SBML Model Report

Model name: "Curien2009_Aspartate_Metabolism"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Lukas Endler[1] and Gilles Curien[2] at May 28th 2009 at 12:57 a. m. and last time modified at December thirteenth 2010 at 9:51 a. m. Table 1 gives an overview of the quantities of all components of this model.

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

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	31
events	0	constraints	0
reactions	18	function definitions	0
global parameters	4	unit definitions	8
rules	3	initial assignments	0

Model Notes

This a model described in the article:
Understanding the regulation of aspartate metabolism using a model based on measured kinetic parameters.
Curien G, Bastien O, Robert-Genthon M, Cornish-Bowden A, Crdenas ML, Dumas R. Mol Syst

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Biol. 2009;5:271. Epub 2009 May 19. PMID: 19455135 , doi: 10.1038/msb.2009.29
Abstract:
The aspartate-derived amino-acid pathway from plants is well suited for analysing the function of the allosteric network of interactions in branched pathways. For this purpose, a detailed kinetic model of the system in the plant model Arabidopsis was constructed on the basis of in vitro kinetic measurements. The data, assembled into a mathematical model, reproduce in vivo measurements and also provide non-intuitive predictions. A crucial result is the identification of allosteric interactions whose function is not to couple demand and supply but to maintain a high independence between fluxes in competing pathways. In addition, the model shows that enzyme isoforms are not functionally redundant, because they contribute unequally to the flux and its regulation. Another result is the identification of the threonine concentration as the most sensitive variable in the system, suggesting a regulatory role for threonine at a higher level of integration.

The limiting rates for the tRNA synthetase reactions, V_Lys_RS, V_Thr_RS and V_Ile_RS, are all assigned a joined value, Vmax_AA_RS, to facilitate reproduction of the results in the publication. To alter these rates seperately these assignments have to be changed or removed.

2 Unit Definitions

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

2.1 Unit `substance`

Name micromole

Definition μmol

2.2 Unit `per_time`

Definition s^{-1}

2.3 Unit `per_litre`

Definition l^{-1}

2.4 Unit umole_per_litre

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

2.5 Unit umole_per_litre_per_time

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

2.6 Unit umole2_per_litre2

Definition $\mu\mathrm{mol}^2 \cdot \mathrm{l}^{-2}$

2.7 Unit litre_per_umole_per_time

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

2.8 Unit umole_per_time

Definition $\mu\mathrm{mol} \cdot \mathrm{s}^{-1}$

2.9 Unit volume

Notes Litre is the predefined SBML unit for `volume`.

Definition l

2.10 Unit area

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

Definition m^2

2.11 Unit length

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

Definition m

2.12 Unit time

Notes Second is the predefined SBML unit for `time`.

Definition s

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
c1	chl		3	1	litre	☑	

3.1 Compartment c1

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

Name chl

4 Species

This model contains 31 species. The boundary condition of 23 of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 8 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
Asp	Aspartate	c1	$\mu mol \cdot l^{-1}$	⊟	☑
AK1	AK1	c1	$\mu mol \cdot l^{-1}$	⊟	☑
Lys	Lysine	c1	$\mu mol \cdot l^{-1}$	⊟	⊟
AdoMet	S-adenosyl-methionine	c1	$\mu mol \cdot l^{-1}$	⊟	☑
AspP	Aspartyl_P	c1	$\mu mol \cdot l^{-1}$	⊟	⊟
AK2	AK2	c1	$\mu mol \cdot l^{-1}$	⊟	☑
AKHSDHI	AKI-HSDHI	c1	$\mu mol \cdot l^{-1}$	⊟	☑
AKHSDHII	AKII-HSDHII	c1	$\mu mol \cdot l^{-1}$	⊟	☑
Thr	Threonine	c1	$\mu mol \cdot l^{-1}$	⊟	⊟
ASADH	ASADH	c1	$\mu mol \cdot l^{-1}$	⊟	☑
ASA	Aspartate semialdehyde	c1	$\mu mol \cdot l^{-1}$	⊟	⊟
DHDPS1	DHDPS1	c1	$\mu mol \cdot l^{-1}$	⊟	☑
DHDPS2	DHDPS2	c1	$\mu mol \cdot l^{-1}$	⊟	☑
Hser	Homoserine	c1	$\mu mol \cdot l^{-1}$	⊟	⊟
PHser	Phosphohomoserine	c1	$\mu mol \cdot l^{-1}$	⊟	⊟
HSK	HSK	c1	$\mu mol \cdot l^{-1}$	⊟	☑
TS1	TS1	c1	$\mu mol \cdot l^{-1}$	⊟	⊟
Phosphate		c1	$\mu mol \cdot l^{-1}$	⊟	☑
Cys	Cysteine	c1	$\mu mol \cdot l^{-1}$	⊟	☑
CGS	CGS	c1	$\mu mol \cdot l^{-1}$	⊟	☑
Cysta	Cystathione	c1	$\mu mol \cdot l^{-1}$	⊟	☑

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
TD	TD	c1	$\mu mol \cdot l^{-1}$	⊟	☑
Ile	Isoleucine	c1	$\mu mol \cdot l^{-1}$	⊟	⊟
Val	Valine	c1	$\mu mol \cdot l^{-1}$	⊟	☑
LysTRNA	Lys-tRNA	c1	$\mu mol \cdot l^{-1}$	⊟	☑
ThrTRNA	Thr-tRNA	c1	$\mu mol \cdot l^{-1}$	⊟	☑
IleTRNA	Ile-tRNA	c1	$\mu mol \cdot l^{-1}$	⊟	☑
LKR	LKR	c1	$\mu mol \cdot l^{-1}$	⊟	☑
Sacc	Saccharopine	c1	$\mu mol \cdot l^{-1}$	⊟	☑
THA	THA	c1	$\mu mol \cdot l^{-1}$	⊟	☑
Gly	Glycine	c1	$\mu mol \cdot l^{-1}$	⊟	☑

5 Parameters

This model contains four global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_Lys_RS			0.43	$\mu mol \cdot l^{-1} \cdot s^{-1}$	⊟
V_Thr_RS			0.43	$\mu mol \cdot l^{-1} \cdot s^{-1}$	⊟
V_Ile_RS			0.43	$\mu mol \cdot l^{-1} \cdot s^{-1}$	⊟
V_AA_RS	Vmax_AA_RS		0.43	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☑

6 Rules

This is an overview of three rules.

6.1 Rule V_Lys_RS

Rule V_Lys_RS is an assignment rule for parameter V_Lys_RS:

$$V\_Lys\_RS = V\_AA\_RS \tag{1}$$

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

6.2 Rule V_Thr_RS

Rule V_Thr_RS is an assignment rule for parameter V_Thr_RS:

$$V\_Thr\_RS = V\_AA\_RS \tag{2}$$

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

6.3 Rule V_Ile_RS

Rule V_Ile_RS is an assignment rule for parameter V_Ile_RS:

$$V\_Ile\_RS = V\_AA\_RS \tag{3}$$

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

7 Reactions

This model contains 18 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	Vak1	Aspartate kinase 1 react.	$\text{Asp} \overset{\text{AK1, Lys, AdoMet}}{\rightleftharpoons} \text{AspP}$	0000402
2	Vak2	Aspartate kinase 2 react.	$\text{Asp} \overset{\text{AK2, Lys}}{\rightleftharpoons} \text{AspP}$	0000402
3	VakI	aspartate kinase react. (AKI-HSDHI)	$\text{Asp} \overset{\text{AKHSDHI, Thr}}{\rightleftharpoons} \text{AspP}$	0000402
4	VakII	aspartate kinase react. (AKII-HSDHII)	$\text{Asp} \overset{\text{AKHSDHII, Thr}}{\rightleftharpoons} \text{AspP}$	0000402
5	Vasadh	Aspartate semialdehyde dehydrogenase react.	$\text{AspP} \overset{\text{ASADH}}{\rightleftharpoons} \text{ASA}$	0000200
6	Vdhdps1	DHDPS1 react.	$\text{ASA} \overset{\text{DHDPS1, Lys}}{\longrightarrow} \text{Lys}$	0000205
7	Vdhdps2	DHDPS2 react.	$\text{ASA} \overset{\text{DHDPS2, Lys}}{\longrightarrow} \text{Lys}$	0000205
8	Vhsdh1	homoserine dehydrogenase react. (AKI-HSDHI)	$\text{ASA} \overset{\text{AKHSDHI, Thr}}{\rightleftharpoons} \text{Hser}$	0000200
9	Vhsdh2	homoserine dehydrogenase react. (AKII-HSDHII)	$\text{ASA} \overset{\text{AKHSDHII, Thr}}{\rightleftharpoons} \text{Hser}$	0000200
10	Vhsk	homoserine kinase react.	$\text{Hser} \overset{\text{HSK}}{\longrightarrow} \text{PHser}$	0000402
11	Vts1	Threonine synthase react. (TS1)	$\text{PHser} \overset{\text{TS1, Phosphate, AdoMet}}{\longrightarrow} \text{Thr}$	0000376
12	Vcgs	Cystathionine gamma synthase react.	$\text{PHser} \overset{\text{CGS, Cys, Phosphate}}{\longrightarrow} \text{Cysta}$	0000402
13	Vtd	Threonine deaminase react.	$\text{Thr} \overset{\text{TD, Val, Ile}}{\longrightarrow} \text{Ile}$	0000205
14	VlysTRNA	Lys aminoacyl tRNA synthetase react.	$\text{Lys} \longrightarrow \text{LysTRNA}$	0000176

№	Id	Name	Reaction Equation	SBO
15	VthrTRNA	Thr aminoacyl tRNA synthetase react.	Thr $\longrightarrow$ ThrTRNA	0000176
16	VileTRNA	Ile aminoacyl tRNA synthetase react.	Ile $\longrightarrow$ IleTRNA	0000176
17	VlysKR	Lys ketoglutarate reductase react.	Lys $\xrightarrow{\text{LKR}}$ Sacc	0000176
18	Vtha	Thr aldolase react.	Thr $\xrightarrow{\text{THA}}$ Gly	0000178

7.1 Reaction `Vak1`

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

Name Aspartate kinase 1 react.

SBO:0000402 transfer of a chemical group

Reaction equation

$$\mathrm{Asp} \xrightleftharpoons{\mathrm{AK1,\ Lys,\ AdoMet}} \mathrm{AspP} \tag{4}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
`Asp`	Aspartate	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
`AK1`	AK1	
`Lys`	Lysine	
`AdoMet`	S-adenosyl-methionine	

Product

Table 8: Properties of each product.

Id	Name	SBO
`AspP`	Aspartyl_P	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}(\mathrm{c1}) \cdot [\mathrm{AK1}] \cdot \frac{\mathrm{AK1\_kforward\_app\_exp} - \mathrm{AK1\_kreverse\_app\_exp} \cdot [\mathrm{AspP}]}{1 + \left(\frac{[\mathrm{Lys}]}{\mathrm{AK1\_Lys\_Ki\_app\_exp}} \Big/ \left(1 + \frac{[\mathrm{AdoMet}]}{\mathrm{AK1\_AdoMet\_Ka\_app\_exp}}\right) \right)^{\mathrm{AK1\_nH\_exp}}} \tag{5}$$

Table 9: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
AK1_kforward_app_exp		0000320	5.65	s^{-1}	☑
AK1_kreverse_app_exp		0000321	1.60	$l \cdot \mu mol^{-1} \cdot s^{-1}$	☑
AK1_Lys_Ki_app_exp		0000288	550.00	$\mu mol \cdot l^{-1}$	☑
AK1_AdoMet_Ka_app_exp		0000363	3.50	$\mu mol \cdot l^{-1}$	☑
AK1_nH_exp		0000190	2.00	dimensionless	☑

7.2 Reaction Vak2

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

Name Aspartate kinase 2 react.

SBO:0000402 transfer of a chemical group

Reaction equation

$$\mathrm{Asp} \overset{\mathrm{AK2,\ Lys}}{\rightleftharpoons} \mathrm{AspP} \tag{6}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
Asp	Aspartate	

Modifiers

Table 11: Properties of each modifier.

Id	Name	SBO
AK2	AK2	
Lys	Lysine	

Product

Table 12: Properties of each product.

Id	Name	SBO
AspP	Aspartyl_P	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}(\mathrm{c1}) \cdot [\mathrm{AK2}] \cdot \frac{\mathrm{AK2\_kforward\_app\_exp} - \mathrm{AK2\_kreverse\_app\_exp} \cdot [\mathrm{AspP}]}{1 + \left(\frac{[\mathrm{Lys}]}{\mathrm{AK2\_Lys\_Ki\_app\_exp}}\right)^{\mathrm{AK2\_nH\_exp}}} \tag{7}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
AK2_kforward_app_exp		0000320	3.15	s^{-1}	☑
AK2_kreverse_app_exp		0000321	0.86	$l \cdot \mu mol^{-1} \cdot s^{-1}$	☑
AK2_Lys_Ki_app_exp		0000363	22.00	$\mu mol \cdot l^{-1}$	☑
AK2_nH_exp		0000190	1.10	dimensionless	☑

7.3 Reaction VakI

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

Name aspartate kinase react. (AKI-HSDHI)

SBO:0000402 transfer of a chemical group

Reaction equation

$$\mathrm{Asp} \xrightleftharpoons{\mathrm{AKHSDHI,\ Thr}} \mathrm{AspP} \tag{8}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
Asp	Aspartate	

Modifiers

Table 15: Properties of each modifier.

Id	Name	SBO
AKHSDHI	AKI-HSDHI	
Thr	Threonine	

Product

Table 16: Properties of each product.

Id	Name	SBO
AspP	Aspartyl_P	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{c1}) \cdot [\mathrm{AKHSDHI}] \cdot \frac{\mathrm{AKI\_kforward\_app\_exp} - \mathrm{AKI\_kreverse\_app\_exp} \cdot [\mathrm{AspP}]}{1 + \left(\frac{[\mathrm{Thr}]}{\mathrm{AKI\_Thr\_Ki\_app\_exp}}\right)^{\mathrm{AKI\_nH\_exp}}} \quad (9)$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
AKI_kforward_app_exp		0000320	0.36	s^{-1}	☑
AKI_kreverse_app_exp		0000321	0.15	$l \cdot \mu mol^{-1} \cdot s^{-1}$	☑
AKI_Thr_Ki_app_exp		0000363	124.00	$\mu mol \cdot l^{-1}$	☑
AKI_nH_exp		0000190	2.00	dimensionless	☑

7.4 Reaction VakII

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

Name aspartate kinase react. (AKII-HSDHII)

SBO:0000402 transfer of a chemical group

Reaction equation

$$\mathrm{Asp} \xrightleftharpoons{\text{AKHSDHII, Thr}} \mathrm{AspP} \tag{10}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
Asp	Aspartate	

Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
AKHSDHII	AKII-HSDHII	
Thr	Threonine	

Product

Table 20: Properties of each product.

Id	Name	SBO
AspP	Aspartyl_P	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}(\mathrm{c1}) \cdot [\mathrm{AKHSDHII}] \cdot \frac{\mathrm{AKII\_kforward\_app\_exp} - \mathrm{AKII\_kreverse\_app\_exp} \cdot [\mathrm{AspP}]}{1 + \left(\frac{[\mathrm{Thr}]}{\mathrm{AKII\_Thr\_Ki\_app\_exp}}\right)^{\mathrm{AKII\_nH\_exp}}} \tag{11}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
AKII_kforward_app_exp		0000320	1.35	s^{-1}	☑
AKII_kreverse_app_exp		0000321	0.22	$1 \cdot \mu mol^{-1} \cdot s^{-1}$	☑
AKII_Thr_Ki_app_exp		0000363	109.00	$\mu mol \cdot l^{-1}$	☑
AKII_nH_exp		0000190	2.00	dimensionless	☑

7.5 Reaction Vasadh

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

Name Aspartate semialdehyde dehydrogenase react.

SBO:0000200 redox reaction

Reaction equation

$$\text{AspP} \overset{\text{ASADH}}{\rightleftharpoons} \text{ASA} \tag{12}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
AspP	Aspartyl_P	

Modifier

Table 23: Properties of each modifier.

Id	Name	SBO
ASADH	ASADH	

Product

Table 24: Properties of each product.

Id	Name	SBO
ASA	Aspartate semialdehyde	

Kinetic Law

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

$$v_5 = \text{vol}(\text{c1}) \cdot [\text{ASADH}] \cdot (\text{ASADH\_kforward\_app\_exp} \cdot [\text{AspP}] - \text{ASADH\_kreverse\_app\_exp} \cdot [\text{ASA}]) \quad (13)$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ASADH_kforward_app_exp		0000320	0.90	$1 \cdot \mu\text{mol}^{-1} \cdot \text{s}^{-1}$	☑
ASADH_kreverse_app_exp		0000321	0.23	$1 \cdot \mu\text{mol}^{-1} \cdot \text{s}^{-1}$	☑

7.6 Reaction Vdhdps1

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

Name DHDPS1 react.

SBO:0000205 composite biochemical process

Reaction equation

$$\text{ASA} \xrightarrow{\text{DHDPS1, Lys}} \text{Lys} \quad (14)$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
ASA	Aspartate semialdehyde	

Modifiers

Table 27: Properties of each modifier.

Id	Name	SBO
DHDPS1	DHDPS1	
Lys	Lysine	

Product

Table 28: Properties of each product.

Id	Name	SBO
Lys	Lysine	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}(\mathrm{c1}) \cdot \mathrm{DHDPS1\_k\_app\_exp} \cdot [\mathrm{DHDPS1}] \cdot [\mathrm{ASA}] \cdot \frac{1}{1 + \left(\frac{[\mathrm{Lys}]}{\mathrm{DHDPS1\_Lys\_Ki\_app\_exp}}\right)^{\mathrm{DHDPS1\_nH\_exp}}} \tag{15}$$

Table 29: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
DHDPS1_k-_app_exp		0000320	1.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
DHDPS1_Lys-_Ki_app_exp		0000363	10.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
DHDPS1_nH-_exp		0000190	2.0	dimensionless	☑

7.7 Reaction Vdhdps2

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

Name DHDPS2 react.

SBO:0000205 composite biochemical process

Reaction equation

$$\mathrm{ASA} \xrightarrow{\text{DHDPS2, Lys}} \mathrm{Lys} \tag{16}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
ASA	Aspartate semialdehyde	

Modifiers

Table 31: Properties of each modifier.

Id	Name	SBO
DHDPS2	DHDPS2	
Lys	Lysine	

Product

Table 32: Properties of each product.

Id	Name	SBO
Lys	Lysine	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}(\mathrm{c1}) \cdot \mathrm{DHDPS2\_k\_app\_exp} \cdot [\mathrm{DHDPS2}] \cdot [\mathrm{ASA}] \cdot \frac{1}{1 + \left(\frac{[\mathrm{Lys}]}{\mathrm{DHDPS2\_Lys\_Ki\_app\_exp}}\right)^{\mathrm{DHDPS2\_nH\_exp}}} \tag{17}$$

Table 33: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
DHDPS2_k_app_exp		0000320	1.0	$\mu\mathrm{mol} \cdot 1^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
DHDPS2_Lys-_Ki_app_exp		0000363	33.0	$\mu mol \cdot l^{-1}$	☑
DHDPS2_nH-_exp		0000190	2.0	dimensionless	☑

7.8 Reaction Vhsdh1

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

Name homoserine dehydrogenase react. (AKI-HSDHI)

SBO:0000200 redox reaction

Reaction equation

$$\mathrm{ASA} \overset{\text{AKHSDHI, Thr}}{\rightleftharpoons} \mathrm{Hser} \tag{18}$$

Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
ASA	Aspartate semialdehyde	

Modifiers

Table 35: Properties of each modifier.

Id	Name	SBO
AKHSDHI	AKI-HSDHI	
Thr	Threonine	

Product

Table 36: Properties of each product.

Id	Name	SBO
Hser	Homoserine	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}(\mathrm{c1}) \cdot \mathrm{HSDHI\_kforward\_app\_exp} \cdot [\mathrm{AKHSDHI}] \cdot [\mathrm{ASA}] \cdot \left(\mathrm{HSDHI\_Thr\_relative\_residual\_activity\_app\_exp} + \frac{\mathrm{HSDHI\_Thr\_relative\_inhibition\_app\_exp}}{1 + \frac{[\mathrm{Thr}]}{\mathrm{HSDHI\_Thr\_Ki\_app\_exp}}} \right) \tag{19}$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
HSDHI_kforward_app_exp			0.84	$1 \cdot \mu\mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑
HSDHI_Thr_relative_residual_activity_app_exp			0.14	dimensionless	☑
HSDHI_Thr_relative_inhibition_app_exp			0.86	dimensionless	☑
HSDHI_Thr_Ki_app_exp			400.00	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑

7.9 Reaction Vhsdh2

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

Name homoserine dehydrogenase react. (AKII-HSDHII)

SBO:0000200 redox reaction

Reaction equation

$$\mathrm{ASA} \underset{\longleftarrow}{\overset{\mathrm{AKHSDHII,\ Thr}}{\longrightarrow}} \mathrm{Hser} \tag{20}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
ASA	Aspartate semialdehyde	

Modifiers

Table 39: Properties of each modifier.

Id	Name	SBO
AKHSDHII	AKII-HSDHII	
Thr	Threonine	

Product

Table 40: Properties of each product.

Id	Name	SBO
Hser	Homoserine	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{c1}) \cdot \mathrm{HSDHII\_kforward\_app\_exp} \cdot [\mathrm{AKHSDHII}] \cdot [\mathrm{ASA}] \cdot \left(\mathrm{HSDHII\_Thr\_relative\_residual\_activity\_app\_exp} + \frac{\mathrm{HSDHII\_Thr\_relative\_inhibition\_app\_exp}}{1 + \frac{[\mathrm{Thr}]}{\mathrm{HSDHII\_Thr\_Ki\_app\_exp}}} \right) \tag{21}$$

Table 41: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
HSDHII-_kforward-_app_exp			0.64	$1 \cdot \mu\mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
HSDHII_Thr-_relative-_residual-_activity-_app_exp			0.25	dimensionless	☑
HSDHII_Thr-_relative-_inhibition-_app_exp			0.75	dimensionless	☑
HSDHII_Thr-_Ki_app_exp			8500.00	$\mu mol \cdot l^{-1}$	☑

7.10 Reaction Vhsk

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

Name homoserine kinase react.

SBO:0000402 transfer of a chemical group

Reaction equation

$$\text{Hser} \xrightarrow{\text{HSK}} \text{PHser} \tag{22}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
Hser	Homoserine	

Modifier

Table 43: Properties of each modifier.

Id	Name	SBO
HSK	HSK	

Product

Table 44: Properties of each product.

Id	Name	SBO
PHser	Phosphohomoserine	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-6}$ mol

$$v_{10} = \frac{\text{vol}(c1) \cdot \text{HSK\_kcat\_app\_exp} \cdot [\text{HSK}] \cdot [\text{Hser}]}{\text{HSK\_Hser\_app\_exp} + [\text{Hser}]} \tag{23}$$

Table 45: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
HSK_kcat_app_exp			2.8	s^{-1}	☑
HSK_Hser_app_exp			14.0	$\mu mol \cdot l^{-1}$	☑

7.11 Reaction Vts1

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

Name Threonine synthase react. (TS1)

SBO:0000376 hydrolysis

Reaction equation

$$\text{PHser} \xrightarrow{\text{TS1, Phosphate, AdoMet}} \text{Thr} \tag{24}$$

Reactant

Table 46: Properties of each reactant.

Id	Name	SBO
PHser	Phosphohomoserine	

Modifiers

Table 47: Properties of each modifier.

Id	Name	SBO
TS1	TS1	
Phosphate		
AdoMet	S-adenosyl-methionine	

Product

Table 48: Properties of each product.

Id	Name	SBO
Thr	Threonine	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}(\mathrm{c1}) \cdot [\mathrm{TS1}] \cdot [\mathrm{PHser}] \cdot \frac{\frac{\mathrm{TS1\_kcatmin\_exp} + \mathrm{TS1\_AdoMet\_kcatmax\_exp} \cdot \frac{[\mathrm{AdoMet}]^{\mathrm{TS1\_nH\_exp}}}{\mathrm{TS1\_AdoMet\_Ka1\_exp}}}{1 + \frac{[\mathrm{AdoMet}]^{\mathrm{TS1\_nH\_exp}}}{\mathrm{TS1\_AdoMet\_Ka1\_exp}}}}{\mathrm{TS1\_AdoMEt\_Km\_no\_AdoMet\_exp} \cdot \frac{1 + \frac{[\mathrm{AdoMet}]}{\mathrm{TS1\_AdoMet\_Ka2\_exp}}}{1 + \frac{[\mathrm{AdoMet}]}{\mathrm{TS1\_AdoMet\_Ka3\_exp}} \cdot \frac{[\mathrm{AdoMet}]^{\mathrm{TS1\_nH\_exp}}}{\mathrm{TS1\_AdoMet\_Ka4\_exp}}} \cdot \left(1 + \frac{[\mathrm{Phosphate}]}{\mathrm{TS1\_Phosphate\_Ki\_exp}}\right) + [\mathrm{PHser}]} \tag{25}$$

Table 49: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
TS1_kcatmin_exp			0.42	dimensionless	☑
TS1_AdoMet_kcatmax_exp			3.50	dimensionless	☑
TS1_AdoMet_Ka1_exp			73.00	$\mu\mathrm{mol}^2 \cdot \mathrm{l}^{-2}$	☑
TS1_nH_exp			2.00	dimensionless	☑
TS1_Phosphate_Ki_exp			1000.00	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
TS1_AdoMEt_Km_no_AdoMet_exp			250.00	dimensionless	☑

Id	Name	SBO	Value	Unit	Constant
TS1_AdoMet-_Ka2_exp			0.50	dimensionless	☑
TS1_AdoMet-_Ka3_exp			1.09	dimensionless	☑
TS1_AdoMet-_Ka4_exp			140.00	$\mu mol^2 \cdot l^{-2}$	☑

7.12 Reaction Vcgs

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

Name Cystathionine gamma synthase react.

SBO:0000402 transfer of a chemical group

Reaction equation

$$\text{PHser} \xrightarrow{\text{CGS, Cys, Phosphate}} \text{Cysta} \tag{26}$$

Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
PHser	Phosphohomoserine	

Modifiers

Table 51: Properties of each modifier.

Id	Name	SBO
CGS	CGS	
Cys	Cysteine	
Phosphate		

Product

Table 52: Properties of each product.

Id	Name	SBO
Cysta	Cystathione	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\,(\mathrm{c1}) \cdot [\mathrm{CGS}] \cdot [\mathrm{PHser}] \cdot \frac{\frac{\mathrm{CGS\_kcat\_exp}}{1+\frac{\mathrm{CGS\_Cys\_Km\_exp}}{[\mathrm{Cys}]}}}{\frac{\mathrm{CGS\_Phser\_Km\_exp}}{1+\frac{\mathrm{CGS\_Cys\_Km\_exp}}{[\mathrm{Cys}]}} \cdot \left(1 + \frac{[\mathrm{Phosphate}]}{\mathrm{CGS\_Phosphate\_Ki\_exp}}\right) + [\mathrm{PHser}]} \tag{27}$$

Table 53: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
CGS_kcat_exp			30.0	dimensionless	☑
CGS_Cys_Km_exp			460.0	dimensionless	☑
CGS_Phser_Km_exp			2500.0	dimensionless	☑
CGS_Phosphate_Ki_exp			2000.0	dimensionless	☑

7.13 Reaction Vtd

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

Name Threonine deaminase react.

SBO:0000205 composite biochemical process

Reaction equation

$$\mathrm{Thr} \xrightarrow{\mathrm{TD,\ Val,\ Ile}} \mathrm{Ile} \tag{28}$$

Reactant

Table 54: Properties of each reactant.

Id	Name	SBO
Thr	Threonine	

Modifiers

Table 55: Properties of each modifier.

Id	Name	SBO
TD	TD	
Val	Valine	
Ile	Isoleucine	

Product

Table 56: Properties of each product.

Id	Name	SBO
Ile	Isoleucine	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}(\mathrm{c1}) \cdot [\mathrm{TD}] \cdot [\mathrm{Thr}] \cdot \frac{\mathrm{TD\_k\_app\_exp}}{1 + \left(\frac{[\mathrm{Ile}]}{\mathrm{TD\_Ile\_Ki\_no\_Val\_app\_exp} + \frac{\mathrm{TD\_Val\_Ka1\_app\_exp} \cdot [\mathrm{Val}]}{\mathrm{TD\_Val\_Ka2\_app\_exp} + [\mathrm{Val}]}} \right)^{\mathrm{TD\_nH\_app\_exp}}} \quad (29)$$

Table 57: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
TD_k_app_exp			0.012	dimensionless	☑
TD_Ile_Ki_no-_Val_app_exp			30.000	dimensionless	☑
TD_Val_Ka1-_app_exp			73.000	dimensionless	☑
TD_Val_Ka2-_app_exp			615.000	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
TD_nH_app_exp			3.000	dimensionless	☑

7.14 Reaction VlysTRNA

This is an irreversible reaction of one reactant forming one product.

Name Lys aminoacyl tRNA synthetase react.

SBO:0000176 biochemical reaction

Reaction equation

$$\text{Lys} \longrightarrow \text{LysTRNA} \tag{30}$$

Reactant

Table 58: Properties of each reactant.

Id	Name	SBO
Lys	Lysine	

Product

Table 59: Properties of each product.

Id	Name	SBO
LysTRNA	Lys-tRNA	

Kinetic Law

Derived unit $10^{-6}\ \text{mol} \cdot \text{s}^{-1}$

$$v_{14} = \frac{\text{vol}(\text{c1}) \cdot \text{V\_Lys\_RS} \cdot [\text{Lys}]}{\text{Lys\_tRNAS\_Lys\_Km} + [\text{Lys}]} \tag{31}$$

Table 60: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Lys_tRNAS-_Lys_Km			25.0	$\mu\text{mol} \cdot \text{l}^{-1}$	☑

7.15 Reaction VthrTRNA

This is an irreversible reaction of one reactant forming one product.

Name Thr aminoacyl tRNA synthetase react.

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{Thr} \longrightarrow \mathrm{ThrTRNA} \tag{32}$$

Reactant

Table 61: Properties of each reactant.

Id	Name	SBO
`Thr`	Threonine	

Product

Table 62: Properties of each product.

Id	Name	SBO
`ThrTRNA`	Thr-tRNA	

Kinetic Law

Derived unit $10^{-6}\,\mathrm{mol}\cdot\mathrm{s}^{-1}$

$$v_{15} = \frac{\mathrm{vol}\,(\mathrm{c1}) \cdot \mathrm{V\_Thr\_RS} \cdot [\mathrm{Thr}]}{\mathrm{Thr\_tRNAS\_Thr\_Km} + [\mathrm{Thr}]} \tag{33}$$

Table 63: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Thr_tRNAS-_Thr_Km`			100.0	$\mu\mathrm{mol}\cdot\mathrm{l}^{-1}$	☑

7.16 Reaction `VileTRNA`

This is an irreversible reaction of one reactant forming one product.

Name Ile aminoacyl tRNA synthetase react.

SBO:0000176 biochemical reaction

Reaction equation

$$\text{Ile} \longrightarrow \text{IleTRNA} \tag{34}$$

Reactant

Table 64: Properties of each reactant.

Id	Name	SBO
Ile	Isoleucine	

Product

Table 65: Properties of each product.

Id	Name	SBO
IleTRNA	Ile-tRNA	

Kinetic Law

Derived unit $10^{-6}\,\text{mol}\cdot\text{s}^{-1}$

$$v_{16} = \frac{\text{vol}(\text{c1}) \cdot \text{V\_Ile\_RS} \cdot [\text{Ile}]}{\text{Ile\_tRNAS\_Ile\_Km} + [\text{Ile}]} \tag{35}$$

Table 66: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Ile_tRNAS-_Ile_Km			20.0	$\mu\text{mol}\cdot\text{l}^{-1}$	☑

7.17 Reaction VlysKR

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

Name Lys ketoglutarate reductase react.

SBO:0000176 biochemical reaction

Reaction equation

$$\text{Lys} \xrightarrow{\text{LKR}} \text{Sacc} \tag{36}$$

Reactant

Table 67: Properties of each reactant.

Id	Name	SBO
Lys	Lysine	

Modifier

Table 68: Properties of each modifier.

Id	Name	SBO
LKR	LKR	

Product

Table 69: Properties of each product.

Id	Name	SBO
Sacc	Saccharopine	

Kinetic Law

Derived unit $s^{-1} \cdot 10^{-6}$ mol

$$v_{17} = \frac{\text{vol}(c1) \cdot \text{LKR\_kcat\_exp} \cdot [\text{LKR}] \cdot [\text{Lys}]}{\text{LKR\_Lys\_Km\_exp} + [\text{Lys}]} \tag{37}$$

Table 70: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
LKR_kcat_exp			3.1	s^{-1}	☑
LKR_Lys_Km_exp			13000.0	$\mu mol \cdot l^{-1}$	☑

7.18 Reaction Vtha

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

Name Thr aldolase react.

SBO:0000178 cleavage

Reaction equation

$$\text{Thr} \xrightarrow{\text{THA}} \text{Gly} \tag{38}$$

Reactant

Table 71: Properties of each reactant.

Id	Name	SBO
Thr	Threonine	

Modifier

Table 72: Properties of each modifier.

Id	Name	SBO
THA	THA	

Product

Table 73: Properties of each product.

Id	Name	SBO
Gly	Glycine	

Kinetic Law

Derived unit $\text{s}^{-1} \cdot 10^{-6}\,\text{mol}$

$$v_{18} = \frac{\text{vol}(\text{c1}) \cdot \text{THA\_kcat\_exp} \cdot [\text{THA}] \cdot [\text{Thr}]}{\text{THA\_Thr\_Km\_exp} + [\text{Thr}]} \tag{39}$$

Table 74: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
THA_kcat_exp			1.7	s^{-1}	☑
THA_Thr_Km_exp			7100.0	$\mu\text{mol} \cdot \text{l}^{-1}$	☑

8 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.

8.1 Species `Asp`

Name Aspartate

SBO:0000327 non-macromolecular ion

Initial concentration $1500\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in `Vak1`, `Vak2`, `VakI`, `VakII`), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\text{d}}{\text{d}t}\text{Asp} = 0 \tag{40}$$

8.2 Species `AK1`

Name AK1

SBO:0000252 polypeptide chain

Initial concentration $0.25\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a modifier in `Vak1`), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\text{d}}{\text{d}t}\text{AK1} = 0 \tag{41}$$

8.3 Species `Lys`

Name Lysine

SBO:0000247 simple chemical

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

This species takes part in eight reactions (as a reactant in VlysTRNA, VlysKR and as a product in Vdhdps1, Vdhdps2 and as a modifier in Vak1, Vak2, Vdhdps1, Vdhdps2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Lys} = v_6 + v_7 - v_{14} - v_{17} \tag{42}$$

8.4 Species AdoMet

Name S-adenosyl-methionine

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a modifier in Vak1, Vts1), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AdoMet} = 0 \tag{43}$$

8.5 Species AspP

Name Aspartyl_P

SBO:0000327 non-macromolecular ion

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

This species takes part in five reactions (as a reactant in Vasadh and as a product in Vak1, Vak2, VakI, VakII).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AspP} = v_1 + v_2 + v_3 + v_4 - v_5 \tag{44}$$

8.6 Species AK2

Name AK2

SBO:0000252 polypeptide chain

Initial concentration $0.25\ \mu\mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a modifier in Vak2), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AK2} = 0 \tag{45}$$

8.7 Species AKHSDHI

Name AKI-HSDHI

SBO:0000252 polypeptide chain

Initial concentration $0.63\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in two reactions (as a modifier in VakI, Vhsdh1), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{AKHSDHI} = 0 \tag{46}$$

8.8 Species AKHSDHII

Name AKII-HSDHII

SBO:0000252 polypeptide chain

Initial concentration $0.63\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in two reactions (as a modifier in VakII, Vhsdh2), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{AKHSDHII} = 0 \tag{47}$$

8.9 Species Thr

Name Threonine

SBO:0000247 simple chemical

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

This species takes part in eight reactions (as a reactant in Vtd, VthrTRNA, Vtha and as a product in Vts1 and as a modifier in VakI, VakII, Vhsdh1, Vhsdh2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Thr} = v_{11} - v_{13} - v_{15} - v_{18} \tag{48}$$

8.10 Species ASADH

Name ASADH

SBO:0000252 polypeptide chain

Initial concentration $11.6\ \mu\text{mol}\cdot\text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{ASADH} = 0 \tag{49}$$

8.11 Species ASA

Name Aspartate semialdehyde

SBO:0000327 non-macromolecular ion

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

This species takes part in five reactions (as a reactant in Vdhdps1, Vdhdps2, Vhsdh1, Vhsdh2 and as a product in Vasadh).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ASA} = v_5 - v_6 - v_7 - v_8 - v_9 \tag{50}$$

8.12 Species DHDPS1

Name DHDPS1

SBO:0000252 polypeptide chain

Initial concentration $1.6\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in one reaction (as a modifier in Vdhdps1), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DHDPS1} = 0 \tag{51}$$

8.13 Species DHDPS2

Name DHDPS2

SBO:0000252 polypeptide chain

Initial concentration $1.6\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in one reaction (as a modifier in Vdhdps2), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DHDPS2} = 0 \tag{52}$$

8.14 Species Hser

Name Homoserine

SBO:0000247 simple chemical

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

This species takes part in three reactions (as a reactant in Vhsk and as a product in Vhsdh1, Vhsdh2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Hser} = v_8 + v_9 - v_{10} \tag{53}$$

8.15 Species PHser

Name Phosphohomoserine

SBO:0000327 non-macromolecular ion

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

This species takes part in three reactions (as a reactant in Vts1, Vcgs and as a product in Vhsk).

$$\frac{\text{d}}{\text{d}t}\text{PHser} = v_{10} - v_{11} - v_{12} \tag{54}$$

8.16 Species HSK

Name HSK

SBO:0000252 polypeptide chain

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

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

$$\frac{\text{d}}{\text{d}t}\text{HSK} = 0 \tag{55}$$

8.17 Species TS1

Name TS1

SBO:0000252 polypeptide chain

Initial concentration $7.4\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a modifier in Vts1).

$$\frac{\text{d}}{\text{d}t}\text{TS1} = 0 \tag{56}$$

8.18 Species Phosphate

SBO:0000327 non-macromolecular ion

Initial concentration $10000\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a modifier in Vts1, Vcgs), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\text{d}}{\text{d}t}\text{Phosphate} = 0 \tag{57}$$

8.19 Species Cys

Name Cysteine

SBO:0000247 simple chemical

Initial concentration 15 $\mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{\text{d}}{\text{d}t}\text{Cys} = 0 \tag{58}$$

8.20 Species CGS

Name CGS

SBO:0000252 polypeptide chain

Initial concentration 0.7 $\mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{\text{d}}{\text{d}t}\text{CGS} = 0 \tag{59}$$

8.21 Species Cysta

Name Cystathione

SBO:0000247 simple chemical

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

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

$$\frac{\text{d}}{\text{d}t}\text{Cysta} = 0 \tag{60}$$

8.22 Species TD

Name TD

SBO:0000252 polypeptide chain

Initial concentration 0.36 $\mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{\text{d}}{\text{d}t}\text{TD} = 0 \tag{61}$$

8.23 Species Ile

Name Isoleucine

SBO:0000247 simple chemical

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

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

$$\frac{\text{d}}{\text{d}t}\text{Ile} = v_{13} - v_{16} \tag{62}$$

8.24 Species Val

Name Valine

SBO:0000247 simple chemical

Initial concentration $100\ \mu\text{mol}\cdot\text{l}^{-1}$

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

$$\frac{\text{d}}{\text{d}t}\text{Val} = 0 \tag{63}$$

8.25 Species LysTRNA

Name Lys-tRNA

SBO:0000245 macromolecule

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

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

$$\frac{\text{d}}{\text{d}t}\text{LysTRNA} = 0 \tag{64}$$

8.26 Species ThrTRNA

Name Thr-tRNA

SBO:0000245 macromolecule

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

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

$$\frac{\text{d}}{\text{d}t}\text{ThrTRNA} = 0 \tag{65}$$

8.27 Species IleTRNA

Name Ile-tRNA

SBO:0000245 macromolecule

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

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

$$\frac{\text{d}}{\text{d}t}\text{IleTRNA} = 0 \tag{66}$$

8.28 Species LKR

Name LKR

SBO:0000252 polypeptide chain

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

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

$$\frac{\text{d}}{\text{d}t}\text{LKR} = 0 \tag{67}$$

8.29 Species Sacc

Name Saccharopine

SBO:0000247 simple chemical

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

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

$$\frac{\text{d}}{\text{d}t}\text{Sacc} = 0 \tag{68}$$

8.30 Species THA

Name THA

SBO:0000252 polypeptide chain

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

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

$$\frac{\text{d}}{\text{d}t}\text{THA} = 0 \tag{69}$$

8.31 Species Gly

Name Glycine

SBO:0000247 simple chemical

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gly} = 0 \tag{70}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000176 biochemical reaction: An event involving one or more chemical entities that modifies the electrochemical structure of at least one of the participants.

SBO:0000178 cleavage: Rupture of a covalent bond resulting in the conversion of one physical entity into several physical entities

SBO:0000190 Hill coefficient: Empirical parameter created by Archibald Vivian Hill to describe the cooperative binding of oxygen on hemoglobine (Hill (1910). The possible effects of the aggregation of the molecules of haemoglobin on its dissociation curves. J Physiol 40: iv-vii)

SBO:0000200 redox reaction: Chemical process in which atoms have their oxidation number (oxidation state) changed

SBO:0000205 composite biochemical process: Process that involves the participation of chemical or biological entities and is composed of several elementary steps or reactions.

SBO:0000245 macromolecule: Molecular entity mainly built-up by the repetition of pseudo-identical units. CHEBI:3383

SBO:0000247 simple chemical: Simple, non-repetitive chemical entity

SBO:0000252 polypeptide chain: Naturally occurring macromolecule formed by the repetition of amino-acid residues linked by peptidic bonds. A polypeptide chain is synthesized by the ribosome. CHEBI:1654

SBO:0000288 IC50: Also called half maximal inhibitory concentration, it represents the concentration of an inhibitor substance that is required to suppress 50% of an effect.

SBO:0000320 product catalytic rate constant: Numerical parameter that quantifies the velocity of product creation by a reversible enzymatic reaction.

SBO:0000321 substrate catalytic rate constant: Numerical parameter that quantifies the velocity of substrate creation by a reversible enzymatic reaction.

SBO:0000327 non-macromolecular ion: Chemical entity having a net electric charge

SBO:0000363 activation constant: Dissociation constant of a potentiator (activator) from a target (e.g. an enzyme) of which it activates the function

SBO:0000376 hydrolysis: Decomposition of a compound by reaction with water, where the hydroxyl and H groups are incorporated into different product

SBO:0000402 transfer of a chemical group: Covalent reaction that results in the transfer of a chemical group from one molecule to another

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