SBML Model Report

Model name: "Rodriguez-Caso2006-_Polyamine_Metabolism"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by the following seven authors: Lukas Endler[1], Armando Reyes-Palomares[2], Carlos Rodrguez-Caso[3], Raul Montaez[4], Marta Cascante[5], Francisca Snchez-Jimnez[6] and Miguel A. Medina[7] at September eighth 2008 at 3:27 p. m. and last time modified at July fifth 2012 at 2:37 p. m. Table 1 shows an overview of the quantities of all components of this model.

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

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	11
events	0	constraints	0
reactions	13	function definitions	0
global parameters	17	unit definitions	10
rules	6	initial assignments	0

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Model Notes

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Metabolic modeling of polyamine metabolism in mammals.
Rodrguez-Caso,C et al.: J Biol Chem 2006 : 281:21799-812.
The model reproduces the dynamical behavior of the polyamine metabolism in mammals. In this model there are some additions and corrections to the publication. All perturbations and analysis have produced results very close to the published experiments. The model was successfully tested on CoPaSi v.4.4 (build 26).

Parameters not included in the publication:

1. Parameters for SSAT kinetic constants:

KmAcCoA = 1.5 M

KmCoA = 40 M

2. Parameters for equation MAT (table 1):

Vmax_MAT = 0.45 M/min

Km_MAT = 41 M

Ki_MET_MAT = 50 M

3. Erratum.: The corrected ODE for time-dependent variable Antz is:

KsANTZ*(1-1/(1+Keq*0.01*([D]+[S])))-KdANTZ*[Antz]

According to these modifications the new steady-state analysis results are:

Metabolites:

[P]= 104.681 M

[D]= 76.7492 M

[S]= 58.0135 M

[SAM]= 52.327 M

[A]= 0.0101962 M

[aS]= 0.0245375 M

[aD]= 0.832236 M

Time-dependent global parameters:

[Antz] = 0.574038 M

Vmaxodc = 1.28315 M/min

Vmaxssat = 0.673814 M/min

Vmaxsamdc = 0.36829 M/min

In summary, you are entitled to use this encoded model in absolutely any manner you deem suitable, verbatim, or with modification, alone or embedded it in a larger context, redistribute it, commercially or not, in a restricted way or not.

To cite BioModels Database, please use: Li C, Donizelli M, Rodriguez N, Dharuri H, Endler L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novre N, Laibe C (2010) BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models. BMC Syst Biol., 4:92.

2 Unit Definitions

This is an overview of 13 unit definitions of which three are predefined by SBML and not mentioned in the model.

2.1 Unit `time`

Name minute

Definition 60 s

2.2 Unit `substance`

Name mole

Definition µmol

2.3 Unit `uM_1`

Name peruM

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

2.4 Unit `uM_min_1`

Name uMpermin

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

2.5 Unit `uM_1_min_1`

Name peruMpermin

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

2.6 Unit uM_1_min_2

Name uM(-1)min(-2)

Definition $\mu\mathrm{mol}^{-1} \cdot (60\ \mathrm{s})^{-2} \cdot 1$

2.7 Unit min_1

Name permin

Definition $(60\ \mathrm{s})^{-1}$

2.8 Unit uM

Name microM

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

2.9 Unit min_uM_1

Name minperuM

Definition $60\ \mathrm{s} \cdot \mu\mathrm{mol}^{-1} \cdot 1$

2.10 Unit uM_min_2

Name uM(min)^2

Definition $\mu\mathrm{mol} \cdot 1^{-1} \cdot (60\ \mathrm{s})^{-2}$

2.11 Unit volume

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

Definition l

2.12 Unit area

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

Definition m^2

2.13 Unit length

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

Definition m

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
`cytosol`	Cytosol		3	1	litre	☑	

3.1 Compartment `cytosol`

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

Name Cytosol

4 Species

This model contains eleven species. The boundary condition of four 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
SAM	S-adenosyl-L-methionine	cytosol	$\mu mol \cdot l^{-1}$	☐	☐
A	S-adenosylmethioninamine	cytosol	$\mu mol \cdot l^{-1}$	☐	☐
P	Putrescine	cytosol	$\mu mol \cdot l^{-1}$	☐	☐
S	Spermine	cytosol	$\mu mol \cdot l^{-1}$	☐	☐
D	Spermidine	cytosol	$\mu mol \cdot l^{-1}$	☐	☐
aS	N1-Acetylspermine	cytosol	$\mu mol \cdot l^{-1}$	☐	☐
aD	N1-Acetylspermidine	cytosol	$\mu mol \cdot l^{-1}$	☐	☐
Met	Methionine	cytosol	$\mu mol \cdot l^{-1}$	☑	☑
ORN	L-Ornithine	cytosol	$\mu mol \cdot l^{-1}$	☑	☑
AcCoA	Acetyl-CoA	cytosol	$\mu mol \cdot l^{-1}$	☑	☑
CoA	CoA	cytosol	$\mu mol \cdot l^{-1}$	☑	☑

5 Parameters

This model contains 17 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Vmaxodc`	Vmaxodc		1.279	$\mu mol \cdot (60\ s)^{-1} \cdot l^{-1}$	⊟
`Vmaxssat`	Vmaxssat		0.677	$\mu mol \cdot (60\ s)^{-1} \cdot l^{-1}$	⊟
`Vmaxsamdc`	Vmaxsamdc		0.367	$\mu mol \cdot (60\ s)^{-1} \cdot l^{-1}$	⊟
`Antz`	Antz		0.575	$\mu mol \cdot (60\ s)^{-1} \cdot l^{-1}$	⊟
`Keq`	Keq		1.000	$\mu mol^{-1} \cdot l$	☑
`Kdodc`	KdODC		0.050	$\mu mol^{-1} \cdot l$	☑
`Ksodc`	KsODC		5.000	$\mu mol \cdot l^{-1} \cdot (60\ s)^{-2}$	☑
`Kdssat`	KdSSAT		0.200	$(60\ s)^{-1}$	☑
`Ksssat`	KsSSAT		0.001	$\mu mol \cdot l^{-1} \cdot (60\ s)^{-2}$	☑
`Kdsamdc`	KdSAMDC		0.020	$(60\ s)^{-1}$	☑
`Kssamdc`	KsSAMDC		1.000	$\mu mol \cdot l^{-1} \cdot (60\ s)^{-2}$	☑
`Kdantz`	KdANTZ		0.020	$(60\ s)^{-1}$	☑
`Ksantz`	KsANTZ		0.020	$\mu mol \cdot l^{-1} \cdot (60\ s)^{-2}$	☑
`R`	R		0.004	$(60\ s)^{-1}$	☑
`C`	C		4.440	dimensionless	☑
`Kaccoa`	Kaccoa		0.004	$(60\ s)^{-1}$	⊟
`Kcoa`	Kcoa		0.012	$(60\ s)^{-1}$	⊟

6 Rules

This is an overview of six rules.

6.1 Rule `Kaccoa`

Rule `Kaccoa` is an assignment rule for parameter `Kaccoa`:

$$\text{Kaccoa} = \text{R} \tag{1}$$

Derived unit $(60\ s)^{-1}$

6.2 Rule `Kcoa`

Rule `Kcoa` is an assignment rule for parameter `Kcoa`:

$$\text{Kcoa} = 3 \cdot \text{R} \tag{2}$$

6.3 Rule Vmaxodc

Rule Vmaxodc is a rate rule for parameter Vmaxodc:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Vmaxodc} = \frac{\mathrm{Ksodc}}{1 + \mathrm{Keq} \cdot (\mathrm{[D]} + \mathrm{[S]})} - \mathrm{Kdodc} \cdot \mathrm{Antz} \cdot \mathrm{Vmaxodc} \tag{3}$$

6.4 Rule Vmaxssat

Rule Vmaxssat is a rate rule for parameter Vmaxssat:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Vmaxssat} = \mathrm{Ksssat} \cdot \left(1 - \frac{1}{1 + \mathrm{Keq} \cdot (\mathrm{[D]} + \mathrm{[S]})}\right) - \mathrm{Kdssat} \cdot \frac{1}{1 + \mathrm{Keq} \cdot (\mathrm{[D]} + \mathrm{[S]})} \cdot \mathrm{Vmaxssat} \tag{4}$$

6.5 Rule Vmaxsamdc

Rule Vmaxsamdc is a rate rule for parameter Vmaxsamdc:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Vmaxsamdc} = \mathrm{Kssamdc} \cdot \frac{1}{1 + \mathrm{Keq} \cdot (\mathrm{[D]} + \mathrm{[S]})} - \mathrm{Kdsamdc} \cdot \mathrm{Vmaxsamdc} \tag{5}$$

6.6 Rule Antz

Rule Antz is a rate rule for parameter Antz:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Antz} = \mathrm{Ksantz} \cdot \left(1 - \frac{1}{1 + \mathrm{Keq} \cdot 0.01 \cdot (\mathrm{[D]} + \mathrm{[S]})}\right) - \mathrm{Kdantz} \cdot \mathrm{Antz} \tag{6}$$

7 Reactions

This model contains 13 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	ODC	Ornithine decarboxylase	$\mathrm{ORN} \longrightarrow \mathrm{P}$	
2	SAMdc	S-adenosylmethionine decarboxylase	$\mathrm{SAM} \xrightarrow{\mathrm{S,\ P}} \mathrm{A}$	
3	SSAT_for_S	Spermidine/Spermine N1-acetyltransferase for S	$\mathrm{S} + \mathrm{AcCoA} \xrightarrow{\mathrm{D}} \mathrm{aS} + \mathrm{CoA}$	
4	SSAT_for_D	Spermidine/spermine N1-acetyltransferase for D	$\mathrm{D} + \mathrm{AcCoA} \xrightarrow{\mathrm{S}} \mathrm{aD} + \mathrm{CoA}$	
5	PAO_for_aD	Polyamine oxidase for aD	$\mathrm{aD} \xrightarrow{\mathrm{aS,\ D,\ S}} \mathrm{P}$	
6	PAO_for_aS	Polyamine oxidase for aS	$\mathrm{aS} \xrightarrow{\mathrm{aD,\ S}} \mathrm{D}$	
7	SpdS	Spermidine synthase	$\mathrm{A} + \mathrm{P} \longrightarrow \mathrm{D}$	
8	SpmS	Spermine synthase	$\mathrm{A} + \mathrm{D} \longrightarrow \mathrm{S}$	
9	MAT	Methionine adenosyltransferase	$\mathrm{Met} \longrightarrow \mathrm{SAM}$	
10	VCoA	VCOA	$\mathrm{AcCoA} \longrightarrow \mathrm{CoA}$	
11	VacCoA	VACCOA	$\mathrm{CoA} \longrightarrow \mathrm{AcCoA}$	
12	P_efflux	Putrescine efflux	$\mathrm{P} \longrightarrow \emptyset$	
13	aD_efflux	aD efflux	$\mathrm{aD} \longrightarrow \emptyset$	

7.1 Reaction ODC

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

Name Ornithine decarboxylase

Reaction equation

$$\mathrm{ORN} \longrightarrow \mathrm{P} \tag{7}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
ORN	L-Ornithine	

Product

Table 7: Properties of each product.

Id	Name	SBO
P	Putrescine	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \frac{\mathrm{Vmaxodc} \cdot [\mathrm{ORN}]}{\mathrm{Kmodc} \cdot \left(1 + \frac{[\mathrm{P}]}{\mathrm{Kipodc}}\right) + [\mathrm{ORN}]} \tag{8}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kipodc			1300.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
Kmodc			60.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑

7.2 Reaction SAMdc

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

Name S-adenosylmethionine decarboxylase

Reaction equation

$$\mathrm{SAM} \xrightarrow{\mathrm{S,\ P}} \mathrm{A} \tag{9}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
SAM	S-adenosyl-L-methionine	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
S	Spermine	
P	Putrescine	

Product

Table 11: Properties of each product.

Id	Name	SBO
A	S-adenosylmethioninamine	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \frac{\frac{\mathrm{Vmaxsamdc}}{1+\frac{[\mathrm{S}]}{\mathrm{Kissamdc}}} \cdot [\mathrm{SAM}]}{\mathrm{Kmsamdc} \cdot \left(1 + \frac{\mathrm{Kapsamdc}}{[\mathrm{P}]} + \frac{[\mathrm{A}]}{\mathrm{Kiasamdc}}\right) + [\mathrm{SAM}]} \tag{10}$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kapsamdc			0.5	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
Kiasamdc			2.5	$\mu mol \cdot l^{-1}$	☑
Kissamdc			500.0	$\mu mol \cdot l^{-1}$	☑
Kmsamdc			50.0	$\mu mol \cdot l^{-1}$	☑

7.3 Reaction SSAT_for_S

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

Name Spermidine/Spermine N1-acetyltransferase for S

Reaction equation

$$S + AcCoA \xrightarrow{D} aS + CoA \tag{11}$$

Reactants

Table 13: Properties of each reactant.

Id	Name	SBO
S	Spermine	
AcCoA	Acetyl-CoA	

Modifier

Table 14: Properties of each modifier.

Id	Name	SBO
D	Spermidine	

Products

Table 15: Properties of each product.

Id	Name	SBO
aS	N1-Acetylspermine	
CoA	CoA	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \frac{\frac{1}{C} \cdot \mathrm{Vmaxssat} \cdot [\mathrm{S}] \cdot [\mathrm{AcCoA}]}{\mathrm{Kmsssat} \cdot \left(1 + \frac{[\mathrm{D}]}{\mathrm{Kmdssat}}\right) \cdot \mathrm{Kmaccoassat} \cdot \left(1 + \frac{[\mathrm{CoA}]}{\mathrm{Kmcoassat}}\right) + \mathrm{Kmaccoassat} \cdot \left(1 + \frac{[\mathrm{CoA}]}{\mathrm{Kmcoassat}}\right) \cdot [\mathrm{S}] + \mathrm{Kmsssat} \cdot \left(1 \right.} \tag{12}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Kmaccoassat`			1.5	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
`Kmcoassat`			40.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
`Kmdssat`			130.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
`Kmsssat`			35.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑

7.4 Reaction `SSAT_for_D`

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

Name Spermidine/spermine N1-acetyltransferase for D

Reaction equation

$$\mathrm{D} + \mathrm{AcCoA} \xrightarrow{\mathrm{S}} \mathrm{aD} + \mathrm{CoA} \tag{13}$$

Reactants

Table 17: Properties of each reactant.

Id	Name	SBO
`D`	Spermidine	
`AcCoA`	Acetyl-CoA	

Modifier

Table 18: Properties of each modifier.

Id	Name	SBO
`S`	Spermine	

Products

Table 19: Properties of each product.

Id	Name	SBO
aD	N1-Acetylspermidine	
CoA	CoA	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \frac{\mathrm{Vmaxssat} \cdot [\mathrm{D}] \cdot [\mathrm{AcCoA}]}{\mathrm{Kmdssat} \cdot \left(1 + \frac{[\mathrm{S}]}{\mathrm{Kmsssat}}\right) \cdot \mathrm{Kmaccoassat} \cdot \left(1 + \frac{[\mathrm{CoA}]}{\mathrm{Kmcoassat}}\right) + \mathrm{Kmaccoassat} \cdot \left(1 + \frac{[\mathrm{CoA}]}{\mathrm{Kmcoassat}}\right) \cdot [\mathrm{D}] + \mathrm{Kmdssat} \cdot \left(1 \right.} \tag{14}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kmaccoassat			1.5	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
Kmcoassat			40.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
Kmdssat			130.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
Kmsssat			35.0	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑

7.5 Reaction PAO_for_aD

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

Name Polyamine oxidase for aD

Reaction equation

$$\mathrm{aD} \xrightarrow{\mathrm{aS,\ D,\ S}} \mathrm{P} \tag{15}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
aD	N1-Acetylspermidine	

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
aS	N1-Acetylspermine	
D	Spermidine	
S	Spermine	

Product

Table 23: Properties of each product.

Id	Name	SBO
P	Putrescine	

Kinetic Law

SBO:0000270 enzymatic rate law for competitive inhibition of irreversible unireactant enzymes by exclusive inhibitors

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \frac{\mathrm{Vmpao} \cdot [\mathrm{aD}]}{\mathrm{Kmadpao} \cdot \left(1 + \frac{[\mathrm{aD}]}{\mathrm{Kmadpao}} + \frac{[\mathrm{aS}]}{\mathrm{Kmaspao}} + \frac{[\mathrm{D}]}{\mathrm{Kmdpao}} + \frac{[\mathrm{S}]}{\mathrm{Kmspao}}\right)} \tag{16}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kmadpao			14.00	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
Kmaspao			0.60	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
Kmdpao			50.00	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
Kmspao			15.00	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑
Vmpao			10.35	$\mu\mathrm{mol} \cdot (60\ \mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$	☑

7.6 Reaction PAO_for_aS

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

Name Polyamine oxidase for aS

Reaction equation

$$\mathrm{aS} \xrightarrow{\mathrm{aD,\ S}} \mathrm{D} \tag{17}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
aS	N1-Acetylspermine	

Modifiers

Table 26: Properties of each modifier.

Id	Name	SBO
aD	N1-Acetylspermidine	
S	Spermine	

Product

Table 27: Properties of each product.

Id	Name	SBO
D	Spermidine	

Kinetic Law

SBO:0000270 enzymatic rate law for competitive inhibition of irreversible unireactant enzymes by exclusive inhibitors

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\left(\mathrm{cytosol}\right) \cdot \frac{\mathrm{Vmpao} \cdot [\mathrm{aS}]}{\mathrm{Kmaspao} \cdot \left(1 + \frac{[\mathrm{aD}]}{\mathrm{Kmadpao}} + \frac{[\mathrm{aS}]}{\mathrm{Kmaspao}} + \frac{[\mathrm{D}]}{\mathrm{Kmdpao}} + \frac{[\mathrm{S}]}{\mathrm{Kmspao}}\right)} \tag{18}$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kmadpao			14.00	$\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
Kmaspao			0.60	$\mu mol \cdot l^{-1}$	☑
Kmdpao			50.00	$\mu mol \cdot l^{-1}$	☑
Kmspao			15.00	$\mu mol \cdot l^{-1}$	☑
Vmpao			10.35	$\mu mol \cdot (60\ s)^{-1} \cdot l^{-1}$	☑

7.7 Reaction SpdS

This is an irreversible reaction of two reactants forming one product.

Name Spermidine synthase

Reaction equation

$$A + P \longrightarrow D \tag{19}$$

Reactants

Table 29: Properties of each reactant.

Id	Name	SBO
A	S-adenosylmethioninamine	
P	Putrescine	

Product

Table 30: Properties of each product.

Id	Name	SBO
D	Spermidine	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}(\mathrm{cytosol}) \cdot \frac{\mathrm{Vmspds} \cdot [A] \cdot [P]}{\mathrm{Kiaspds} \cdot \mathrm{Kpspds} \cdot \left(1 + \frac{[D]}{\mathrm{Kidspds}}\right) + \mathrm{Kpspds} \cdot [A] + \mathrm{KaSpds} \cdot \left(1 + \frac{[D]}{\mathrm{Kidspds}}\right) \cdot [P] + [A] \cdot [P]} \tag{20}$$

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KaSpds			0.30	$\mu mol \cdot l^{-1}$	☑
Kiaspds			0.80	$\mu mol \cdot l^{-1}$	☑
Kidspds			100.00	$\mu mol \cdot l^{-1}$	☑
Kpspds			40.00	$\mu mol \cdot l^{-1}$	☑
Vmspds			10.95	$\mu mol \cdot (60\ s)^{-1} \cdot l^{-1}$	☑

7.8 Reaction SpmS

This is an irreversible reaction of two reactants forming one product.

Name Spermine synthase

Reaction equation

$$A + D \longrightarrow S \tag{21}$$

Reactants

Table 32: Properties of each reactant.

Id	Name	SBO
A	S-adenosylmethioninamine	
D	Spermidine	

Product

Table 33: Properties of each product.

Id	Name	SBO
S	Spermine	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}(\mathrm{cytosol}) \cdot \frac{\mathrm{Vmspms} \cdot [A] \cdot [D]}{\mathrm{Kiaspms} \cdot \mathrm{Kdspms} \cdot \left(1 + \frac{[S]}{\mathrm{Kisspms}}\right) + \mathrm{Kdspms} \cdot [A] + \mathrm{Kaspms} \cdot \left(1 + \frac{[S]}{\mathrm{Kisspms}}\right) \cdot [D] + [A] \cdot [D]} \tag{22}$$

Table 34: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kaspms			0.10	$\mu mol \cdot l^{-1}$	☑
Kdspms			60.00	$\mu mol \cdot l^{-1}$	☑
Kiaspms			0.06	$\mu mol \cdot l^{-1}$	☑
Kisspms			25.00	$\mu mol \cdot l^{-1}$	☑
Vmspms			3.23	$\mu mol \cdot (60\ s)^{-1} \cdot l^{-1}$	☑

7.9 Reaction MAT

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

Name Methionine adenosyltransferase

Reaction equation

$$\text{Met} \longrightarrow \text{SAM} \tag{23}$$

Reactant

Table 35: Properties of each reactant.

Id	Name	SBO
Met	Methionine	

Product

Table 36: Properties of each product.

Id	Name	SBO
SAM	S-adenosyl-L-methionine	

Kinetic Law

SBO:0000260 enzymatic rate law for simple competitive inhibition of irreversible unireactant enzymes by one inhibitor

Derived unit contains undeclared units

$$v_9 = \text{vol}(\text{cytosol}) \cdot \frac{\text{Vmmat}}{1 + \frac{\text{Kmmat}}{[\text{Met}]} \cdot \left(1 + \frac{[\text{SAM}]}{\text{Kimetmat}}\right)} \tag{24}$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Kimetmat`			50.00	$\mu mol \cdot l^{-1}$	☑
`Kmmat`			41.00	$\mu mol \cdot l^{-1}$	☑
`Vmmat`			0.45	$\mu mol \cdot (60\ s)^{-1} \cdot l^{-1}$	☑

7.10 Reaction `VCoA`

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

Name VCOA

Reaction equation

$$\text{AcCoA} \longrightarrow \text{CoA} \tag{25}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
`AcCoA`	Acetyl-CoA	

Product

Table 39: Properties of each product.

Id	Name	SBO
`CoA`	CoA	

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

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

$$v_{10} = \text{vol}\,(\text{cytosol}) \cdot \text{Kcoa} \cdot [\text{AcCoA}] \tag{26}$$

7.11 Reaction `VacCoA`

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

Name VACCOA

Reaction equation

$$\mathrm{CoA} \longrightarrow \mathrm{AcCoA} \tag{27}$$

Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
CoA	CoA	

Product

Table 41: Properties of each product.

Id	Name	SBO
AcCoA	Acetyl-CoA	

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

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

$$v_{11} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Kaccoa} \cdot [\mathrm{CoA}] \tag{28}$$

7.12 Reaction P_efflux

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

Name Putrescine efflux

Reaction equation

$$\mathrm{P} \longrightarrow \emptyset \tag{29}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
P	Putrescine	

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

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

$$v_{12} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Kpefflux} \cdot [\mathrm{P}] \tag{30}$$

Table 43: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kpefflux			0.01	$(60\ \mathrm{s})^{-1}$	☑

7.13 Reaction aD_efflux

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

Name aD efflux

Reaction equation

$$\mathrm{aD} \longrightarrow \emptyset \tag{31}$$

Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
aD	N1-Acetylspermidine	

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

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

$$v_{13} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Kadefflux} \cdot [\mathrm{aD}] \tag{32}$$

Table 45: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kadefflux			0.01	$(60\ \mathrm{s})^{-1}$	☑

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.

8.1 Species SAM

Name S-adenosyl-L-methionine

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

This species takes part in two reactions (as a reactant in SAMdc and as a product in MAT).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{SAM} = v_9 - v_2 \tag{33}$$

8.2 Species A

Name S-adenosylmethioninamine

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

This species takes part in three reactions (as a reactant in SpdS, SpmS and as a product in SAMdc).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A} = v_2 - v_7 - v_8 \tag{34}$$

8.3 Species P

Name Putrescine

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

This species takes part in five reactions (as a reactant in SpdS, P_efflux and as a product in ODC, PAO_for_aD and as a modifier in SAMdc).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P} = v_1 + v_5 - v_7 - v_{12} \tag{35}$$

8.4 Species S

Name Spermine

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

This species takes part in six reactions (as a reactant in SSAT_for_S and as a product in SpmS and as a modifier in SAMdc, SSAT_for_D, PAO_for_aD, PAO_for_aS).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S} = v_8 - v_3 \tag{36}$$

8.5 Species D

Name Spermidine

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

This species takes part in six reactions (as a reactant in SSAT_for_D, SpmS and as a product in PAO_for_aS, SpdS and as a modifier in SSAT_for_S, PAO_for_aD).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{D} = v_6 + v_7 - v_4 - v_8 \tag{37}$$

8.6 Species aS

Name N1-Acetylspermine

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

This species takes part in three reactions (as a reactant in PAO_for_aS and as a product in SSAT-_for_S and as a modifier in PAO_for_aD).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{aS} = v_3 - v_6 \tag{38}$$

8.7 Species aD

Name N1-Acetylspermidine

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

This species takes part in four reactions (as a reactant in PAO_for_aD, aD_efflux and as a product in SSAT_for_D and as a modifier in PAO_for_aS).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{aD} = v_4 - v_5 - v_{13} \tag{39}$$

8.8 Species Met

Name Methionine

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Met} = 0 \tag{40}$$

8.9 Species ORN

Name L-Ornithine

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ORN} = 0 \tag{41}$$

8.10 Species AcCoA

Name Acetyl-CoA

Initial concentration $39.5\ \mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AcCoA} = 0 \tag{42}$$

8.11 Species CoA

Name CoA

Initial concentration $160\ \mu\text{mol} \cdot \text{l}^{-1}$

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

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

A Glossary of Systems Biology Ontology Terms

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme: Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does not include any reverse process that creates the reactants from the products. The change of a product quantity is proportional to the quantity of one reactant. It is to be used in a reaction modelled using a continuous framework.

SBO:0000260 enzymatic rate law for simple competitive inhibition of irreversible unireactant enzymes by one inhibitor: Inhibition of a unireactant enzyme by one inhibitor that binds once to the free enzyme and prevents the binding of the substrate. The enzymes do not catalyse the reactions in both directions.

SBO:0000270 enzymatic rate law for competitive inhibition of irreversible unireactant enzymes by exclusive inhibitors: Inhibition of a unireactant enzyme by inhibitors that bind to the free enzyme on the same binding site than the substrate. The enzymes do not catalyse the reactions in both directions.

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