrm{Vf\_mMTCH}, \mathrm{K\_1cf\_MTCH}, [\mathrm{m\_1cf}])\\ - \mathrm{MM}\,(\mathrm{Vr\_MTCH}, \mathrm{K\_10f\_MTCH}, [\mathrm{m\_10f}])\end{aligned} \tag{190}$$

9.30 Reaction VmSERc

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

Name VmSERc

Reaction equation

$$3\,\mathrm{m\_ser} \xrightleftharpoons{\mathrm{c\_ser},\ \mathrm{m\_ser}} \mathrm{c\_ser} \tag{191}$$

Reactant

Table 81: Properties of each reactant.

Id	Name	SBO
m_ser	m_Serine	

Modifiers

Table 82: Properties of each modifier.

Id	Name	SBO
c_ser	c_Serine	
m_ser	m_Serine	

Product

Table 83: Properties of each product.

Id	Name	SBO
c_ser	c_Serine	

Kinetic Law

Derived unit contains undeclared units

$$v_{30} = \text{function\_4\_VmSERc\_1}\left(\text{K\_cser}, \text{K\_mser}, \text{V\_cser}, \text{V\_mser}, [\text{c\_ser}], \text{vol}\left(\text{cytosol}\right), [\text{m\_ser}], \text{vol}\left(\text{mito}\right)\right) \tag{192}$$

$$\text{function\_4\_VmSERc\_1}\left(\text{K\_cser}, \text{K\_mser}, \text{V\_cser}, \text{V\_mser}, [\text{c\_ser}], \text{vol}\left(\text{cytosol}\right), [\text{m\_ser}], \text{vol}\left(\text{mito}\right)\right) = \left(\frac{\text{MM}\left(\text{V\_mser}, \text{K\_mser}, [\text{m\_ser}]\right) \cdot \text{vol}\left(\text{mito}\right)}{3} - \text{MM}\left(\text{V\_cser}, \text{K\_cser}, [\text{c\_ser}]\right)\right) \cdot \text{vol}\left(\text{cytosol}\right) \tag{193}$$

9.31 Reaction VmHCOOHc

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

Name VmHCOOHc

Reaction equation

$$3\,\mathrm{m\_coo} \xrightleftharpoons{\mathrm{c\_coo},\ \mathrm{m\_coo}} \mathrm{c\_coo} \tag{194}$$

Reactant

Table 84: Properties of each reactant.

Id	Name	SBO
m_coo	m_Formate	

Modifiers

Table 85: Properties of each modifier.

Id	Name	SBO
c_coo	c_Formate	
m_coo	m_Formate	

Product

Table 86: Properties of each product.

Id	Name	SBO
c_coo	c_Formate	

Kinetic Law

Derived unit contains undeclared units

$$v_{31} = \mathrm{function\_4\_VmHCOOHc\_1}\left([\mathrm{c\_coo}], \mathrm{vol}\left(\mathrm{cytosol}\right), \mathrm{k\_in\_coo}, \mathrm{k\_out\_coo}, [\mathrm{m\_coo}], \mathrm{vol}\left(\mathrm{mito}\right)\right) \tag{195}$$

$$\mathrm{function\_4\_VmHCOOHc\_1}\left([\mathrm{c\_coo}], \mathrm{vol}\left(\mathrm{cytosol}\right), \mathrm{k\_in\_coo}, \mathrm{k\_out\_coo}, [\mathrm{m\_coo}], \mathrm{vol}\left(\mathrm{mito}\right)\right) = \frac{\mathrm{k\_in\_coo} \cdot [\mathrm{m\_coo}] \cdot \mathrm{vol}\left(\mathrm{mito}\right)}{3} - \mathrm{k\_out\_coo} \cdot [\mathrm{c\_coo}] \cdot \mathrm{vol}\left(\mathrm{cytosol}\right) \tag{196}$$

9.32 Reaction VmGLYc

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

Name VmGLYc

Reaction equation

$$3\,\mathrm{m\_gly} \xrightleftharpoons{\mathrm{c\_gly},\ \mathrm{m\_gly}} \mathrm{c\_gly} \tag{197}$$

Reactant

Table 87: Properties of each reactant.

Id	Name	SBO
m_gly	m_Glycine	

Modifiers

Table 88: Properties of each modifier.

Id	Name	SBO
c_gly	c_Glycine	
m_gly	m_Glycine	

Product

Table 89: Properties of each product.

Id	Name	SBO
c_gly	c_Glycine	

Kinetic Law

Derived unit contains undeclared units

$$v_{32} = \mathrm{function\_4\_VmGLYc\_1}\left(\mathrm{K\_cgly}, \mathrm{K\_mgly}, \mathrm{V\_cgly}, \mathrm{V\_mgly}, [\mathrm{c\_gly}], \mathrm{vol}\left(\mathrm{cytosol}\right), [\mathrm{m\_gly}], \mathrm{vol}\left(\mathrm{mito}\right)\right) \tag{198}$$

$$\begin{aligned}&\text{function\_4\_VmGLYc\_1}\left(\text{K\_cgly}, \text{K\_mgly}, \text{V\_cgly}, \text{V\_mgly}, [\text{c\_gly}],\right.\\&\left.\text{vol}\left(\text{cytosol}\right), [\text{m\_gly}], \text{vol}\left(\text{mito}\right)\right) = \text{MM}\left(\text{V\_mgly}, \text{K\_mgly}, [\text{m\_gly}]\right)\\&\cdot \text{vol}\left(\text{mito}\right) \cdot \frac{1}{3} - \text{MM}\left(\text{V\_cgly}, \text{K\_cgly}, [\text{c\_gly}]\right) \cdot \text{vol}\left(\text{cytosol}\right)\end{aligned} \tag{199}$$

9.33 Reaction V_MS

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

Name V_MS

Reaction equation

$$\text{c\_5mf} + \text{hcy} \xrightleftharpoons{\text{H2O2, c\_5mf, hcy}} \text{c\_thf} + \text{met} \tag{200}$$

Reactants

Table 90: Properties of each reactant.

Id	Name	SBO
c_5mf	c_5-methyl-THF	
hcy	Homocysteine	

Modifiers

Table 91: Properties of each modifier.

Id	Name	SBO
H2O2	H2O2	
c_5mf	c_5-methyl-THF	
hcy	Homocysteine	

Products

Table 92: Properties of each product.

Id	Name	SBO
c_thf	c_THF	
met	c_Methionine	

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_{33} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{function\_4\_V\_MS\_1}\,([\mathrm{H2O2}], \mathrm{K\_5mf\_MS}, \mathrm{K\_hcy\_MS}, \mathrm{Ki\_MS}, \mathrm{Vm\_MS}, [\mathrm{c\_5mf}], [\mathrm{hcy}], \mathrm{ssH2O2}) \tag{201}$$

$$\mathrm{function\_4\_V\_MS\_1}\,([\mathrm{H2O2}], \mathrm{K\_5mf\_MS}, \mathrm{K\_hcy\_MS}, \mathrm{Ki\_MS}, \mathrm{Vm\_MS}, [\mathrm{c\_5mf}], [\mathrm{hcy}], \mathrm{ssH2O2}) = \frac{\mathrm{MM\_twosubst}\,(\mathrm{Vm\_MS}, \mathrm{K\_5mf\_MS}, \mathrm{K\_hcy\_MS}, [\mathrm{c\_5mf}], [\mathrm{hcy}]) \cdot (\mathrm{ssH2O2} + \mathrm{Ki\_MS})}{[\mathrm{H2O2}] + \mathrm{Ki\_MS}} \tag{202}$$

$$\mathrm{function\_4\_V\_MS\_1}\,([\mathrm{H2O2}], \mathrm{K\_5mf\_MS}, \mathrm{K\_hcy\_MS}, \mathrm{Ki\_MS}, \mathrm{Vm\_MS}, [\mathrm{c\_5mf}], [\mathrm{hcy}], \mathrm{ssH2O2}) = \frac{\mathrm{MM\_twosubst}\,(\mathrm{Vm\_MS}, \mathrm{K\_5mf\_MS}, \mathrm{K\_hcy\_MS}, [\mathrm{c\_5mf}], [\mathrm{hcy}]) \cdot (\mathrm{ssH2O2} + \mathrm{Ki\_MS})}{[\mathrm{H2O2}] + \mathrm{Ki\_MS}} \tag{203}$$

9.34 Reaction V_DHFR

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

Name V_DHFR

Reaction equation

$$\mathrm{c\_dhf} + \mathrm{NADPH} \xrightleftharpoons{\mathrm{NADPH},\ \mathrm{c\_dhf}} \mathrm{c\_thf} \tag{204}$$

Reactants

Table 93: Properties of each reactant.

Id	Name	SBO
c_dhf	c_DHF	
NADPH	NADPH	

Modifiers

Table 94: Properties of each modifier.

Id	Name	SBO
NADPH	NADPH	
c_dhf	c_DHF	

Product

Table 95: Properties of each product.

Id	Name	SBO
c_thf	c_THF	

Kinetic Law

Derived unit contains undeclared units

$$v_{34} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{function\_4\_V\_DHFR\_1}\,(\mathrm{K\_NADPH\_DHFR}, \mathrm{K\_dhf\_DHFR}, [\mathrm{NADPH}], \mathrm{Vm\_DHFR}, [\mathrm{c\_dhf}]) \tag{205}$$

$$\mathrm{function\_4\_V\_DHFR\_1}\,(\mathrm{K\_NADPH\_DHFR}, \mathrm{K\_dhf\_DHFR}, [\mathrm{NADPH}], \mathrm{Vm\_DHFR}, [\mathrm{c\_dhf}]) = \frac{\mathrm{Vm\_DHFR} \cdot [\mathrm{c\_dhf}] \cdot [\mathrm{NADPH}]}{(\mathrm{K\_dhf\_DHFR} + [\mathrm{c\_dhf}]) \cdot (\mathrm{K\_NADPH\_DHFR} + [\mathrm{NADPH}])} \tag{206}$$

$$\mathrm{function\_4\_V\_DHFR\_1}\,(\mathrm{K\_NADPH\_DHFR}, \mathrm{K\_dhf\_DHFR}, [\mathrm{NADPH}], \mathrm{Vm\_DHFR}, [\mathrm{c\_dhf}]) = \frac{\mathrm{Vm\_DHFR} \cdot [\mathrm{c\_dhf}] \cdot [\mathrm{NADPH}]}{(\mathrm{K\_dhf\_DHFR} + [\mathrm{c\_dhf}]) \cdot (\mathrm{K\_NADPH\_DHFR} + [\mathrm{NADPH}])} \tag{207}$$

9.35 Reaction VcFTD

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

Name VcFTD

Reaction equation

$$\mathrm{c\_10f} \overset{\mathrm{c\_10f}}{\rightleftharpoons} \mathrm{c\_thf} \tag{208}$$

Reactant

Table 96: Properties of each reactant.

Id	Name	SBO
c_10f	c_10-formyl-THF	

Modifier

Table 97: Properties of each modifier.

Id	Name	SBO
c_10f	c_10-formyl-THF	

Product

Table 98: Properties of each product.

Id	Name	SBO
c_thf	c_THF	

Kinetic Law

Derived unit contains undeclared units

$$v_{35} = \text{vol}\,(\text{cytosol}) \cdot \text{function\_4\_VcFTD\_1}\,(\text{K\_10f\_FTD}, \text{Vm\_cFTD}, [\text{c\_10f}]) \tag{209}$$

$$\text{function\_4\_VcFTD\_1}\,(\text{K\_10f\_FTD}, \text{Vm\_cFTD}, [\text{c\_10f}]) = \frac{\text{Vm\_cFTD} \cdot [\text{c\_10f}]}{\text{K\_10f\_FTD} + [\text{c\_10f}]} \tag{210}$$

$$\text{function\_4\_VcFTD\_1}\,(\text{K\_10f\_FTD}, \text{Vm\_cFTD}, [\text{c\_10f}]) = \frac{\text{Vm\_cFTD} \cdot [\text{c\_10f}]}{\text{K\_10f\_FTD} + [\text{c\_10f}]} \tag{211}$$

9.36 Reaction V_PGT

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

Name V_PGT

Reaction equation

$$\text{c\_10f} + \text{GAR} \overset{\text{GAR, c\_10f}}{\rightleftharpoons} \text{aic} + \text{c\_thf} \tag{212}$$

Reactants

Table 99: Properties of each reactant.

Id	Name	SBO
c_10f	c_10-formyl-THF	
GAR	GAR	

Modifiers

Table 100: Properties of each modifier.

Id	Name	SBO
GAR	GAR	
c_10f	c_10-formyl-THF	

Products

Table 101: Properties of each product.

Id	Name	SBO
aic	AICAR	
c_thf	c_THF	

Kinetic Law

Derived unit contains undeclared units

$$v_{36} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{function\_4\_V\_PGT\_1}\,([\mathrm{GAR}], \mathrm{K\_10f\_PGT}, \mathrm{K\_GAR\_PGT}, \mathrm{Vm\_PGT}, [\mathrm{c\_10f}]) \tag{213}$$

$$\mathrm{function\_4\_V\_PGT\_1}\,([\mathrm{GAR}], \mathrm{K\_10f\_PGT}, \mathrm{K\_GAR\_PGT}, \mathrm{Vm\_PGT}, [\mathrm{c\_10f}]) = \frac{\mathrm{Vm\_PGT} \cdot [\mathrm{c\_10f}] \cdot [\mathrm{GAR}]}{(\mathrm{K\_10f\_PGT} + [\mathrm{c\_10f}]) \cdot (\mathrm{K\_GAR\_PGT} + [\mathrm{GAR}])} \tag{214}$$

$$\mathrm{function\_4\_V\_PGT\_1}\,([\mathrm{GAR}], \mathrm{K\_10f\_PGT}, \mathrm{K\_GAR\_PGT}, \mathrm{Vm\_PGT}, [\mathrm{c\_10f}]) = \frac{\mathrm{Vm\_PGT} \cdot [\mathrm{c\_10f}] \cdot [\mathrm{GAR}]}{(\mathrm{K\_10f\_PGT} + [\mathrm{c\_10f}]) \cdot (\mathrm{K\_GAR\_PGT} + [\mathrm{GAR}])} \tag{215}$$

9.37 Reaction VcFTS

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

Name VcFTS

Reaction equation

$$\text{c\_thf} + \text{c\_coo} \overset{\text{c\_coo, c\_thf}}{\rightleftharpoons} \text{c\_10f} \tag{216}$$

Reactants

Table 102: Properties of each reactant.

Id	Name	SBO
c_thf	c_THF	
c_coo	c_Formate	

Modifiers

Table 103: Properties of each modifier.

Id	Name	SBO
c_coo	c_Formate	
c_thf	c_THF	

Product

Table 104: Properties of each product.

Id	Name	SBO
c_10f	c_10-formyl-THF	

Kinetic Law

Derived unit contains undeclared units

$$v_{37} = \text{vol}(\text{cytosol}) \cdot \text{function\_4\_VcFTS\_1}(\text{K\_coo\_cFTS}, \text{K\_thf\_cFTS}, \text{Vm\_cFTS}, [\text{c\_coo}], [\text{c\_thf}]) \tag{217}$$

$$\text{function\_4\_VcFTS\_1}(\text{K\_coo\_cFTS}, \text{K\_thf\_cFTS}, \text{Vm\_cFTS}, [\text{c\_coo}], [\text{c\_thf}]) = \frac{\text{Vm\_cFTS} \cdot [\text{c\_thf}] \cdot [\text{c\_coo}]}{(\text{K\_thf\_cFTS} + [\text{c\_thf}]) \cdot (\text{K\_coo\_cFTS} + [\text{c\_coo}])} \tag{218}$$

$$\text{function\_4\_VcFTS\_1}(\text{K\_coo\_cFTS}, \text{K\_thf\_cFTS}, \text{Vm\_cFTS}, [\text{c\_coo}], [\text{c\_thf}]) = \frac{\text{Vm\_cFTS} \cdot [\text{c\_thf}] \cdot [\text{c\_coo}]}{(\text{K\_thf\_cFTS} + [\text{c\_thf}]) \cdot (\text{K\_coo\_cFTS} + [\text{c\_coo}])} \tag{219}$$

9.38 Reaction VcSHMT

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

Name VcSHMT

Reaction equation

$$\text{c\_ser} + \text{c\_thf} \xrightleftharpoons{\text{c\_2cf, c\_gly, c\_ser, c\_thf}} \text{c\_gly} + \text{c\_2cf} \tag{220}$$

Reactants

Table 105: Properties of each reactant.

Id	Name	SBO
c_ser	c_Serine	
c_thf	c_THF	

Modifiers

Table 106: Properties of each modifier.

Id	Name	SBO
c_2cf	c_5-10-methylene-THF	
c_gly	c_Glycine	
c_ser	c_Serine	
c_thf	c_THF	

Products

Table 107: Properties of each product.

Id	Name	SBO
c_gly	c_Glycine	
c_2cf	c_5-10-methylene-THF	

Kinetic Law

Derived unit contains undeclared units

$$v_{38} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{function\_4\_VcSHMT\_1}\,(\mathrm{K\_2cf\_SHMT}, \mathrm{K\_gly\_SHMT}, \mathrm{K\_ser\_SHMT}, \mathrm{K\_thf\_SHMT}, \mathrm{Vf\_cSHMT}, \mathrm{Vr\_cSHMT}, [\mathrm{c\_2cf}], [\mathrm{c\_gly}], [\mathrm{c\_ser}], [\mathrm{c\_thf}]) \tag{221}$$

$$\mathrm{function\_4\_VcSHMT\_1}\,(\mathrm{K\_2cf\_SHMT}, \mathrm{K\_gly\_SHMT}, \mathrm{K\_ser\_SHMT}, \mathrm{K\_thf\_SHMT}, \mathrm{Vf\_cSHMT}, \mathrm{Vr\_cSHMT}, [\mathrm{c\_2cf}], [\mathrm{c\_gly}], [\mathrm{c\_ser}], [\mathrm{c\_thf}]) = \mathrm{MM\_twosubst}\,(\mathrm{Vf\_cSHMT}, \mathrm{K\_thf\_SHMT}, \mathrm{K\_ser\_SHMT}, [\mathrm{c\_thf}], [\mathrm{c\_ser}]) - \mathrm{MM\_twosubst}\,(\mathrm{Vr\_cSHMT}, \mathrm{K\_gly\_SHMT}, \mathrm{K\_2cf\_SHMT}, [\mathrm{c\_gly}], [\mathrm{c\_2cf}]) \tag{222}$$

$$\mathrm{function\_4\_VcSHMT\_1}\,(\mathrm{K\_2cf\_SHMT}, \mathrm{K\_gly\_SHMT}, \mathrm{K\_ser\_SHMT}, \mathrm{K\_thf\_SHMT}, \mathrm{Vf\_cSHMT}, \mathrm{Vr\_cSHMT}, [\mathrm{c\_2cf}], [\mathrm{c\_gly}], [\mathrm{c\_ser}], [\mathrm{c\_thf}]) = \mathrm{MM\_twosubst}\,(\mathrm{Vf\_cSHMT}, \mathrm{K\_thf\_SHMT}, \mathrm{K\_ser\_SHMT}, [\mathrm{c\_thf}], [\mathrm{c\_ser}]) - \mathrm{MM\_twosubst}\,(\mathrm{Vr\_cSHMT}, \mathrm{K\_gly\_SHMT}, \mathrm{K\_2cf\_SHMT}, [\mathrm{c\_gly}], [\mathrm{c\_2cf}]) \tag{223}$$

9.39 Reaction VcNE

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

Name VcNE

Reaction equation

$$\mathrm{c\_thf} + \mathrm{HCHO} \xrightleftharpoons{\mathrm{HCHO},\ \mathrm{c\_2cf},\ \mathrm{c\_thf}} \mathrm{c\_2cf} \tag{224}$$

Reactants

Table 108: Properties of each reactant.

Id	Name	SBO
c_thf	c_THF	
HCHO	Formaldehyde	

Modifiers

Table 109: Properties of each modifier.

Id	Name	SBO
HCHO	Formaldehyde	
c_2cf	c_5-10-methylene-THF	
c_thf	c_THF	

Product

Table 110: Properties of each product.

Id	Name	SBO
c_2cf	c_5-10-methylene-THF	

Kinetic Law

Derived unit contains undeclared units

$$v_{39} = \text{function\_4\_VcNE\_1}\left([\text{HCHO}], [\text{c\_2cf}], [\text{c\_thf}], \text{vol}\left(\text{cytosol}\right), \text{k1\_cNE}, \text{k2\_cNE}\right) \quad (225)$$

$$\begin{aligned} &\text{function\_4\_VcNE\_1}\left([\text{HCHO}], [\text{c\_2cf}], [\text{c\_thf}], \text{vol}\left(\text{cytosol}\right), \text{k1\_cNE}, \text{k2\_cNE}\right) \\ &= \text{vol}\left(\text{cytosol}\right) \cdot \left(\text{k1\_cNE} \cdot [\text{c\_thf}] \cdot [\text{HCHO}] - \text{k2\_cNE} \cdot [\text{c\_2cf}]\right) \end{aligned} \quad (226)$$

9.40 Reaction V_TS

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

Name V_TS

Reaction equation

$$\text{DUMP} + \text{c\_2cf} \overset{\text{DUMP, c\_2cf}}{\rightleftharpoons} \text{c\_dhf} \quad (227)$$

Reactants

Table 111: Properties of each reactant.

Id	Name	SBO
DUMP	dUMP	
c_2cf	c_5-10-methylene-THF	

Modifiers

Table 112: Properties of each modifier.

Id	Name	SBO
DUMP	dUMP	
c_2cf	c_5-10-methylene-THF	

Product

Table 113: Properties of each product.

Id	Name	SBO
c_dhf	c_DHF	

Kinetic Law

Derived unit contains undeclared units

$$v_{40} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{function\_4\_V\_TS\_1}\,([\mathrm{DUMP}], \mathrm{K\_2cf\_TS}, \mathrm{K\_DUMP\_TS}, \mathrm{Vm\_TS}, [\mathrm{c\_2cf}]) \tag{228}$$

$$\mathrm{function\_4\_V\_TS\_1}\,([\mathrm{DUMP}], \mathrm{K\_2cf\_TS}, \mathrm{K\_DUMP\_TS}, \mathrm{Vm\_TS}, [\mathrm{c\_2cf}]) = \frac{\mathrm{Vm\_TS} \cdot [\mathrm{DUMP}] \cdot [\mathrm{c\_2cf}]}{(\mathrm{K\_DUMP\_TS} + [\mathrm{DUMP}]) \cdot (\mathrm{K\_2cf\_TS} + [\mathrm{c\_2cf}])} \tag{229}$$

$$\mathrm{function\_4\_V\_TS\_1}\,([\mathrm{DUMP}], \mathrm{K\_2cf\_TS}, \mathrm{K\_DUMP\_TS}, \mathrm{Vm\_TS}, [\mathrm{c\_2cf}]) = \frac{\mathrm{Vm\_TS} \cdot [\mathrm{DUMP}] \cdot [\mathrm{c\_2cf}]}{(\mathrm{K\_DUMP\_TS} + [\mathrm{DUMP}]) \cdot (\mathrm{K\_2cf\_TS} + [\mathrm{c\_2cf}])} \tag{230}$$

9.41 Reaction V_MTHFR

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

Name V_MTHFR

Reaction equation

$$\text{c\_2cf} + \text{NADPH} \xrightleftharpoons{\text{sah, sam, NADPH, c\_2cf}} \text{c\_5mf} \tag{231}$$

Reactants

Table 114: Properties of each reactant.

Id	Name	SBO
c_2cf	c_5-10-methylene-THF	
NADPH	NADPH	

Modifiers

Table 115: Properties of each modifier.

Id	Name	SBO
sah	SAH	
sam	SAM	
NADPH	NADPH	
c_2cf	c_5-10-methylene-THF	

Product

Table 116: Properties of each product.

Id	Name	SBO
c_5mf	c_5-methyl-THF	

Kinetic Law

Derived unit contains undeclared units

$$v_{41} = \text{vol}\,(\text{cytosol}) \cdot \text{function\_4\_V\_MTHFR\_1}\,(\text{K\_2cf\_MTHFR}, \text{K\_NADPH\_MTHFR}, [\text{NADPH}], \text{Vm\_MTHFR}, [\text{c\_2cf}], [\text{sah}], [\text{sam}]) \tag{232}$$

$$\text{function\_4\_V\_MTHFR\_1}\,(\text{K\_2cf\_MTHFR}, \text{K\_NADPH\_MTHFR}, [\text{NADPH}], \text{Vm\_MTHFR}, [\text{c\_2cf}], [\text{sah}], [\text{sam}]) = \frac{\text{MM\_twosubst}\,(\text{Vm\_MTHFR}, \text{K\_2cf\_MTHFR}, \text{K\_NADPH\_MTHFR}, [\text{c\_2cf}], [\text{NADPH}]) \cdot 72}{10 + [\text{sam}] - [\text{sah}]} \tag{233}$$

$$\text{function\_4\_V\_MTHFR\_1}\,(\text{K\_2cf\_MTHFR}, \text{K\_NADPH\_MTHFR}, [\text{NADPH}], \text{Vm\_MTHFR}, [\text{c\_2cf}], [\text{sah}], [\text{sam}]) = \frac{\text{MM\_twosubst}\,(\text{Vm\_MTHFR}, \text{K\_2cf\_MTHFR}, \text{K\_NADPH\_MTHFR}, [\text{c\_2cf}], [\text{NADPH}]) \cdot 72}{10 + [\text{sam}] - [\text{sah}]} \tag{234}$$

9.42 Reaction `VcMTD`

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

Name VcMTD

Reaction equation

$$\text{c\_2cf} \xrightleftharpoons{\text{c\_1cf, c\_2cf}} \text{c\_1cf} + \text{NADPH} \tag{235}$$

Reactant

Table 117: Properties of each reactant.

Id	Name	SBO
`c_2cf`	c_5-10-methylene-THF	

Modifiers

Table 118: Properties of each modifier.

Id	Name	SBO
`c_1cf`	c_5-10-methenyl-THF	
`c_2cf`	c_5-10-methylene-THF	

Id	Name	SBO

Products

Table 119: Properties of each product.

Id	Name	SBO
c_1cf	c_5-10-methenyl-THF	
NADPH	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_{42} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{function\_4\_VcMTD\_1}\,(\mathrm{K\_1cf\_MTD}, \mathrm{K\_2cf\_MTD}, \mathrm{Vf\_cMTD}, \mathrm{Vr\_cMTD}, [\mathrm{c\_1cf}], [\mathrm{c\_2cf}]) \tag{236}$$

$$\mathrm{function\_4\_VcMTD\_1}\,(\mathrm{K\_1cf\_MTD}, \mathrm{K\_2cf\_MTD}, \mathrm{Vf\_cMTD}, \mathrm{Vr\_cMTD}, [\mathrm{c\_1cf}], [\mathrm{c\_2cf}]) = \mathrm{MM}\,(\mathrm{Vf\_cMTD}, \mathrm{K\_2cf\_MTD}, [\mathrm{c\_2cf}]) - \mathrm{MM}\,(\mathrm{Vr\_cMTD}, \mathrm{K\_1cf\_MTD}, [\mathrm{c\_1cf}]) \tag{237}$$

$$\mathrm{function\_4\_VcMTD\_1}\,(\mathrm{K\_1cf\_MTD}, \mathrm{K\_2cf\_MTD}, \mathrm{Vf\_cMTD}, \mathrm{Vr\_cMTD}, [\mathrm{c\_1cf}], [\mathrm{c\_2cf}]) = \mathrm{MM}\,(\mathrm{Vf\_cMTD}, \mathrm{K\_2cf\_MTD}, [\mathrm{c\_2cf}]) - \mathrm{MM}\,(\mathrm{Vr\_cMTD}, \mathrm{K\_1cf\_MTD}, [\mathrm{c\_1cf}]) \tag{238}$$

9.43 Reaction VcMTCH

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

Name VcMTCH

Reaction equation

$$\mathrm{c\_1cf} \xrightleftharpoons{\mathrm{c\_10f,\ c\_1cf}} \mathrm{c\_10f} \tag{239}$$

Reactant

Table 120: Properties of each reactant.

Id	Name	SBO
c_1cf	c_5-10-methenyl-THF	

Modifiers

Table 121: Properties of each modifier.

Id	Name	SBO
c_10f	c_10-formyl-THF	
c_1cf	c_5-10-methenyl-THF	

Product

Table 122: Properties of each product.

Id	Name	SBO
c_10f	c_10-formyl-THF	

Kinetic Law

Derived unit contains undeclared units

$$v_{43} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{function\_4\_VcMTCH\_1}\,(\mathrm{K\_10f\_MTCH}, \mathrm{K\_1cf\_MTCH}, \mathrm{Vf\_cMTCH}, \mathrm{Vr\_MTCH}, [\mathrm{c\_10f}], [\mathrm{c\_1cf}]) \tag{240}$$

$$\mathrm{function\_4\_VcMTCH\_1}\,(\mathrm{K\_10f\_MTCH}, \mathrm{K\_1cf\_MTCH}, \mathrm{Vf\_cMTCH}, \mathrm{Vr\_MTCH}, [\mathrm{c\_10f}], [\mathrm{c\_1cf}]) = \mathrm{MM}\,(\mathrm{Vf\_cMTCH}, \mathrm{K\_1cf\_MTCH}, [\mathrm{c\_1cf}]) - \mathrm{MM}\,(\mathrm{Vr\_MTCH}, \mathrm{K\_10f\_MTCH}, [\mathrm{c\_10f}]) \tag{241}$$

$$\mathrm{function\_4\_VcMTCH\_1}\,(\mathrm{K\_10f\_MTCH}, \mathrm{K\_1cf\_MTCH}, \mathrm{Vf\_cMTCH}, \mathrm{Vr\_MTCH}, [\mathrm{c\_10f}], [\mathrm{c\_1cf}]) = \mathrm{MM}\,(\mathrm{Vf\_cMTCH}, \mathrm{K\_1cf\_MTCH}, [\mathrm{c\_1cf}]) - \mathrm{MM}\,(\mathrm{Vr\_MTCH}, \mathrm{K\_10f\_MTCH}, [\mathrm{c\_10f}]) \tag{242}$$

9.44 Reaction V_ART

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

Name V_ART

Reaction equation

$$\text{c\_10f} + \text{aic} \xrightleftharpoons{\text{aic, c\_10f}} \text{c\_thf} \tag{243}$$

Reactants

Table 123: Properties of each reactant.

Id	Name	SBO
c_10f	c_10-formyl-THF	
aic	AICAR	

Modifiers

Table 124: Properties of each modifier.

Id	Name	SBO
aic	AICAR	
c_10f	c_10-formyl-THF	

Product

Table 125: Properties of each product.

Id	Name	SBO
c_thf	c_THF	

Kinetic Law

Derived unit contains undeclared units

$$v_{44} = \text{vol}\,(\text{cytosol}) \cdot \text{function\_4\_V\_ART\_1}\,(\text{K\_10f\_ART}, \text{K\_aic\_ART}, \text{Vm\_ART}, [\text{aic}], [\text{c\_10f}]) \tag{244}$$

$$\begin{aligned} &\text{function\_4\_V\_ART\_1}\,(\text{K\_10f\_ART}, \text{K\_aic\_ART}, \text{Vm\_ART}, [\text{aic}], [\text{c\_10f}]) \\ &= \frac{\text{Vm\_ART} \cdot [\text{c\_10f}] \cdot [\text{aic}]}{(\text{K\_10f\_ART} + [\text{c\_10f}]) \cdot (\text{K\_aic\_ART} + [\text{aic}])} \end{aligned} \tag{245}$$

$$\begin{aligned}&\text{function\_4\_V\_ART\_1}\left(\text{K\_10f\_ART}, \text{K\_aic\_ART}, \text{Vm\_ART}, [\text{aic}], [\text{c\_10f}]\right)\\ &= \frac{\text{Vm\_ART} \cdot [\text{c\_10f}] \cdot [\text{aic}]}{(\text{K\_10f\_ART} + [\text{c\_10f}]) \cdot (\text{K\_aic\_ART} + [\text{aic}])}\end{aligned} \tag{246}$$

9.45 Reaction V_BHMT

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

Name V_BHMT

Reaction equation

$$\text{hcy} + \text{BET} \overset{\text{H2O2, sah, sam, BET, hcy}}{\rightleftharpoons} \text{met} + \text{dmg} \tag{247}$$

Reactants

Table 126: Properties of each reactant.

Id	Name	SBO
hcy	Homocysteine	
BET	Betaine	

Modifiers

Table 127: Properties of each modifier.

Id	Name	SBO
H2O2	H2O2	
sah	SAH	
sam	SAM	
BET	Betaine	
hcy	Homocysteine	

Products

Table 128: Properties of each product.

Id	Name	SBO
met	c_Methionine	

Id	Name	SBO
dmg	Dimethylglycine	

Kinetic Law

Derived unit contains undeclared units

$$v_{45} = \text{function\_4\_V\_BHMT\_1}\left([\text{BET}], [\text{H2O2}], \text{K\_bet\_BHMT}, \text{K\_hcy\_BHMT}, \text{Ki\_BHMT}, \text{Vm\_BHMT}, \text{vol}\left(\text{cytosol}\right), [\text{hcy}], [\text{sah}], [\text{sam}], \text{ssH2O2}\right) \tag{248}$$

$$\begin{aligned}\text{function\_4\_V\_BHMT\_1}\left([\text{BET}], [\text{H2O2}], \text{K\_bet\_BHMT}, \text{K\_hcy\_BHMT}, \text{Ki\_BHMT}, \text{Vm\_BHMT}, \text{vol}\left(\text{cytosol}\right), [\text{hcy}], [\text{sah}], [\text{sam}], \text{ssH2O2}\right) &= \text{vol}\left(\text{cytosol}\right) \\ &\cdot \exp\left(0.0021 \cdot \left([\text{sam}] + [\text{sah}]\right)\right) \cdot \exp\left(0.0021 \cdot 102.6\right) \\ &\cdot \text{MM\_twosubst}\left(\text{Vm\_BHMT}, \text{K\_hcy\_BHMT}, \text{K\_bet\_BHMT}, [\text{hcy}], [\text{BET}]\right) \\ &\cdot \frac{\text{ssH2O2} + \text{Ki\_BHMT}}{[\text{H2O2}] + \text{Ki\_BHMT}}\end{aligned} \tag{249}$$

9.46 Reaction V_MATI

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

Name V_MATI

Reaction equation

$$\text{met} \overset{\text{c\_gsg, met, sam}}{\rightleftharpoons} \text{sam} \tag{250}$$

Reactant

Table 129: Properties of each reactant.

Id	Name	SBO
met	c_Methionine	

Modifiers

Table 130: Properties of each modifier.

Id	Name	SBO
c_gsg	c_GSSG	
met	c_Methionine	
sam	SAM	

Product

Table 131: Properties of each product.

Id	Name	SBO
sam	SAM	

Kinetic Law

Derived unit contains undeclared units

$$v_{46} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{function\_4\_V\_MATI\_1}\,(\mathrm{Ki\_MAT1}, \mathrm{Km\_MAT1}, \mathrm{Vm\_MAT1}, [\mathrm{c\_gsg}], [\mathrm{met}], [\mathrm{sam}]) \tag{251}$$

$$\mathrm{function\_4\_V\_MATI\_1}\,(\mathrm{Ki\_MAT1}, \mathrm{Km\_MAT1}, \mathrm{Vm\_MAT1}, [\mathrm{c\_gsg}], [\mathrm{met}], [\mathrm{sam}]) = \mathrm{Vm\_MAT1} \cdot \frac{[\mathrm{met}]}{\mathrm{Km\_MAT1} + [\mathrm{met}]} \cdot (0.23 + 0.8 \cdot \exp\,(0.0026 \cdot [\mathrm{sam}])) \cdot \frac{\mathrm{Ki\_MAT1} + 66.71}{\mathrm{Ki\_MAT1} + [\mathrm{c\_gsg}]} \tag{252}$$

$$\mathrm{function\_4\_V\_MATI\_1}\,(\mathrm{Ki\_MAT1}, \mathrm{Km\_MAT1}, \mathrm{Vm\_MAT1}, [\mathrm{c\_gsg}], [\mathrm{met}], [\mathrm{sam}]) = \mathrm{Vm\_MAT1} \cdot \frac{[\mathrm{met}]}{\mathrm{Km\_MAT1} + [\mathrm{met}]} \cdot (0.23 + 0.8 \cdot \exp\,(0.0026 \cdot [\mathrm{sam}])) \cdot \frac{\mathrm{Ki\_MAT1} + 66.71}{\mathrm{Ki\_MAT1} + [\mathrm{c\_gsg}]} \tag{253}$$

9.47 Reaction V_MATIII

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

Name V_MATIII

Reaction equation

$$\mathrm{met} \overset{\mathrm{c\_gsg,\ met,\ sam}}{\rightleftharpoons} \mathrm{sam} \tag{254}$$

Reactant

Table 132: Properties of each reactant.

Id	Name	SBO
met	c_Methionine	

Modifiers

Table 133: Properties of each modifier.

Id	Name	SBO
c_gsg	c_GSSG	
met	c_Methionine	
sam	SAM	

Product

Table 134: Properties of each product.

Id	Name	SBO
sam	SAM	

Kinetic Law

Derived unit contains undeclared units

$$v_{47} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{function\_4\_V\_MATIII\_1}\,(\mathrm{Ka\_MAT3}, \mathrm{Ki\_MAT3}, \mathrm{Km\_MAT3}, \mathrm{Vm\_MAT3}, [\mathrm{c\_gsg}], [\mathrm{met}], [\mathrm{sam}]) \tag{255}$$

$$\mathrm{function\_4\_V\_MATIII\_1}\,(\mathrm{Ka\_MAT3}, \mathrm{Ki\_MAT3}, \mathrm{Km\_MAT3}, \mathrm{Vm\_MAT3}, [\mathrm{c\_gsg}], [\mathrm{met}], [\mathrm{sam}]) = \mathrm{Vm\_MAT3} \cdot \frac{[\mathrm{met}]^{1.21}}{\mathrm{Km\_MAT3} + [\mathrm{met}]^{1.21}} \cdot \left(1 + \frac{7.2 \cdot [\mathrm{sam}]^2}{\mathrm{Ka\_MAT3}^2 + [\mathrm{sam}]^2}\right) \cdot \frac{\mathrm{Ki\_MAT3} + 66.71}{\mathrm{Ki\_MAT3} + [\mathrm{c\_gsg}]} \tag{256}$$

$$\mathrm{function\_4\_V\_MATIII\_1}\,(\mathrm{Ka\_MAT3}, \mathrm{Ki\_MAT3}, \mathrm{Km\_MAT3}, \mathrm{Vm\_MAT3}, [\mathrm{c\_gsg}], [\mathrm{met}], [\mathrm{sam}]) = \mathrm{Vm\_MAT3} \cdot \frac{[\mathrm{met}]^{1.21}}{\mathrm{Km\_MAT3} + [\mathrm{met}]^{1.21}} \cdot \left(1 + \frac{7.2 \cdot [\mathrm{sam}]^2}{\mathrm{Ka\_MAT3}^2 + [\mathrm{sam}]^2}\right) \cdot \frac{\mathrm{Ki\_MAT3} + 66.71}{\mathrm{Ki\_MAT3} + [\mathrm{c\_gsg}]} \tag{257}$$

9.48 Reaction V_GNMT

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

Name V_GNMT

Reaction equation

$$\mathrm{sam} + \mathrm{c\_gly} \xrightleftharpoons{\mathrm{c\_5mf,\ c\_gly,\ sah,\ sam}} \mathrm{sah} + \mathrm{src} \tag{258}$$

Reactants

Table 135: Properties of each reactant.

Id	Name	SBO
sam	SAM	
c_gly	c_Glycine	

Modifiers

Table 136: Properties of each modifier.

Id	Name	SBO
c_5mf	c_5-methyl-THF	
c_gly	c_Glycine	
sah	SAH	
sam	SAM	

Products

Table 137: Properties of each product.

Id	Name	SBO
sah	SAH	
src	Sarcosine	

Kinetic Law

Derived unit contains undeclared units

$$v_{48} = \text{function\_4\_V\_GNMT\_1}\left(\text{K\_gly\_GNMT}, \text{K\_sam\_GNMT}, \text{Ki\_GNMT}, \text{Vm\_GNMT}, [\text{c\_5mf}], [\text{c\_gly}], \text{vol}\left(\text{cytosol}\right), [\text{sah}], [\text{sam}]\right) \tag{259}$$

$$\begin{aligned}\text{function\_4\_V\_GNMT\_1}&\left(\text{K\_gly\_GNMT}, \text{K\_sam\_GNMT}, \text{Ki\_GNMT}, \right.\\ &\left.\text{Vm\_GNMT}, [\text{c\_5mf}], [\text{c\_gly}], \text{vol}\left(\text{cytosol}\right), [\text{sah}], [\text{sam}]\right) = \text{vol}\left(\text{cytosol}\right)\\ &\cdot \text{MM\_twosubst}\left(\text{Vm\_GNMT}, \text{K\_sam\_GNMT}, \text{K\_gly\_GNMT}, [\text{sam}], [\text{c\_gly}]\right)\\ &\cdot \frac{1}{1 + \frac{[\text{sah}]}{\text{Ki\_GNMT}}} \cdot \frac{4.8}{0.35 + [\text{c\_5mf}]}\end{aligned} \tag{260}$$

9.49 Reaction V_DNMT

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

Name V_DNMT

Reaction equation

$$\text{sam} \overset{\text{sah, sam}}{\rightleftharpoons} \text{sah} \tag{261}$$

Reactant

Table 138: Properties of each reactant.

Id	Name	SBO
sam	SAM	

Modifiers

Table 139: Properties of each modifier.

Id	Name	SBO
sah	SAH	
sam	SAM	

Product

Table 140: Properties of each product.

Id	Name	SBO
sah	SAH	

Kinetic Law

Derived unit contains undeclared units

$$v_{49} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{function\_4\_V\_DNMT\_1}\,(\mathrm{Ki\_DNMT}, \mathrm{Km\_DNMT}, \mathrm{Vm\_DNMT}, [\mathrm{sah}], [\mathrm{sam}]) \tag{262}$$

$$\begin{aligned} &\mathrm{function\_4\_V\_DNMT\_1}\,(\mathrm{Ki\_DNMT}, \mathrm{Km\_DNMT}, \mathrm{Vm\_DNMT}, [\mathrm{sah}], [\mathrm{sam}]) \\ &= \mathrm{Vm\_DNMT} \cdot \frac{[\mathrm{sam}]}{\mathrm{Km\_DNMT} \cdot \left(1 + \frac{[\mathrm{sah}]}{\mathrm{Ki\_DNMT}}\right) + [\mathrm{sam}]} \end{aligned} \tag{263}$$

$$\begin{aligned} &\mathrm{function\_4\_V\_DNMT\_1}\,(\mathrm{Ki\_DNMT}, \mathrm{Km\_DNMT}, \mathrm{Vm\_DNMT}, [\mathrm{sah}], [\mathrm{sam}]) \\ &= \mathrm{Vm\_DNMT} \cdot \frac{[\mathrm{sam}]}{\mathrm{Km\_DNMT} \cdot \left(1 + \frac{[\mathrm{sah}]}{\mathrm{Ki\_DNMT}}\right) + [\mathrm{sam}]} \end{aligned} \tag{264}$$

9.50 Reaction V_SAHH

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

Name V_SAHH

Reaction equation

$$\mathrm{sah} \underset{\text{hcy, sah}}{\rightleftharpoons} \mathrm{hcy} \tag{265}$$

Reactant

Table 141: Properties of each reactant.

Id	Name	SBO
sah	SAH	

Modifiers

Table 142: Properties of each modifier.

Id	Name	SBO
hcy	Homocysteine	
sah	SAH	

Product

Table 143: Properties of each product.

Id	Name	SBO
hcy	Homocysteine	

Kinetic Law

Derived unit contains undeclared units

$$v_{50} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{function\_4\_V\_SAHH\_1}\,(\mathrm{K\_hcy\_SAHH}, \mathrm{K\_sah\_SAHH}, \mathrm{Vf\_SAHH}, \mathrm{Vr\_SAHH}, [\mathrm{hcy}], [\mathrm{sah}]) \tag{266}$$

$$\mathrm{function\_4\_V\_SAHH\_1}\,(\mathrm{K\_hcy\_SAHH}, \mathrm{K\_sah\_SAHH}, \mathrm{Vf\_SAHH}, \mathrm{Vr\_SAHH}, [\mathrm{hcy}], [\mathrm{sah}]) = \mathrm{MM}\,(\mathrm{Vf\_SAHH}, \mathrm{K\_sah\_SAHH}, [\mathrm{sah}]) - \mathrm{MM}\,(\mathrm{Vr\_SAHH}, \mathrm{K\_hcy\_SAHH}, [\mathrm{hcy}]) \tag{267}$$

$$\mathrm{function\_4\_V\_SAHH\_1}\,(\mathrm{K\_hcy\_SAHH}, \mathrm{K\_sah\_SAHH}, \mathrm{Vf\_SAHH}, \mathrm{Vr\_SAHH}, [\mathrm{hcy}], [\mathrm{sah}]) = \mathrm{MM}\,(\mathrm{Vf\_SAHH}, \mathrm{K\_sah\_SAHH}, [\mathrm{sah}]) - \mathrm{MM}\,(\mathrm{Vr\_SAHH}, \mathrm{K\_hcy\_SAHH}, [\mathrm{hcy}]) \tag{268}$$

9.51 Reaction gluconeogenesis_ser

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

Name gluconeogenesis_ser

Reaction equation

$$\mathrm{c\_ser} \overset{\mathrm{c\_ser}}{\rightleftharpoons} \emptyset \tag{269}$$

Reactant

Table 144: Properties of each reactant.

Id	Name	SBO
c_ser	c_Serine	

Modifier

Table 145: Properties of each modifier.

Id	Name	SBO
c_ser	c_Serine	

Kinetic Law

Derived unit contains undeclared units

$$v_{51} = \text{vol}(\text{cytosol}) \cdot \text{function\_4\_gluconeogenesis\_ser\_1}([\text{c\_ser}]) \tag{270}$$

$$\text{function\_4\_gluconeogenesis\_ser\_1}([\text{c\_ser}]) = 1.2 \cdot [\text{c\_ser}] \tag{271}$$

$$\text{function\_4\_gluconeogenesis\_ser\_1}([\text{c\_ser}]) = 1.2 \cdot [\text{c\_ser}] \tag{272}$$

9.52 Reaction V_CBS

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

Name V_CBS

Reaction equation

$$\text{hcy} + \text{c\_ser} \xrightleftharpoons{\text{H2O2, sah, sam, c\_ser, hcy}} \text{cyt} \tag{273}$$

Reactants

Table 146: Properties of each reactant.

Id	Name	SBO
hcy	Homocysteine	
c_ser	c_Serine	

Modifiers

Table 147: Properties of each modifier.

Id	Name	SBO
H2O2	H2O2	
sah	SAH	
sam	SAM	
c_ser	c_Serine	
hcy	Homocysteine	

Product

Table 148: Properties of each product.

Id	Name	SBO
cyt	Cystathionine	

Kinetic Law

Derived unit contains undeclared units

$$v_{52} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{function\_4\_V\_CBS\_1}\,([\mathrm{H2O2}], \mathrm{K\_hcy\_CBS}, \mathrm{K\_ser\_CBS}, \mathrm{Ka\_CBS}, \mathrm{Vm\_CBS}, [\mathrm{c\_ser}], [\mathrm{hcy}], [\mathrm{sah}], [\mathrm{sam}], \mathrm{ssH2O2}) \tag{274}$$

$$\mathrm{function\_4\_V\_CBS\_1}\,([\mathrm{H2O2}], \mathrm{K\_hcy\_CBS}, \mathrm{K\_ser\_CBS}, \mathrm{Ka\_CBS}, \mathrm{Vm\_CBS}, [\mathrm{c\_ser}], [\mathrm{hcy}], [\mathrm{sah}], [\mathrm{sam}], \mathrm{ssH2O2}) = \mathrm{MM\_twosubst}\,(\mathrm{Vm\_CBS}, \mathrm{K\_hcy\_CBS}, \mathrm{K\_ser\_CBS}, [\mathrm{hcy}], [\mathrm{c\_ser}]) \cdot \frac{\left(\frac{30}{102.59}\right)^2 + 1}{\left(\frac{30}{[\mathrm{sam}]+[\mathrm{sah}]}\right)^2 + 1} \cdot \frac{[\mathrm{H2O2}] + \mathrm{Ka\_CBS}}{\mathrm{ssH2O2} + \mathrm{Ka\_CBS}} \tag{275}$$

$$\mathrm{function\_4\_V\_CBS\_1}\,([\mathrm{H2O2}], \mathrm{K\_hcy\_CBS}, \mathrm{K\_ser\_CBS}, \mathrm{Ka\_CBS}, \mathrm{Vm\_CBS}, [\mathrm{c\_ser}], [\mathrm{hcy}], [\mathrm{sah}], [\mathrm{sam}], \mathrm{ssH2O2}) = \mathrm{MM\_twosubst}\,(\mathrm{Vm\_CBS}, \mathrm{K\_hcy\_CBS}, \mathrm{K\_ser\_CBS}, [\mathrm{hcy}], [\mathrm{c\_ser}]) \cdot \frac{\left(\frac{30}{102.59}\right)^2 + 1}{\left(\frac{30}{[\mathrm{sam}]+[\mathrm{sah}]}\right)^2 + 1} \cdot \frac{[\mathrm{H2O2}] + \mathrm{Ka\_CBS}}{\mathrm{ssH2O2} + \mathrm{Ka\_CBS}} \tag{276}$$

9.53 Reaction V_CTGL

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

Name V_CTGL

Reaction equation

$$\text{cyt} \overset{\text{cyt}}{\rightleftharpoons} \text{c\_cys} \tag{277}$$

Reactant

Table 149: Properties of each reactant.

Id	Name	SBO
cyt	Cystathionine	

Modifier

Table 150: Properties of each modifier.

Id	Name	SBO
cyt	Cystathionine	

Product

Table 151: Properties of each product.

Id	Name	SBO
c_cys	c_Cysteine	

Kinetic Law

Derived unit contains undeclared units

$$v_{53} = \text{vol}(\text{cytosol}) \cdot \text{function\_4\_V\_CTGL\_1}(\text{K\_cyt\_CTGL}, \text{Vm\_CTGL}, [\text{cyt}]) \tag{278}$$

$$\text{function\_4\_V\_CTGL\_1}(\text{K\_cyt\_CTGL}, \text{Vm\_CTGL}, [\text{cyt}]) = \frac{\text{Vm\_CTGL} \cdot [\text{cyt}]}{\text{K\_cyt\_CTGL} + [\text{cyt}]} \tag{279}$$

$$\text{function\_4\_V\_CTGL\_1}\left(\text{K\_cyt\_CTGL}, \text{Vm\_CTGL}, [\text{cyt}]\right) = \frac{\text{Vm\_CTGL} \cdot [\text{cyt}]}{\text{K\_cyt\_CTGL} + [\text{cyt}]} \quad (280)$$

9.54 Reaction V_GCS

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

Name V_GCS

Reaction equation

$$\text{c\_cys} + \text{c\_glu} \xrightleftharpoons{\text{H2O2, c\_gsh, c\_cys, c\_glu, glc}} \text{glc} \quad (281)$$

Reactants

Table 152: Properties of each reactant.

Id	Name	SBO
c_cys	c_Cysteine	
c_glu	c_Glutamate	

Modifiers

Table 153: Properties of each modifier.

Id	Name	SBO
H2O2	H2O2	
c_gsh	c_GSH	
c_cys	c_Cysteine	
c_glu	c_Glutamate	
glc	Glutamyl-Cysteine	

Product

Table 154: Properties of each product.

Id	Name	SBO
glc	Glutamyl-Cysteine	

Kinetic Law

Derived unit contains undeclared units

$$v_{54} = \text{vol}\,(\text{cytosol}) \cdot \text{function\_4\_V\_GCS\_1}\,([\text{H2O2}], \text{K\_cys\_GCS}, \text{K\_glu\_GCS}, \text{Ka\_GCS}, \text{Ke\_GCS}, \text{Ki\_GCS}, \text{Kp\_GCS}, \text{Vm\_GCS}, [\text{c\_cys}], [\text{c\_glu}], [\text{c\_gsh}], [\text{glc}], \text{ssH2O2}) \tag{282}$$

$$\text{function\_4\_V\_GCS\_1}\,([\text{H2O2}], \text{K\_cys\_GCS}, \text{K\_glu\_GCS}, \text{Ka\_GCS}, \text{Ke\_GCS}, \text{Ki\_GCS}, \text{Kp\_GCS}, \text{Vm\_GCS}, [\text{c\_cys}], [\text{c\_glu}], [\text{c\_gsh}], [\text{glc}], \text{ssH2O2}) \tag{283}$$

$$= \frac{\text{Vm\_GCS} \cdot \left([\text{c\_cys}] \cdot [\text{c\_glu}] - \frac{[\text{glc}]}{\text{Ke\_GCS}}\right)}{\text{K\_cys\_GCS} \cdot \text{K\_glu\_GCS} + [\text{c\_glu}] \cdot \text{K\_cys\_GCS} + [\text{c\_cys}] \cdot \left(\text{K\_glu\_GCS} \cdot \left(1 + \frac{[\text{c\_gsh}]}{\text{Ki\_GCS}}\right) + [\text{c\_glu}]\right) + \frac{[\text{glc}]}{\text{Kp\_GCS}} + \cdot \frac{[\text{H2O2}] + \text{Ka\_GCS}}{\text{ssH2O2} + \text{Ka\_GCS}}}$$

$$\text{function\_4\_V\_GCS\_1}\,([\text{H2O2}], \text{K\_cys\_GCS}, \text{K\_glu\_GCS}, \text{Ka\_GCS}, \text{Ke\_GCS}, \text{Ki\_GCS}, \text{Kp\_GCS}, \text{Vm\_GCS}, [\text{c\_cys}], [\text{c\_glu}], [\text{c\_gsh}], [\text{glc}], \text{ssH2O2}) \tag{284}$$

$$= \frac{\text{Vm\_GCS} \cdot \left([\text{c\_cys}] \cdot [\text{c\_glu}] - \frac{[\text{glc}]}{\text{Ke\_GCS}}\right)}{\text{K\_cys\_GCS} \cdot \text{K\_glu\_GCS} + [\text{c\_glu}] \cdot \text{K\_cys\_GCS} + [\text{c\_cys}] \cdot \left(\text{K\_glu\_GCS} \cdot \left(1 + \frac{[\text{c\_gsh}]}{\text{Ki\_GCS}}\right) + [\text{c\_glu}]\right) + \frac{[\text{glc}]}{\text{Kp\_GCS}} + \cdot \frac{[\text{H2O2}] + \text{Ka\_GCS}}{\text{ssH2O2} + \text{Ka\_GCS}}}$$

9.55 Reaction `cys_usage`

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

Name cys_usage

Reaction equation

$$\text{c\_cys} \overset{\text{c\_cys}}{\rightleftharpoons} \emptyset \tag{285}$$

Reactant

Table 155: Properties of each reactant.

Id	Name	SBO
c_cys	c_Cysteine	

Modifier

Table 156: Properties of each modifier.

Id	Name	SBO
c_cys	c_Cysteine	

Kinetic Law

Derived unit contains undeclared units

$$v_{55} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{function\_4\_cys\_usage\_1}\,([\mathrm{c\_cys}]) \tag{286}$$

$$\mathrm{function\_4\_cys\_usage\_1}\,([\mathrm{c\_cys}]) = \frac{0.35 \cdot [\mathrm{c\_cys}]^2}{200} \tag{287}$$

$$\mathrm{function\_4\_cys\_usage\_1}\,([\mathrm{c\_cys}]) = \frac{0.35 \cdot [\mathrm{c\_cys}]^2}{200} \tag{288}$$

9.56 Reaction c_glu_usage

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

Name c_glu_usage

Reaction equation

$$\mathrm{c\_glu} \overset{\mathrm{c\_glu}}{\rightleftharpoons} \emptyset \tag{289}$$

Reactant

Table 157: Properties of each reactant.

Id	Name	SBO
c_glu	c_Glutamate	

Modifier

Table 158: Properties of each modifier.

Id	Name	SBO
c_glu	c_Glutamate	

Kinetic Law

Derived unit contains undeclared units

$$v_{56} = \text{vol}(\text{cytosol}) \cdot \text{function\_4\_c\_glu\_usage\_1}([\text{c\_glu}]) \tag{290}$$

$$\text{function\_4\_c\_glu\_usage\_1}([\text{c\_glu}]) = 0.07 \cdot [\text{c\_glu}] \tag{291}$$

$$\text{function\_4\_c\_glu\_usage\_1}([\text{c\_glu}]) = 0.07 \cdot [\text{c\_glu}] \tag{292}$$

9.57 Reaction V_GS

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

Name V_GS

Reaction equation

$$\text{glc} + \text{c\_gly} \overset{\text{c\_gly, c\_gsh, glc}}{\rightleftharpoons} \text{c\_gsh} \tag{293}$$

Reactants

Table 159: Properties of each reactant.

Id	Name	SBO
glc	Glutamyl-Cysteine	
c_gly	c_Glycine	

Modifiers

Table 160: Properties of each modifier.

Id	Name	SBO
c_gly	c_Glycine	

Id	Name	SBO
c_gsh	c_GSH	
glc	Glutamyl-Cysteine	

Product

Table 161: Properties of each product.

Id	Name	SBO
c_gsh	c_GSH	

Kinetic Law

Derived unit contains undeclared units

$$v_{57} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{function\_4\_V\_GS\_1}\,(\mathrm{K\_glc\_GS}, \mathrm{K\_gly\_GS}, \mathrm{Ke\_GS}, \mathrm{Kp\_GS}, \mathrm{Vm\_GS}, [\mathrm{c\_gly}], [\mathrm{c\_gsh}], [\mathrm{glc}]) \tag{294}$$

$$\mathrm{function\_4\_V\_GS\_1}\,(\mathrm{K\_glc\_GS}, \mathrm{K\_gly\_GS}, \mathrm{Ke\_GS}, \mathrm{Kp\_GS}, \mathrm{Vm\_GS}, [\mathrm{c\_gly}], [\mathrm{c\_gsh}], [\mathrm{glc}]) = \frac{\mathrm{Vm\_GS} \cdot \left([\mathrm{c\_gly}] \cdot [\mathrm{glc}] - \frac{[\mathrm{c\_gsh}]}{\mathrm{Ke\_GS}}\right)}{\mathrm{K\_gly\_GS} \cdot \mathrm{K\_glc\_GS} + [\mathrm{glc}] \cdot \mathrm{K\_gly\_GS} + [\mathrm{c\_gly}] \cdot (\mathrm{K\_glc\_GS} + [\mathrm{glc}]) + \frac{[\mathrm{c\_gsh}]}{\mathrm{Kp\_GS}}} \tag{295}$$

$$\mathrm{function\_4\_V\_GS\_1}\,(\mathrm{K\_glc\_GS}, \mathrm{K\_gly\_GS}, \mathrm{Ke\_GS}, \mathrm{Kp\_GS}, \mathrm{Vm\_GS}, [\mathrm{c\_gly}], [\mathrm{c\_gsh}], [\mathrm{glc}]) = \frac{\mathrm{Vm\_GS} \cdot \left([\mathrm{c\_gly}] \cdot [\mathrm{glc}] - \frac{[\mathrm{c\_gsh}]}{\mathrm{Ke\_GS}}\right)}{\mathrm{K\_gly\_GS} \cdot \mathrm{K\_glc\_GS} + [\mathrm{glc}] \cdot \mathrm{K\_gly\_GS} + [\mathrm{c\_gly}] \cdot (\mathrm{K\_glc\_GS} + [\mathrm{glc}]) + \frac{[\mathrm{c\_gsh}]}{\mathrm{Kp\_GS}}} \tag{296}$$

9.58 Reaction V_GPX

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

Name V_GPX

Reaction equation

$$2\,\mathrm{c\_gsh} + \mathrm{H2O2} \xrightleftharpoons{\mathrm{H2O2,\ c\_gsh}} \mathrm{c\_gsg} \tag{297}$$

Reactants

Table 162: Properties of each reactant.

Id	Name	SBO
c_gsh	c_GSH	
H2O2	H2O2	

Modifiers

Table 163: Properties of each modifier.

Id	Name	SBO
H2O2	H2O2	
c_gsh	c_GSH	

Product

Table 164: Properties of each product.

Id	Name	SBO
c_gsg	c_GSSG	

Kinetic Law

Derived unit contains undeclared units

$$v_{58} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{function\_4\_V\_GPX\_1}\,([\mathrm{H2O2}], \mathrm{K\_H2O2\_GPX}, \mathrm{K\_gsh\_GPX}, \mathrm{Vm\_GPX}, [\mathrm{c\_gsh}]) \tag{298}$$

$$\mathrm{function\_4\_V\_GPX\_1}\,([\mathrm{H2O2}], \mathrm{K\_H2O2\_GPX}, \mathrm{K\_gsh\_GPX}, \mathrm{Vm\_GPX}, [\mathrm{c\_gsh}]) = \mathrm{Vm\_GPX} \cdot \left(\frac{[\mathrm{c\_gsh}]}{\mathrm{K\_gsh\_GPX} + [\mathrm{c\_gsh}]}\right)^2 \cdot \frac{[\mathrm{H2O2}]}{\mathrm{K\_H2O2\_GPX} + [\mathrm{H2O2}]} \tag{299}$$

$$\mathrm{function\_4\_V\_GPX\_1}\,([\mathrm{H2O2}], \mathrm{K\_H2O2\_GPX}, \mathrm{K\_gsh\_GPX}, \mathrm{Vm\_GPX}, [\mathrm{c\_gsh}]) = \mathrm{Vm\_GPX} \cdot \left(\frac{[\mathrm{c\_gsh}]}{\mathrm{K\_gsh\_GPX} + [\mathrm{c\_gsh}]}\right)^2 \cdot \frac{[\mathrm{H2O2}]}{\mathrm{K\_H2O2\_GPX} + [\mathrm{H2O2}]} \tag{300}$$

9.59 Reaction V_GR

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

Name V_GR

Reaction equation

$$\mathrm{c\_gsg} + \mathrm{NADPH} \overset{\mathrm{NADPH,\ c\_gsg}}{\rightleftharpoons} 2\,\mathrm{c\_gsh} \tag{301}$$

Reactants

Table 165: Properties of each reactant.

Id	Name	SBO
c_gsg	c_GSSG	
NADPH	NADPH	

Modifiers

Table 166: Properties of each modifier.

Id	Name	SBO
NADPH	NADPH	
c_gsg	c_GSSG	

Product

Table 167: Properties of each product.

Id	Name	SBO
c_gsh	c_GSH	

Kinetic Law

Derived unit contains undeclared units

$$\begin{aligned} v_{59} = {} & \mathrm{vol}\,(\mathrm{cytosol}) \\ & \cdot \mathrm{function\_4\_V\_GR\_1}\,(\mathrm{K\_NADPH\_GR}, \mathrm{K\_gsg\_GR}, [\mathrm{NADPH}], \mathrm{Vm\_GR}, [\mathrm{c\_gsg}]) \end{aligned} \tag{302}$$

$$\begin{aligned}&\text{function\_4\_V\_GR\_1}\left(\text{K\_NADPH\_GR}, \text{K\_gsg\_GR}, [\text{NADPH}], \text{Vm\_GR}, [\text{c\_gsg}]\right)\\&= \frac{\text{Vm\_GR} \cdot [\text{c\_gsg}] \cdot [\text{NADPH}]}{(\text{K\_gsg\_GR} + [\text{c\_gsg}]) \cdot (\text{K\_NADPH\_GR} + [\text{NADPH}])}\end{aligned} \tag{303}$$

$$\begin{aligned}&\text{function\_4\_V\_GR\_1}\left(\text{K\_NADPH\_GR}, \text{K\_gsg\_GR}, [\text{NADPH}], \text{Vm\_GR}, [\text{c\_gsg}]\right)\\&= \frac{\text{Vm\_GR} \cdot [\text{c\_gsg}] \cdot [\text{NADPH}]}{(\text{K\_gsg\_GR} + [\text{c\_gsg}]) \cdot (\text{K\_NADPH\_GR} + [\text{NADPH}])}\end{aligned} \tag{304}$$

9.60 Reaction c_gsh_degr

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

Name c_gsh_degr

Reaction equation

$$\text{c\_gsh} \overset{\text{c\_gsh}}{\rightleftharpoons} \emptyset \tag{305}$$

Reactant

Table 168: Properties of each reactant.

Id	Name	SBO
c_gsh	c_GSH	

Modifier

Table 169: Properties of each modifier.

Id	Name	SBO
c_gsh	c_GSH	

Kinetic Law

Derived unit contains undeclared units

$$v_{60} = \text{vol}\left(\text{cytosol}\right) \cdot \text{function\_4\_c\_gsh\_degr\_1}\left([\text{c\_gsh}]\right) \tag{306}$$

$$\text{function\_4\_c\_gsh\_degr\_1}\left([\text{c\_gsh}]\right) = 0.0020 \cdot [\text{c\_gsh}] \tag{307}$$

$$\text{function\_4\_c\_gsh\_degr\_1}\left([\text{c\_gsh}]\right) = 0.0020 \cdot [\text{c\_gsh}] \tag{308}$$

9.61 Reaction c_gsg_degr

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

Name c_gsg_degr

Reaction equation

$$\text{c\_gsg} \overset{\text{c\_gsg}}{\rightleftharpoons} \emptyset \tag{309}$$

Reactant

Table 170: Properties of each reactant.

Id	Name	SBO
c_gsg	c_GSSG	

Modifier

Table 171: Properties of each modifier.

Id	Name	SBO
c_gsg	c_GSSG	

Kinetic Law

Derived unit contains undeclared units

$$v_{61} = \text{vol}\left(\text{cytosol}\right) \cdot \text{function\_4\_c\_gsg\_degr\_1}\left([\text{c\_gsg}]\right) \tag{310}$$

$$\text{function\_4\_c\_gsg\_degr\_1}\left([\text{c\_gsg}]\right) = 0.1 \cdot [\text{c\_gsg}] \tag{311}$$

$$\text{function\_4\_c\_gsg\_degr\_1}\left([\text{c\_gsg}]\right) = 0.1 \cdot [\text{c\_gsg}] \tag{312}$$

9.62 Reaction reaction_1

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

Name V_ODC

Reaction equation

$$\text{species\_7} \xrightleftharpoons{\text{species\_2, species\_7}} \text{species\_2} \tag{313}$$

Reactant

Table 172: Properties of each reactant.

Id	Name	SBO
species_7	Ornithine	

Modifiers

Table 173: Properties of each modifier.

Id	Name	SBO
species_2	Putrescine	
species_7	Ornithine	

Product

Table 174: Properties of each product.

Id	Name	SBO
species_2	Putrescine	

Kinetic Law

Derived unit contains undeclared units

$$v_{62} = \text{vol}\,(\text{cytosol}) \cdot \text{function\_4\_V\_ODC\_1}\,(\text{Kipodc}, \text{Kmodc}, \text{parameter\_1}, [\text{species\_2}], [\text{species\_7}]) \tag{314}$$

$$\begin{aligned} &\text{function\_4\_V\_ODC\_1}\,(\text{Kipodc}, \text{Kmodc}, \text{parameter\_1}, [\text{species\_2}], [\text{species\_7}]) \\ &= \frac{\text{parameter\_1} \cdot [\text{species\_7}]}{\text{Kmodc} \cdot \left(1 + \frac{[\text{species\_2}]}{\text{Kipodc}}\right) + [\text{species\_7}]} \end{aligned} \tag{315}$$

$$\begin{aligned}&\text{function\_4\_V\_ODC\_1}\left(\text{Kipodc}, \text{Kmodc}, \text{parameter\_1}, [\text{species\_2}], [\text{species\_7}]\right)\\&= \frac{\text{parameter\_1} \cdot [\text{species\_7}]}{\text{Kmodc} \cdot \left(1 + \frac{[\text{species\_2}]}{\text{Kipodc}}\right) + [\text{species\_7}]}\end{aligned} \tag{316}$$

Table 175: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Kipodc`	Kipodc		1300.0		☑
`Kmodc`	Kmodc		60.0		☑

9.63 Reaction `reaction_2`

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

Name V_SAMDC

Reaction equation

$$\text{sam} \xrightleftharpoons{\text{species\_3, species\_2, sam, species\_1}} \text{species\_1} \tag{317}$$

Reactant

Table 176: Properties of each reactant.

Id	Name	SBO
`sam`	SAM	

Modifiers

Table 177: Properties of each modifier.

Id	Name	SBO
`species_3`	Spermine	
`species_2`	Putrescine	
`sam`	SAM	
`species_1`	dcSAM	

Product

Table 178: Properties of each product.

Id	Name	SBO
species_1	dcSAM	

Kinetic Law

Derived unit contains undeclared units

$$v_{63} = \text{vol}\,(\text{cytosol}) \cdot \text{function\_4\_V\_SAMDC\_1}\,(\text{Kapsamdc}, \text{Kiasamdc}, \text{Kissamdc}, \text{Kmsamdc}, \text{parameter\_3}, [\text{sam}], [\text{species\_1}], [\text{species\_2}], [\text{species\_3}]) \tag{318}$$

$$\text{function\_4\_V\_SAMDC\_1}\,(\text{Kapsamdc}, \text{Kiasamdc}, \text{Kissamdc}, \text{Kmsamdc}, \text{parameter\_3}, [\text{sam}], [\text{species\_1}], [\text{species\_2}], [\text{species\_3}]) = \frac{\frac{\text{parameter\_3}}{1+\frac{[\text{species\_3}]}{\text{Kissamdc}}} \cdot [\text{sam}]}{\text{Kmsamdc} \cdot \left(1 + \frac{\text{Kapsamdc}}{[\text{species\_2}]} + \frac{[\text{species\_1}]}{\text{Kiasamdc}}\right) + [\text{sam}]} \tag{319}$$

$$\text{function\_4\_V\_SAMDC\_1}\,(\text{Kapsamdc}, \text{Kiasamdc}, \text{Kissamdc}, \text{Kmsamdc}, \text{parameter\_3}, [\text{sam}], [\text{species\_1}], [\text{species\_2}], [\text{species\_3}]) = \frac{\frac{\text{parameter\_3}}{1+\frac{[\text{species\_3}]}{\text{Kissamdc}}} \cdot [\text{sam}]}{\text{Kmsamdc} \cdot \left(1 + \frac{\text{Kapsamdc}}{[\text{species\_2}]} + \frac{[\text{species\_1}]}{\text{Kiasamdc}}\right) + [\text{sam}]} \tag{320}$$

Table 179: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kapsamdc	Kapsamdc		0.5		☑
Kiasamdc	Kiasamdc		2.5		☑
Kissamdc	Kissamdc		500.0		☑
Kmsamdc	Kmsamdc		50.0		☑

9.64 Reaction reaction_3

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

Name V_SSAT_S

Reaction equation

$$\text{species\_3} + \text{species\_8} \xrightleftharpoons{\text{species\_4, species\_3, species\_8, species\_9}} \text{species\_5} + \text{species\_9} \quad (321)$$

Reactants

Table 180: Properties of each reactant.

Id	Name	SBO
species_3	Spermine	
species_8	Acetyl-CoA	

Modifiers

Table 181: Properties of each modifier.

Id	Name	SBO
species_4	Spermidine	
species_3	Spermine	
species_8	Acetyl-CoA	
species_9	CoA	

Products

Table 182: Properties of each product.

Id	Name	SBO
species_5	Acetylspermine	
species_9	CoA	

Kinetic Law

Derived unit contains undeclared units

$$v_{64} = \text{vol}(\text{cytosol}) \cdot \text{function\_4\_V\_SSAT\_S\_1}(\text{C}, \text{Kmaccoassat}, \text{Kmcoassat}, \text{Kmdssat}, \text{Kmsssat}, \text{parameter\_2}, [\text{species\_3}], [\text{species\_4}], [\text{species\_8}], [\text{species\_9}]) \quad (322)$$

$$\text{function\_4\_V\_SSAT\_S\_1}(\text{C}, \text{Kmaccoassat}, \text{Kmcoassat}, \text{Kmdssat}, \text{Kmsssat}, \text{parameter\_2}, [\text{species\_3}], [\text{species\_4}], [\text{species\_8}], [\text{species\_9}]) \quad (323)$$
$$= \frac{\frac{1}{\text{C}} \cdot \text{parameter\_2} \cdot [\text{species\_3}] \cdot [\text{species\_8}]}{\text{Kmsssat} \cdot \left(1 + \frac{[\text{species\_4}]}{\text{Kmdssat}}\right) \cdot \text{Kmaccoassat} \cdot \left(1 + \frac{[\text{species\_9}]}{\text{Kmcoassat}}\right) + \text{Kmaccoassat} \cdot \left(1 + \frac{[\text{species\_9}]}{\text{Kmcoassat}}\right) \cdot [\text{species\_3}] + \text{Kmss}}$$

$$\text{function\_4\_V\_SSAT\_S\_1}(\text{C}, \text{Kmaccoassat}, \text{Kmcoassat}, \text{Kmdssat}, \text{Kmsssat}, \text{parameter\_2}, [\text{species\_3}], [\text{species\_4}], [\text{species\_8}], [\text{species\_9}]) \quad (324)$$
$$= \frac{\frac{1}{\text{C}} \cdot \text{parameter\_2} \cdot [\text{species\_3}] \cdot [\text{species\_8}]}{\text{Kmsssat} \cdot \left(1 + \frac{[\text{species\_4}]}{\text{Kmdssat}}\right) \cdot \text{Kmaccoassat} \cdot \left(1 + \frac{[\text{species\_9}]}{\text{Kmcoassat}}\right) + \text{Kmaccoassat} \cdot \left(1 + \frac{[\text{species\_9}]}{\text{Kmcoassat}}\right) \cdot [\text{species\_3}] + \text{Kmss}}$$

Table 183: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
C	C		4.44		☑
Kmaccoassat	Kmaccoassat		1.50		☑
Kmcoassat	Kmcoassat		40.00		☑
Kmdssat	Kmdssat		130.00		☑
Kmsssat	Kmsssat		35.00		☑

9.65 Reaction reaction_4

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

Name V_SSAT_D

Reaction equation

$$\text{species\_4} + \text{species\_8} \xrightleftharpoons{\text{species\_3, species\_4, species\_8, species\_9}} \text{species\_6} + \text{species\_9} \quad (325)$$

Reactants

Table 184: Properties of each reactant.

Id	Name	SBO
species_4	Spermidine	
species_8	Acetyl-CoA	

Modifiers

Table 185: Properties of each modifier.

Id	Name	SBO
species_3	Spermine	
species_4	Spermidine	
species_8	Acetyl-CoA	
species_9	CoA	

Products

Table 186: Properties of each product.

Id	Name	SBO
species_6	Acetylspermidine	
species_9	CoA	

Kinetic Law

Derived unit contains undeclared units

$$v_{65} = \mathrm{vol}\left(\mathrm{cytosol}\right) \cdot \mathrm{function\_4\_V\_SSAT\_D\_1}\left(\mathrm{Kmaccoassat}, \mathrm{Kmcoassat}, \mathrm{Kmdssat}, \mathrm{Kmsssat}, \mathrm{parameter\_2}, [\mathrm{species\_3}], [\mathrm{species\_4}], [\mathrm{species\_8}], [\mathrm{species\_9}]\right) \tag{326}$$

$$\mathrm{function\_4\_V\_SSAT\_D\_1}\left(\mathrm{Kmaccoassat}, \mathrm{Kmcoassat}, \mathrm{Kmdssat}, \mathrm{Kmsssat}, \mathrm{parameter\_2}, [\mathrm{species\_3}], [\mathrm{species\_4}], [\mathrm{species\_8}], [\mathrm{species\_9}]\right) \tag{327}$$

$$= \frac{\mathrm{parameter\_2} \cdot [\mathrm{species\_4}] \cdot [\mathrm{species\_8}]}{\mathrm{Kmdssat} \cdot \left(1 + \frac{[\mathrm{species\_3}]}{\mathrm{Kmsssat}}\right) \cdot \mathrm{Kmaccoassat} \cdot \left(1 + \frac{[\mathrm{species\_9}]}{\mathrm{Kmcoassat}}\right) + \mathrm{Kmaccoassat} \cdot \left(1 + \frac{[\mathrm{species\_9}]}{\mathrm{Kmcoassat}}\right) \cdot [\mathrm{species\_4}] + \mathrm{Kmd}}$$

$$\mathrm{function\_4\_V\_SSAT\_D\_1}\left(\mathrm{Kmaccoassat}, \mathrm{Kmcoassat}, \mathrm{Kmdssat}, \mathrm{Kmsssat}, \mathrm{parameter\_2}, [\mathrm{species\_3}], [\mathrm{species\_4}], [\mathrm{species\_8}], [\mathrm{species\_9}]\right) \tag{328}$$

$$= \frac{\mathrm{parameter\_2} \cdot [\mathrm{species\_4}] \cdot [\mathrm{species\_8}]}{\mathrm{Kmdssat} \cdot \left(1 + \frac{[\mathrm{species\_3}]}{\mathrm{Kmsssat}}\right) \cdot \mathrm{Kmaccoassat} \cdot \left(1 + \frac{[\mathrm{species\_9}]}{\mathrm{Kmcoassat}}\right) + \mathrm{Kmaccoassat} \cdot \left(1 + \frac{[\mathrm{species\_9}]}{\mathrm{Kmcoassat}}\right) \cdot [\mathrm{species\_4}] + \mathrm{Kmd}}$$

Table 187: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kmaccoassat	Kmaccoassat		1.5		☑
Kmcoassat	Kmcoassat		40.0		☑
Kmdssat	Kmdssat		130.0		☑
Kmsssat	Kmsssat		35.0		☑

9.66 Reaction reaction_5

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

Name V_PAO_AD

Reaction equation

$$\text{species\_6} \xrightleftharpoons{\text{species\_5, species\_4, species\_3, species\_6}} \text{species\_2} \tag{329}$$

Reactant

Table 188: Properties of each reactant.

Id	Name	SBO
species_6	Acetylspermidine	

Modifiers

Table 189: Properties of each modifier.

Id	Name	SBO
species_5	Acetylspermine	
species_4	Spermidine	
species_3	Spermine	
species_6	Acetylspermidine	

Product

Table 190: Properties of each product.

Id	Name	SBO
species_2	Putrescine	

Kinetic Law

Derived unit contains undeclared units

$$v_{66} = \text{vol}\,(\text{cytosol}) \cdot \text{function\_4\_V\_PAO\_AD\_1}\,(\text{Kmadpao}, \text{Kmaspao}, \text{Kmdpao}, \text{Kmspao}, \text{Vmpao}, [\text{species\_3}], [\text{species\_4}], [\text{species\_5}], [\text{species\_6}]) \tag{330}$$

$$\text{function\_4\_V\_PAO\_AD\_1}\,(\text{Kmadpao}, \text{Kmaspao}, \text{Kmdpao}, \text{Kmspao}, \text{Vmpao}, [\text{species\_3}], [\text{species\_4}], [\text{species\_5}], [\text{species\_6}]) = \frac{\text{Vmpao} \cdot [\text{species\_6}]}{\text{Kmadpao} \cdot \left(1 + \frac{[\text{species\_6}]}{\text{Kmadpao}} + \frac{[\text{species\_5}]}{\text{Kmaspao}} + \frac{[\text{species\_4}]}{\text{Kmdpao}} + \frac{[\text{species\_3}]}{\text{Kmspao}}\right)} \tag{331}$$

$$\text{function\_4\_V\_PAO\_AD\_1}\,(\text{Kmadpao}, \text{Kmaspao}, \text{Kmdpao}, \text{Kmspao}, \text{Vmpao}, [\text{species\_3}], [\text{species\_4}], [\text{species\_5}], [\text{species\_6}]) = \frac{\text{Vmpao} \cdot [\text{species\_6}]}{\text{Kmadpao} \cdot \left(1 + \frac{[\text{species\_6}]}{\text{Kmadpao}} + \frac{[\text{species\_5}]}{\text{Kmaspao}} + \frac{[\text{species\_4}]}{\text{Kmdpao}} + \frac{[\text{species\_3}]}{\text{Kmspao}}\right)} \tag{332}$$

Table 191: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kmadpao	Kmadpao		14.0		☑
Kmaspao	Kmaspao		0.6		☑
Kmdpao	Kmdpao		50.0		☑
Kmspao	Kmspao		15.0		☑
Vmpao	Vmpao		621.0		☑

9.67 Reaction reaction_6

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

Name V_PAO_AS

Reaction equation

$$\text{species\_5} \xrightleftharpoons{\text{species\_6, species\_3, species\_4, species\_5}} \text{species\_4} \tag{333}$$

Reactant

Table 192: Properties of each reactant.

Id	Name	SBO
species_5	Acetylspermine	

Modifiers

Table 193: Properties of each modifier.

Id	Name	SBO
species_6	Acetylspermidine	
species_3	Spermine	
species_4	Spermidine	
species_5	Acetylspermine	

Product

Table 194: Properties of each product.

Id	Name	SBO
species_4	Spermidine	

Kinetic Law

Derived unit contains undeclared units

$$v_{67} = \text{vol}(\text{cytosol}) \cdot \text{function\_4\_V\_PAO\_AS\_1}(\text{Kmadpao}, \text{Kmaspao}, \text{Kmdpao}, \text{Kmspao}, \text{Vmpao}, [\text{species\_3}], [\text{species\_4}], [\text{species\_5}], [\text{species\_6}]) \tag{334}$$

$$\text{function\_4\_V\_PAO\_AS\_1}\left(\text{Kmadpao}, \text{Kmaspao}, \text{Kmdpao}, \text{Kmspao}, \text{Vmpao}, [\text{species\_3}], [\text{species\_4}], [\text{species\_5}], [\text{species\_6}]\right) = \frac{\text{Vmpao} \cdot [\text{species\_5}]}{\text{Kmaspao} \cdot \left(1 + \frac{[\text{species\_6}]}{\text{Kmadpao}} + \frac{[\text{species\_5}]}{\text{Kmaspao}} + \frac{[\text{species\_4}]}{\text{Kmdpao}} + \frac{[\text{species\_3}]}{\text{Kmspao}}\right)} \tag{335}$$

$$\text{function\_4\_V\_PAO\_AS\_1}\left(\text{Kmadpao}, \text{Kmaspao}, \text{Kmdpao}, \text{Kmspao}, \text{Vmpao}, [\text{species\_3}], [\text{species\_4}], [\text{species\_5}], [\text{species\_6}]\right) = \frac{\text{Vmpao} \cdot [\text{species\_5}]}{\text{Kmaspao} \cdot \left(1 + \frac{[\text{species\_6}]}{\text{Kmadpao}} + \frac{[\text{species\_5}]}{\text{Kmaspao}} + \frac{[\text{species\_4}]}{\text{Kmdpao}} + \frac{[\text{species\_3}]}{\text{Kmspao}}\right)} \tag{336}$$

Table 195: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Kmadpao`	Kmadpao		14.0		☑
`Kmaspao`	Kmaspao		0.6		☑
`Kmdpao`	Kmdpao		50.0		☑
`Kmspao`	Kmspao		15.0		☑
`Vmpao`	Vmpao		621.0		☑

9.68 Reaction `reaction_7`

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

Name V_SPDS

Reaction equation

$$\text{species\_1} + \text{species\_2} \xrightleftharpoons{\text{species\_1, species\_2, species\_4}} \text{species\_4} \tag{337}$$

Reactants

Table 196: Properties of each reactant.

Id	Name	SBO
`species_1`	dcSAM	
`species_2`	Putrescine	

Modifiers

Table 197: Properties of each modifier.

Id	Name	SBO
species_1	dcSAM	
species_2	Putrescine	
species_4	Spermidine	

Product

Table 198: Properties of each product.

Id	Name	SBO
species_4	Spermidine	

Kinetic Law

Derived unit contains undeclared units

$$v_{68} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{function\_4\_V\_SPDS\_1}\,(\mathrm{KaSpds}, \mathrm{Kiaspds}, \mathrm{Kidspds}, \mathrm{Kpspds}, \mathrm{Vmspds}, [\mathrm{species\_1}], [\mathrm{species\_2}], [\mathrm{species\_4}]) \tag{338}$$

$$\mathrm{function\_4\_V\_SPDS\_1}\,(\mathrm{KaSpds}, \mathrm{Kiaspds}, \mathrm{Kidspds}, \mathrm{Kpspds}, \mathrm{Vmspds}, [\mathrm{species\_1}], [\mathrm{species\_2}], [\mathrm{species\_4}]) \tag{339}$$
$$= \frac{\mathrm{Vmspds} \cdot [\mathrm{species\_1}] \cdot [\mathrm{species\_2}]}{\mathrm{Kiaspds} \cdot \mathrm{Kpspds} \cdot \left(1 + \frac{[\mathrm{species\_4}]}{\mathrm{Kidspds}}\right) + \mathrm{Kpspds} \cdot [\mathrm{species\_1}] + \mathrm{KaSpds} \cdot \left(1 + \frac{[\mathrm{species\_4}]}{\mathrm{Kidspds}}\right) \cdot [\mathrm{species\_2}] + [\mathrm{species\_1}]}$$

$$\mathrm{function\_4\_V\_SPDS\_1}\,(\mathrm{KaSpds}, \mathrm{Kiaspds}, \mathrm{Kidspds}, \mathrm{Kpspds}, \mathrm{Vmspds}, [\mathrm{species\_1}], [\mathrm{species\_2}], [\mathrm{species\_4}]) \tag{340}$$
$$= \frac{\mathrm{Vmspds} \cdot [\mathrm{species\_1}] \cdot [\mathrm{species\_2}]}{\mathrm{Kiaspds} \cdot \mathrm{Kpspds} \cdot \left(1 + \frac{[\mathrm{species\_4}]}{\mathrm{Kidspds}}\right) + \mathrm{Kpspds} \cdot [\mathrm{species\_1}] + \mathrm{KaSpds} \cdot \left(1 + \frac{[\mathrm{species\_4}]}{\mathrm{Kidspds}}\right) \cdot [\mathrm{species\_2}] + [\mathrm{species\_1}]}$$

Table 199: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KaSpds	KaSpds		0.3		☑
Kiaspds	Kiaspds		0.8		☑
Kidspds	Kidspds		100.0		☑
Kpspds	Kpspds		40.0		☑
Vmspds	Vmspds		657.0		☑

9.69 Reaction reaction_8

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

Name V_SPMS

Reaction equation

$$\text{species\_1} + \text{species\_4} \xrightleftharpoons{\text{species\_1, species\_3, species\_4}} \text{species\_3} \tag{341}$$

Reactants

Table 200: Properties of each reactant.

Id	Name	SBO
species_1	dcSAM	
species_4	Spermidine	

Modifiers

Table 201: Properties of each modifier.

Id	Name	SBO
species_1	dcSAM	
species_3	Spermine	
species_4	Spermidine	

Product

Table 202: Properties of each product.

Id	Name	SBO
species_3	Spermine	

Kinetic Law

Derived unit contains undeclared units

$$v_{69} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{function\_4\_V\_SPMS\_1}\,(\mathrm{Kaspms}, \mathrm{Kdspms}, \mathrm{Kiaspms}, \mathrm{Kisspms}, \mathrm{Vmspms}, [\mathrm{species\_1}], [\mathrm{species\_3}], [\mathrm{species\_4}]) \quad (342)$$

$$\mathrm{function\_4\_V\_SPMS\_1}\,(\mathrm{Kaspms}, \mathrm{Kdspms}, \mathrm{Kiaspms}, \mathrm{Kisspms}, \mathrm{Vmspms}, [\mathrm{species\_1}], [\mathrm{species\_3}], [\mathrm{species\_4}]) \quad (343)$$
$$= \frac{\mathrm{Vmspms} \cdot [\mathrm{species\_1}] \cdot [\mathrm{species\_4}]}{\mathrm{Kiaspms} \cdot \mathrm{Kdspms} \cdot \left(1 + \frac{[\mathrm{species\_3}]}{\mathrm{Kisspms}}\right) + \mathrm{Kdspms} \cdot [\mathrm{species\_1}] + \mathrm{Kaspms} \cdot \left(1 + \frac{[\mathrm{species\_3}]}{\mathrm{Kisspms}}\right) \cdot [\mathrm{species\_4}] + [\mathrm{species\_}}$$

$$\mathrm{function\_4\_V\_SPMS\_1}\,(\mathrm{Kaspms}, \mathrm{Kdspms}, \mathrm{Kiaspms}, \mathrm{Kisspms}, \mathrm{Vmspms}, [\mathrm{species\_1}], [\mathrm{species\_3}], [\mathrm{species\_4}]) \quad (344)$$
$$= \frac{\mathrm{Vmspms} \cdot [\mathrm{species\_1}] \cdot [\mathrm{species\_4}]}{\mathrm{Kiaspms} \cdot \mathrm{Kdspms} \cdot \left(1 + \frac{[\mathrm{species\_3}]}{\mathrm{Kisspms}}\right) + \mathrm{Kdspms} \cdot [\mathrm{species\_1}] + \mathrm{Kaspms} \cdot \left(1 + \frac{[\mathrm{species\_3}]}{\mathrm{Kisspms}}\right) \cdot [\mathrm{species\_4}] + [\mathrm{species\_}}$$

Table 203: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kaspms	Kaspms		0.10		☑
Kdspms	Kdspms		60.00		☑
Kiaspms	Kiaspms		0.06		☑
Kisspms	Kisspms		25.00		☑
Vmspms	Vmspms		193.80		☑

9.70 Reaction reaction_9

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

Name V_COA

Reaction equation

$$\text{species\_8} \xrightarrow{\text{species\_8}} \text{species\_9} \tag{345}$$

Reactant

Table 204: Properties of each reactant.

Id	Name	SBO
species_8	Acetyl-CoA	

Modifier

Table 205: Properties of each modifier.

Id	Name	SBO
species_8	Acetyl-CoA	

Product

Table 206: Properties of each product.

Id	Name	SBO
species_9	CoA	

Kinetic Law

Derived unit contains undeclared units

$$v_{70} = \text{vol}\,(\text{cytosol}) \cdot \text{parameter\_15} \cdot [\text{species\_8}] \tag{346}$$

9.71 Reaction reaction_10

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

Name V_ACCOA

Reaction equation

$$\text{species\_9} \xrightarrow{\text{species\_9}} \text{species\_8} \tag{347}$$

Reactant

Table 207: Properties of each reactant.

Id	Name	SBO
species_9	CoA	

Modifier

Table 208: Properties of each modifier.

Id	Name	SBO
species_9	CoA	

Product

Table 209: Properties of each product.

Id	Name	SBO
species_8	Acetyl-CoA	

Kinetic Law

Derived unit contains undeclared units

$$v_{71} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{parameter\_14} \cdot [\mathrm{species\_9}] \tag{348}$$

9.72 Reaction reaction_11

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

Name V_PUT_efflux

Reaction equation

$$\mathrm{species\_2} \xrightarrow{\mathrm{species\_2}} \emptyset \tag{349}$$

Reactant

Table 210: Properties of each reactant.

Id	Name	SBO
species_2	Putrescine	

Modifier

Table 211: Properties of each modifier.

Id	Name	SBO
species_2	Putrescine	

Kinetic Law

Derived unit contains undeclared units

$$v_{72} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{k1} \cdot [\mathrm{species\_2}] \tag{350}$$

Table 212: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.6		☑

9.73 Reaction reaction_12

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

Name V_AD_efflux

Reaction equation

$$\mathrm{species\_6} \xrightarrow{\mathrm{species\_6}} \emptyset \tag{351}$$

Reactant

Table 213: Properties of each reactant.

Id	Name	SBO
species_6	Acetylspermidine	

Modifier

Table 214: Properties of each modifier.

Id	Name	SBO
species_6	Acetylspermidine	

Kinetic Law

Derived unit contains undeclared units

$$v_{73} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{k1} \cdot [\mathrm{species\_6}] \tag{352}$$

Table 215: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.6		☑

10 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.

10.1 Species b_met

Name b_Methionine

Initial concentration 7.5 $\mu\text{mol} \cdot \text{l}^{-1}$

Involved in rule b_met

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

10.2 Species b_ser

Name b_Serine

Initial concentration 37.5 $\mu\text{mol} \cdot \text{l}^{-1}$

Involved in rule b_ser

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

10.3 Species b_gly

Name b_Glycine

Initial concentration 218.733171504338 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in seven reactions (as a reactant in b_gly_loss, V_b_GLY_c and as a product in b_gsh_decomp, b_gsg_decomp, b_gly_import and as a modifier in b_gly_loss, V_b_GLY_c).

$$\frac{\text{d}}{\text{d}t}\text{b\_gly} = v_1 + 2\,v_2 + v_{10} - v_6 - v_{18} \tag{353}$$

10.4 Species b_glu

Name b_Glutamate

Initial concentration 60.4651616225031 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in seven reactions (as a reactant in b_glu_loss, V_b_GLU_c and as a product in b_gsh_decomp, b_gsg_decomp, b_glu_import and as a modifier in b_glu_loss, V_b_GLU_c).

$$\frac{\text{d}}{\text{d}t}\text{b\_glu} = v_1 + 2\,v_2 + v_{11} - v_5 - v_{17} \tag{354}$$

10.5 Species b_cys

Name b_Cysteine

Initial concentration 183.099466381356 $\mu mol \cdot l^{-1}$

This species takes part in nine reactions (as a reactant in b_cys_cystine_conv, b_cys_loss, V_b_CYS_c and as a product in b_gsh_decomp, b_gsg_decomp, b_cys_import and as a modifier in b_cys_cystine_conv, b_cys_loss, V_b_CYS_c).

$$\frac{d}{dt}\text{b\_cys} = v_1 + 2\,v_2 + v_9 - v_3 - v_4 - v_{16} \tag{355}$$

10.6 Species b_gsg

Name b_GSSG

Initial concentration 0.472632922783833 $\mu mol \cdot l^{-1}$

This species takes part in six reactions (as a reactant in b_gsg_decomp, b_gsg_loss and as a product in V_c_gsgHb, V_c_gsgLb and as a modifier in b_gsg_decomp, b_gsg_loss).

$$\frac{d}{dt}\text{b\_gsg} = v_{14} + v_{15} - v_2 - v_8 \tag{356}$$

10.7 Species b_gsh

Name b_GSH

Initial concentration 12.5470655822207 $\mu mol \cdot l^{-1}$

This species takes part in six reactions (as a reactant in b_gsh_decomp, b_gsh_loss and as a product in V_c_gshHb, V_c_gshLb and as a modifier in b_gsh_decomp, b_gsh_loss).

$$\frac{d}{dt}\text{b\_gsh} = v_{12} + v_{13} - v_1 - v_7 \tag{357}$$

10.8 Species GAR

Name GAR

Initial concentration 10 $\mu mol \cdot l^{-1}$

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

$$\frac{d}{dt}\text{GAR} = 0 \tag{358}$$

10.9 Species NADPH

Name NADPH

Initial concentration $50\ \mu\text{mol}\cdot\text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADPH} = 0 \tag{359}$$

10.10 Species BET

Name Betaine

Initial concentration $50\ \mu\text{mol}\cdot\text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{BET} = 0 \tag{360}$$

10.11 Species DUMP

Name dUMP

Initial concentration $20\ \mu\text{mol}\cdot\text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DUMP} = 0 \tag{361}$$

10.12 Species H2O2

Name H2O2

Initial concentration $0.01\ \mu\text{mol}\cdot\text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{H2O2} = 0 \tag{362}$$

10.13 Species c_thf

Name c_THF

Initial concentration 4.0250933022918 $\mu\text{mol} \cdot \text{l}^{-1}$

Initial assignment c_thf

This species takes part in eleven reactions (as a reactant in VcFTS, VcSHMT, VcNE and as a product in V_MS, V_DHFR, VcFTD, V_PGT, V_ART and as a modifier in VcFTS, VcSHMT, VcNE).

$$\frac{\text{d}}{\text{d}t}\text{c\_thf} = v_{33} + v_{34} + v_{35} + v_{36} + v_{44} - v_{37} - v_{38} - v_{39} \tag{363}$$

10.14 Species c_5mf

Name c_5-methyl-THF

Initial concentration 5.36079859230553 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in V_MS and as a product in V_MTHFR and as a modifier in V_MS, V_GNMT).

$$\frac{\text{d}}{\text{d}t}\text{c\_5mf} = v_{41} - v_{33} \tag{364}$$

10.15 Species c_2cf

Name c_5-10-methylene-THF

Initial concentration 0.463962655701761 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in ten reactions (as a reactant in V_TS, V_MTHFR, VcMTD and as a product in VcSHMT, VcNE and as a modifier in VcSHMT, VcNE, V_TS, V_MTHFR, VcMTD).

$$\frac{\text{d}}{\text{d}t}\text{c\_2cf} = v_{38} + v_{39} - v_{40} - v_{41} - v_{42} \tag{365}$$

10.16 Species c_1cf

Name c_5-10-methenyl-THF

Initial concentration 0.259497676806752 $\mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{\text{d}}{\text{d}t}\text{c\_1cf} = v_{42} - v_{43} \tag{366}$$

10.17 Species c_10f

Name c_10-formyl-THF

Initial concentration 3.25539505319571 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in nine reactions (as a reactant in VcFTD, V_PGT, V_ART and as a product in VcFTS, VcMTCH and as a modifier in VcFTD, V_PGT, VcMTCH, V_ART).

$$\frac{\text{d}}{\text{d}t}\text{c\_10f} = v_{37} + v_{43} - v_{35} - v_{36} - v_{44} \tag{367}$$

10.18 Species c_dhf

Name c_DHF

Initial concentration 0.0352527196984464 $\mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{\text{d}}{\text{d}t}\text{c\_dhf} = v_{40} - v_{34} \tag{368}$$

10.19 Species aic

Name AICAR

Initial concentration 0.944676738309717 $\mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{\text{d}}{\text{d}t}\text{aic} = v_{36} - v_{44} \tag{369}$$

10.20 Species c_glu

Name c_Glutamate

Initial concentration 3236.78229408139 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in V_GCS, c_glu_usage and as a product in V_b_GLU_c and as a modifier in V_b_GLU_c, V_GCS, c_glu_usage).

$$\frac{\text{d}}{\text{d}t}\text{c\_glu} = v_{17} - v_{54} - v_{56} \tag{370}$$

10.21 Species c_cys

Name c_Cysteine

Initial concentration 179.792196767939 $\mu mol \cdot l^{-1}$

This species takes part in six reactions (as a reactant in V_GCS, cys_usage and as a product in V_b_CYS_c, V_CTGL and as a modifier in V_GCS, cys_usage).

$$\frac{d}{dt}c\_cys = v_{16} + v_{53} - v_{54} - v_{55} \tag{371}$$

10.22 Species glc

Name Glutamyl-Cysteine

Initial concentration 9.60706615144005 $\mu mol \cdot l^{-1}$

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

$$\frac{d}{dt}glc = v_{54} - v_{57} \tag{372}$$

10.23 Species c_gly

Name c_Glycine

Initial concentration 927.560131015361 $\mu mol \cdot l^{-1}$

This species takes part in ten reactions (as a reactant in V_GNMT, V_GS and as a product in V_b_GLY_c, VmGLYc, VcSHMT and as a modifier in V_b_GLY_c, VmGLYc, VcSHMT, V_GNMT, V_GS).

$$\frac{d}{dt}c\_gly = v_{18} + v_{32} + v_{38} - v_{48} - v_{57} \tag{373}$$

10.24 Species c_gsg

Name c_GSSG

Initial concentration 59.8062682413464 $\mu mol \cdot l^{-1}$

This species takes part in eleven reactions (as a reactant in V_c_gsgHb, V_c_gsgLb, V_GR, c_gsg_degr and as a product in V_GPX and as a modifier in V_c_gsgHb, V_c_gsgLb, V_MATI, V_MATIII, V_GR, c_gsg_degr).

$$\frac{d}{dt}c\_gsg = v_{58} - v_{14} - v_{15} - v_{59} - v_{61} \tag{374}$$

10.25 Species c_gsh

Name c_GSH

Initial concentration 6272.51492720171 $\mu mol \cdot l^{-1}$

This species takes part in twelve reactions (as a reactant in V_c_gshHb, V_c_gshLb, V_GPX, c_gsh_degr and as a product in V_GS, V_GR and as a modifier in V_c_gshHb, V_c_gshLb, V_GCS, V_GS, V_GPX, c_gsh_degr).

$$\frac{d}{dt}\text{c\_gsh} = v_{57} + 2\,v_{59} - v_{12} - v_{13} - 2\,v_{58} - v_{60} \tag{375}$$

10.26 Species cyt

Name Cystathionine

Initial concentration 32.3047581589977 $\mu mol \cdot l^{-1}$

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

$$\frac{d}{dt}\text{cyt} = v_{52} - v_{53} \tag{376}$$

10.27 Species hcy

Name Homocysteine

Initial concentration 1.02425194863179 $\mu mol \cdot l^{-1}$

This species takes part in eight reactions (as a reactant in V_MS, V_BHMT, V_CBS and as a product in V_SAHH and as a modifier in V_MS, V_BHMT, V_SAHH, V_CBS).

$$\frac{d}{dt}\text{hcy} = v_{50} - v_{33} - v_{45} - v_{52} \tag{377}$$

10.28 Species c_ser

Name c_Serine

Initial concentration 571.225285800751 $\mu mol \cdot l^{-1}$

This species takes part in ten reactions (as a reactant in VcSHMT, gluconeogenesis_ser, V_CBS and as a product in V_b_SER_c, VmSERc and as a modifier in V_b_SER_c, VmSERc, VcSHMT, gluconeogenesis_ser, V_CBS).

$$\frac{d}{dt}\text{c\_ser} = v_{19} + v_{30} - v_{38} - v_{51} - v_{52} \tag{378}$$

10.29 Species sah

Name SAH

Initial concentration 15.5626693211634 $\mu mol \cdot l^{-1}$

This species takes part in nine reactions (as a reactant in V_SAHH and as a product in V_GNMT, V_DNMT and as a modifier in V_MTHFR, V_BHMT, V_GNMT, V_DNMT, V_SAHH, V_CBS).

$$\frac{d}{dt}\text{sah} = v_{48} + v_{49} - v_{50} \tag{379}$$

10.30 Species sam

Name SAM

Initial concentration 65.0613824844853 $\mu mol \cdot l^{-1}$

This species takes part in 13 reactions (as a reactant in V_GNMT, V_DNMT, reaction_2 and as a product in V_MATI, V_MATIII and as a modifier in V_MTHFR, V_BHMT, V_MATI, V_MATIII, V_GNMT, V_DNMT, V_CBS, reaction_2).

$$\frac{d}{dt}\text{sam} = v_{46} + v_{47} - v_{48} - v_{49} - v_{63} \tag{380}$$

10.31 Species met

Name c_Methionine

Initial concentration 50.6006924474774 $\mu mol \cdot l^{-1}$

This species takes part in eight reactions (as a reactant in V_MATI, V_MATIII and as a product in V_b_MET_c, V_MS, V_BHMT and as a modifier in V_b_MET_c, V_MATI, V_MATIII).

$$\frac{d}{dt}\text{met} = v_{20} + v_{33} + v_{45} - v_{46} - v_{47} \tag{381}$$

10.32 Species c_coo

Name c_Formate

Initial concentration 13.9758110645557 $\mu mol \cdot l^{-1}$

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

$$\frac{d}{dt}\text{c\_coo} = v_{31} - v_{37} \tag{382}$$

10.33 Species species_1

Name dcSAM

Initial concentration $0.011178638638793\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in six reactions (as a reactant in reaction_7, reaction_8 and as a product in reaction_2 and as a modifier in reaction_2, reaction_7, reaction_8).

$$\frac{\text{d}}{\text{d}t}\text{species\_1} = v_{63} - v_{68} - v_{69} \tag{383}$$

10.34 Species species_2

Name Putrescine

Initial concentration $98.2036296721139\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in eight reactions (as a reactant in reaction_7, reaction_11 and as a product in reaction_1, reaction_5 and as a modifier in reaction_1, reaction_2, reaction_7, reaction_11).

$$\frac{\text{d}}{\text{d}t}\text{species\_2} = v_{62} + v_{66} - v_{68} - v_{72} \tag{384}$$

10.35 Species species_3

Name Spermine

Initial concentration $61.3595114874529\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in eight reactions (as a reactant in reaction_3 and as a product in reaction_8 and as a modifier in reaction_2, reaction_3, reaction_4, reaction_5, reaction_6, reaction_8).

$$\frac{\text{d}}{\text{d}t}\text{species\_3} = v_{69} - v_{64} \tag{385}$$

10.36 Species species_4

Name Spermidine

Initial concentration $79.5917525310194\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in ten reactions (as a reactant in reaction_4, reaction_8 and as a product in reaction_6, reaction_7 and as a modifier in reaction_3, reaction_4, reaction_5, reaction_6, reaction_7, reaction_8).

$$\frac{\text{d}}{\text{d}t}\text{species\_4} = v_{67} + v_{68} - v_{65} - v_{69} \tag{386}$$

10.37 Species species_5

Name Acetylspermine

Initial concentration $0.0272742537826481\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in four reactions (as a reactant in reaction_6 and as a product in reaction_3 and as a modifier in reaction_5, reaction_6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_5} = v_{64} - v_{67} \tag{387}$$

10.38 Species species_6

Name Acetylspermidine

Initial concentration $0.903751442137693\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in six reactions (as a reactant in reaction_5, reaction_12 and as a product in reaction_4 and as a modifier in reaction_5, reaction_6, reaction_12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_6} = v_{65} - v_{66} - v_{73} \tag{388}$$

10.39 Species species_7

Name Ornithine

Initial concentration $300\ \mu\text{mol}\cdot\text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_7} = 0 \tag{389}$$

10.40 Species species_8

Name Acetyl-CoA

Initial concentration $38.833390762794\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in seven reactions (as a reactant in reaction_3, reaction_4, reaction_9 and as a product in reaction_10 and as a modifier in reaction_3, reaction_4, reaction_9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_8} = v_{71} - v_{64} - v_{65} - v_{70} \tag{390}$$

10.41 Species species_9

Name CoA

Initial concentration 160.666609237206 $\mu mol \cdot l^{-1}$

This species takes part in seven reactions (as a reactant in reaction_10 and as a product in reaction_3, reaction_4, reaction_9 and as a modifier in reaction_3, reaction_4, reaction_10).

$$\frac{d}{dt}\text{species\_9} = v_{64} + v_{65} + v_{70} - v_{71} \tag{391}$$

10.42 Species CO

Name CO2

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

This species takes part in one reaction (as a product in V_GDC), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{CO} = 0 \tag{392}$$

10.43 Species m_thf

Name m_THF

Initial concentration 20.989363966111 $\mu mol \cdot l^{-1}$

Initial assignment m_thf

This species takes part in 13 reactions (as a reactant in VmSHMT, VmFTS, VmNE, V_GDC, V_SDH, V_DMGD and as a product in VmFTD and as a modifier in VmSHMT, VmFTS, VmNE, V_GDC, V_SDH, V_DMGD).

$$\frac{d}{dt}\text{m\_thf} = v_{21} - v_{22} - v_{23} - v_{24} - v_{25} - v_{26} - v_{27} \tag{393}$$

10.44 Species m_2cf

Name m_5-10-methylene-THF

Initial concentration 1.66729681864136 $\mu mol \cdot l^{-1}$

This species takes part in nine reactions (as a reactant in VmMTD and as a product in VmSHMT, VmNE, V_GDC, V_SDH, V_DMGD and as a modifier in VmSHMT, VmNE, VmMTD).

$$\frac{d}{dt}\text{m\_2cf} = v_{22} + v_{24} + v_{25} + v_{26} + v_{27} - v_{28} \tag{394}$$

10.45 Species m_1cf

Name m_5-10-methenyl-THF

Initial concentration 1.55022131198345 $\mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{\text{d}}{\text{d}t}\text{m\_1cf} = v_{28} - v_{29} \tag{395}$$

10.46 Species m_10f

Name m_10-formyl-THF

Initial concentration 15.9931179032642 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in VmFTD and as a product in VmFTS, VmMTCH and as a modifier in VmFTD, VmFTS, VmMTCH).

$$\frac{\text{d}}{\text{d}t}\text{m\_10f} = v_{23} + v_{29} - v_{21} \tag{396}$$

10.47 Species m_ser

Name m_Serine

Initial concentration 2150.05782513217 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in VmSHMT, VmSERc and as a modifier in VmSHMT, VmSERc).

$$\frac{\text{d}}{\text{d}t}\text{m\_ser} = -v_{22} - 3\,v_{30} \tag{397}$$

10.48 Species m_gly

Name m_Glycine

Initial concentration 2043.470284255 $\mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in seven reactions (as a reactant in V_GDC, VmGLYc and as a product in VmSHMT, V_SDH and as a modifier in VmSHMT, V_GDC, VmGLYc).

$$\frac{\text{d}}{\text{d}t}\text{m\_gly} = v_{22} + v_{26} - v_{25} - 3\,v_{32} \tag{398}$$

10.49 Species m_coo

Name m_Formate

Initial concentration 58.3710073680041 $\mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in four reactions (as a reactant in VmFTS, VmHCOOHc and as a modifier in VmFTS, VmHCOOHc).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{m\_coo} = -v_{23} - 3\,v_{31} \tag{399}$$

10.50 Species Fol

Name Folate

Initial concentration 20.1 $\mu\text{mol}\cdot\text{l}^{-1}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Fol} = 0 \tag{400}$$

10.51 Species HCHO

Name Formaldehyde

Initial concentration 500 $\mu\text{mol}\cdot\text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{HCHO} = 0 \tag{401}$$

10.52 Species src

Name Sarcosine

Initial concentration 8.25411023033989 $\mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in four reactions (as a reactant in V_SDH and as a product in V_DMGD, V_GNMT and as a modifier in V_SDH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{src} = v_{27} + v_{48} - v_{26} \tag{402}$$

10.53 Species dmg

Name Dimethylglycine

Initial concentration $0.677559463168903\ \mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{\text{d}}{\text{d}t}\text{dmg} = v_{45} - v_{27} \tag{403}$$

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