SBML Model Report

Model name: "Curto1998 - purine metabolism"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Nicolas Le Novre[1] and Tomas Radivoyevitch[2] at March sixth 2005 at 1:52 p.m. and last time modified at July second 2014 at 4:48 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	1
species types	0	species	18
events	0	constraints	0
reactions	37	function definitions	0
global parameters	0	unit definitions	2
rules	0	initial assignments	0

Model Notes

Curto1998 - purine metabolism

This is a purine metabolism model that is geared toward studies of gout.

The model uses Generalized Mass Action (GMA; i.e. power law) descriptions of reaction rate laws.

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[1] EMBL-EBI, lenov@ebi.ac.uk

[2] CASE western research university, txr24@po.cwru.edu

Such descriptions are local approximations that assume independent substrate binding.

This model is described in the article:Mathematical models of purine metabolism in man.Curto R, Voit EO, Sorribas A, Cascante M.Math Biosci 1998 Jul; 151(1): 1-49

Abstract:

Experimental and clinical data on purine metabolism are collated and analyzed with three mathematical models. The first model is the result of an attempt to construct a traditional kinetic model based on Michaelis-Menten rate laws. This attempt is only partially successful, since kinetic information, while extensive, is not complete, and since qualitative information is difficult to incorporate into this type of model. The data gaps necessitate the complementation of the Michaelis-Menten model with other functional forms that can incorporate different types of data. The most convenient and established representations for this purpose are rate laws formulated as power-law functions, and these are used to construct a Complemented Michaelis-Menten (CMM) model. The other two models are pure power-law-representations, one in the form of a Generalized Mass Action (GMA) system, and the other one in the form of an S-system. The first part of the paper contains a compendium of experimental data necessary for any model of purine metabolism. This is followed by the formulation of the three models and a comparative analysis. For physiological and moderately pathological perturbations in metabolites or enzymes, the results of the three models are very similar and consistent with clinical findings. This is an encouraging result since the three models have different structures and data requirements and are based on different mathematical assumptions. Significant enzyme deficiencies are not so well modeled by the S-system model. The CMM model captures the dynamics better, but judging by comparisons with clinical observations, the best model in this case is the GMA model. The model results are discussed in some detail, along with advantages and disadvantages of each modeling strategy.

This model is hosted on BioModels Database and identified by: BIOMD0000000015.

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

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 `substance`

Name micromole (default)

Notes Default unit of substance redefined to micromole by comparison with the article. Nicolas Le Novere

Definition μmol

2.2 Unit `time`

Name minute (default)

Notes Default unit of time redefined to minute by comparison with the article. Nicolas Le Novere

Definition 60 s

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 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

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

3.1 Compartment `cell`

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

4 Species

This model contains 18 species. The boundary condition of two of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 6 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
PRPP	phosphoribosylpyrophosphate	cell	μmol	⊟	⊟
IMP	inosine monophosphate	cell	μmol	⊟	⊟
SAMP	adenylosuccinate	cell	μmol	⊟	⊟
ATP	ATP_ADP_AMP_Ado	cell	μmol	⊟	⊟
SAM	s-adenosyl-L-methionine	cell	μmol	⊟	⊟
Ade	adenine	cell	μmol	⊟	⊟
XMP	xanthosine monophosphate	cell	μmol	⊟	⊟
GTP	GTP_GDP_GMP	cell	μmol	⊟	⊟
dATP	dATP_dADP_dAMP_dAdo	cell	μmol	⊟	⊟
dGTP	dGTP_dGDP_dGMP	cell	μmol	⊟	⊟
RNA		cell	μmol	⊟	⊟
DNA		cell	μmol	⊟	⊟
HX	dIno_Ino_HX	cell	μmol	⊟	⊟
Xa	xanthine	cell	μmol	⊟	⊟
Gua	guanine	cell	μmol	⊟	⊟
UA	uric acid	cell	μmol	⊟	⊟
R5P	ribose-5-phosphate	cell	μmol	⊟	☑
Pi	phosphate	cell	μmol	⊟	☑

5 Reactions

This model contains 37 reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 4: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	ada		$\text{ATP} \longrightarrow \text{HX}$	
2	ade		$\text{Ade} \longrightarrow \emptyset$	
3	adna		$\text{dATP} \xrightarrow{\text{dGTP}} \text{DNA}$	
4	adrnr		$\text{ATP} \xrightarrow{\text{dGTP, dATP}} \text{dATP}$	
5	ampd		$\text{ATP} \xrightarrow{\text{GTP, Pi}} \text{IMP}$	
6	aprt		$\text{PRPP} + \text{Ade} \xrightarrow{\text{ATP}} \text{ATP}$	
7	arna		$\text{ATP} \xrightarrow{\text{GTP}} \text{RNA}$	
8	asuc		$\text{IMP} \xrightarrow{\text{ATP, GTP, Pi}} \text{SAMP}$	
9	asli		$\text{SAMP} \xrightarrow{\text{ATP}} \text{ATP}$	
10	dada		$\text{dATP} \longrightarrow \text{HX}$	
11	den		$\text{PRPP} \xrightarrow{\text{dGTP, IMP, ATP, GTP, Pi}} \text{IMP}$	
12	dgnuc		$\text{dGTP} \longrightarrow \text{Gua}$	
13	dnaa		$\text{DNA} \longrightarrow \text{dATP}$	
14	dnag		$\text{DNA} \longrightarrow \text{dGTP}$	
15	gdna		$\text{dGTP} \xrightarrow{\text{dATP}} \text{DNA}$	
16	gdrnr		$\text{GTP} \xrightarrow{\text{dATP, dGTP}} \text{dGTP}$	
17	gmpr		$\text{GTP} \xrightarrow{\text{XMP, ATP, IMP}} \text{IMP}$	
18	gmps		$\text{XMP} \xrightarrow{\text{ATP}} \text{GTP}$	

№	Id	Name	Reaction Equation	SBO
19	gnuc		$GTP \xrightarrow{Pi} Gua$	
20	gprt		$Gua + PRPP \xrightarrow{GTP} GTP$	
21	grna		$GTP \xrightarrow{ATP} RNA$	
22	gua		$Gua \longrightarrow Xa$	
23	hprt		$HX + PRPP \xrightarrow{IMP} IMP$	
24	hx		$HX \longrightarrow \emptyset$	
25	hxd		$HX \longrightarrow Xa$	
26	impd		$IMP \xrightarrow{GTP,\ XMP} XMP$	
27	inuc		$IMP \xrightarrow{Pi} HX$	
28	mat		$ATP \xrightarrow{SAM} SAM$	
29	polyam		$SAM \longrightarrow Ade$	
30	prpps		$R5P \xrightarrow{ATP,\ GTP,\ Pi,\ PRPP} PRPP$	
31	pyr		$PRPP \longrightarrow \emptyset$	
32	rnaa		$RNA \longrightarrow ATP$	
33	rnag		$RNA \longrightarrow GTP$	
34	trans		$SAM \longrightarrow ATP$	
35	ua		$UA \longrightarrow \emptyset$	
36	x		$Xa \longrightarrow \emptyset$	
37	xd		$Xa \longrightarrow UA$	

5.1 Reaction `ada`

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

Reaction equation

$$ATP \longrightarrow HX \tag{1}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
ATP	ATP_ADP_AMP_Ado	

Product

Table 6: Properties of each product.

Id	Name	SBO
HX	dIno_Ino_HX	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{aada} \cdot \text{ATP}^{\text{fada4}} \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
aada			0.001		☑
fada4			0.970		☑

5.2 Reaction `ade`

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

Reaction equation

$$\text{Ade} \longrightarrow \emptyset \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
Ade	adenine	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{aade} \cdot \text{Ade}^{\text{fade6}} \tag{4}$$

Table 9: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
aade			0.01		☑
fade6			0.55		☑

5.3 Reaction `adna`

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

Reaction equation

$$\text{dATP} \xrightarrow{\text{dGTP}} \text{DNA} \tag{5}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
dATP	dATP_dADP_dAMP_dAdo	

Modifier

Table 11: Properties of each modifier.

Id	Name	SBO
dGTP	dGTP_dGDP_dGMP	

Product

Table 12: Properties of each product.

Id	Name	SBO
DNA		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{aadna} \cdot \text{dATP}^{\text{fdnap9}} \cdot \text{dGTP}^{\text{fdnap10}} \tag{6}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
aadna			3.279		☑
fdnap9			0.420		☑
fdnap10			0.330		☑

5.4 Reaction `adrnr`

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

Reaction equation

$$\text{ATP} \xrightarrow{\text{dGTP, dATP}} \text{dATP} \tag{7}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
ATP	ATP_ADP_AMP_Ado	

Modifiers

Table 15: Properties of each modifier.

Id	Name	SBO
dGTP	dGTP_dGDP_dGMP	
dATP	dATP_dADP_dAMP_dAdo	

Product

Table 16: Properties of each product.

Id	Name	SBO
dATP	dATP_dADP_dAMP_dAdo	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{aadrnr} \cdot \text{ATP}^{\text{fadrnr4}} \cdot \text{dATP}^{\text{fadrnr9}} \cdot \text{dGTP}^{\text{fadrnr10}} \tag{8}$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
aadrnr			0.060		☑
fadrnr4			0.100		☑
fadrnr9			-0.300		☑
fadrnr10			0.870		☑

5.5 Reaction ampd

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

Reaction equation

$$\text{ATP} \xrightarrow{\text{GTP, Pi}} \text{IMP} \tag{9}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
ATP	ATP_ADP_AMP_Ado	

Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
GTP	GTP_GDP_GMP	
Pi	phosphate	

Product

Table 20: Properties of each product.

Id	Name	SBO
IMP	inosine monophosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{aampd} \cdot \text{ATP}^{\text{fampd4}} \cdot \text{GTP}^{\text{fampd8}} \cdot \text{Pi}^{\text{fampd18}} \tag{10}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
aampd			0.027		☑
fampd4			0.800		☑
fampd8			−0.030		☑
fampd18			−0.100		☑

5.6 Reaction `aprt`

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

Reaction equation

$$PRPP + Ade \xrightarrow{ATP} ATP \tag{11}$$

Reactants

Table 22: Properties of each reactant.

Id	Name	SBO
PRPP	phosphoribosylpyrophosphate	
Ade	adenine	

Modifier

Table 23: Properties of each modifier.

Id	Name	SBO
ATP	ATP_ADP_AMP_Ado	

Product

Table 24: Properties of each product.

Id	Name	SBO
ATP	ATP_ADP_AMP_Ado	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = aaprt \cdot PRPP^{faprt1} \cdot ATP^{faprt4} \cdot Ade^{faprt6} \tag{12}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
aaprt			233.80		☑
faprt1			0.50		☑
faprt4			-0.80		☑
faprt6			0.75		☑

5.7 Reaction `arna`

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

Reaction equation

$$ATP \xrightarrow{GTP} RNA \tag{13}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
ATP	ATP_ADP_AMP_Ado	

Modifier

Table 27: Properties of each modifier.

Id	Name	SBO
GTP	GTP_GDP_GMP	

Product

Table 28: Properties of each product.

Id	Name	SBO
RNA		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{aarna} \cdot ATP^{\text{frnap4}} \cdot GTP^{\text{frnap8}} \tag{14}$$

Table 29: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
aarna			614.50		☑
frnap4			0.05		☑
frnap8			0.13		☑

5.8 Reaction `asuc`

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

Reaction equation

$$IMP \xrightarrow{ATP, \; GTP, \; Pi} SAMP \tag{15}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
IMP	inosine monophosphate	

Modifiers

Table 31: Properties of each modifier.

Id	Name	SBO
ATP	ATP_ADP_AMP_Ado	
GTP	GTP_GDP_GMP	
Pi	phosphate	

Product

Table 32: Properties of each product.

Id	Name	SBO
SAMP	adenylosuccinate	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{aasuc} \cdot IMP^{\text{fasuc2}} \cdot ATP^{\text{fasuc4}} \cdot GTP^{\text{fasuc8}} \cdot Pi^{\text{fasuc18}} \tag{16}$$

Table 33: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
aasuc			3.593		☑

Id	Name	SBO	Value	Unit	Constant
fasuc2			0.400		☑
fasuc4			−0.240		☑
fasuc8			0.200		☑
fasuc18			−0.050		☑

5.9 Reaction `asli`

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

Reaction equation

$$\text{SAMP} \xrightarrow{\text{ATP}} \text{ATP} \tag{17}$$

Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
SAMP	adenylosuccinate	

Modifier

Table 35: Properties of each modifier.

Id	Name	SBO
ATP	ATP_ADP_AMP_Ado	

Product

Table 36: Properties of each product.

Id	Name	SBO
ATP	ATP_ADP_AMP_Ado	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{aasli} \cdot \text{SAMP}^{\text{fasli3}} \cdot \text{ATP}^{\text{fasli4}} \tag{18}$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
aasli			66544.00		☑
fasli3			0.99		☑
fasli4			−0.95		☑

5.10 Reaction dada

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

Reaction equation

$$\text{dATP} \longrightarrow \text{HX} \tag{19}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
dATP	dATP_dADP_dAMP_dAdo	

Product

Table 39: Properties of each product.

Id	Name	SBO
HX	dIno_Ino_HX	

Kinetic Law

Derived unit contains undeclared units

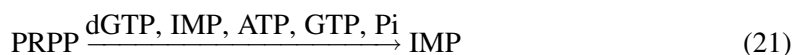$$v_{10} = \text{adada} \cdot \text{dATP}^{\text{fdada9}} \tag{20}$$

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
adada			0.033		☑
fdada9			1.000		☑

5.11 Reaction `den`

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

Reaction equation

$$\text{PRPP} \xrightarrow{\text{dGTP, IMP, ATP, GTP, Pi}} \text{IMP} \tag{21}$$

Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
PRPP	phosphoribosylpyrophosphate	

Modifiers

Table 42: Properties of each modifier.

Id	Name	SBO
dGTP	dGTP_dGDP_dGMP	
IMP	inosine monophosphate	
ATP	ATP_ADP_AMP_Ado	
GTP	GTP_GDP_GMP	
Pi	phosphate	

Product

Table 43: Properties of each product.

Id	Name	SBO
IMP	inosine monophosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \text{aden} \cdot \text{PRPP}^{\text{fden1}} \cdot \text{IMP}^{\text{fden2}} \cdot \text{ATP}^{\text{fden4}} \cdot \text{GTP}^{\text{fden8}} \cdot \text{Pi}^{\text{fden18}} \tag{22}$$

Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
aden			5.273		✓
fden1			2.000		✓
fden2			−0.060		✓
fden4			−0.250		✓
fden8			−0.200		✓
fden18			−0.080		✓

5.12 Reaction dgnuc

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

Reaction equation

$$\text{dGTP} \longrightarrow \text{Gua} \tag{23}$$

Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
dGTP	dGTP_dGDP_dGMP	

Product

Table 46: Properties of each product.

Id	Name	SBO
Gua	guanine	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \text{adgnuc} \cdot \text{dGTP}^{\text{fdgnuc10}} \tag{24}$$

Table 47: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
adgnuc			0.033		☑
fdgnuc10			1.000		☑

5.13 Reaction `dnaa`

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

Reaction equation

$$DNA \longrightarrow dATP \tag{25}$$

Reactant

Table 48: Properties of each reactant.

Id	Name	SBO
DNA		

Product

Table 49: Properties of each product.

Id	Name	SBO
dATP	dATP_dADP_dAMP_dAdo	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \text{adnaa} \cdot \text{DNA}^{\text{fdnan12}} \tag{26}$$

Table 50: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
adnaa			0.002		☑
fdnan12			1.000		☑

5.14 Reaction dnag

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

Reaction equation

$$\text{DNA} \longrightarrow \text{dGTP} \tag{27}$$

Reactant

Table 51: Properties of each reactant.

Id	Name	SBO
DNA		

Product

Table 52: Properties of each product.

Id	Name	SBO
dGTP	dGTP_dGDP_dGMP	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \text{adnag} \cdot \text{DNA}^{\text{fdnan12}} \tag{28}$$

Table 53: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
adnag			0.001		☑
fdnan12			1.000		☑

5.15 Reaction gdna

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

Reaction equation

$$\text{dGTP} \xrightarrow{\text{dATP}} \text{DNA} \tag{29}$$

Reactant

Table 54: Properties of each reactant.

Id	Name	SBO
dGTP	dGTP_dGDP_dGMP	

Modifier

Table 55: Properties of each modifier.

Id	Name	SBO
dATP	dATP_dADP_dAMP_dAdo	

Product

Table 56: Properties of each product.

Id	Name	SBO
DNA		

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{agdna} \cdot \text{dATP}^{\text{fdnap9}} \cdot \text{dGTP}^{\text{fdnap10}} \tag{30}$$

Table 57: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
agdna			2.230		☑
fdnap9			0.420		☑
fdnap10			0.330		☑

5.16 Reaction `gdrnr`

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

Reaction equation

$$GTP \xrightarrow{\text{dATP, dGTP}} dGTP \qquad (31)$$

Reactant

Table 58: Properties of each reactant.

Id	Name	SBO
GTP	GTP_GDP_GMP	

Modifiers

Table 59: Properties of each modifier.

Id	Name	SBO
dATP	dATP_dADP_dAMP_dAdo	
dGTP	dGTP_dGDP_dGMP	

Product

Table 60: Properties of each product.

Id	Name	SBO
dGTP	dGTP_dGDP_dGMP	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \text{agdrnr} \cdot \text{GTP}^{\text{fgdrnr8}} \cdot \text{dATP}^{\text{fgdrnr9}} \cdot \text{dGTP}^{\text{fgdrnr10}} \qquad (32)$$

Table 61: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
agdrnr			0.120		☑
fgdrnr8			0.400		☑
fgdrnr9			−1.200		☑
fgdrnr10			−0.390		☑

5.17 Reaction `gmpr`

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

Reaction equation

$$\text{GTP} \xrightarrow{\text{XMP, ATP, IMP}} \text{IMP} \tag{33}$$

Reactant

Table 62: Properties of each reactant.

Id	Name	SBO
GTP	GTP_GDP_GMP	

Modifiers

Table 63: Properties of each modifier.

Id	Name	SBO
XMP	xanthosine monophosphate	
ATP	ATP_ADP_AMP_Ado	
IMP	inosine monophosphate	

Product

Table 64: Properties of each product.

Id	Name	SBO
IMP	inosine monophosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \text{agmpr} \cdot \text{IMP}^{\text{fgmpr2}} \cdot \text{ATP}^{\text{fgmpr4}} \cdot \text{XMP}^{\text{fgmpr7}} \cdot \text{GTP}^{\text{fgmpr8}} \tag{34}$$

Table 65: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
agmpr			0.301		✓

Id	Name	SBO	Value	Unit	Constant
fgmpr2			-0.150		☑
fgmpr4			-0.070		☑
fgmpr7			-0.760		☑
fgmpr8			0.700		☑

5.18 Reaction `gmps`

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

Reaction equation

$$\text{XMP} \xrightarrow{\text{ATP}} \text{GTP} \tag{35}$$

Reactant

Table 66: Properties of each reactant.

Id	Name	SBO
XMP	xanthosine monophosphate	

Modifier

Table 67: Properties of each modifier.

Id	Name	SBO
ATP	ATP_ADP_AMP_Ado	

Product

Table 68: Properties of each product.

Id	Name	SBO
GTP	GTP_GDP_GMP	

Kinetic Law

Derived unit contains undeclared units

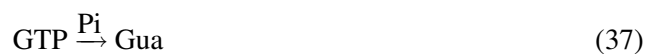$$v_{18} = \text{agmps} \cdot \text{ATP}^{\text{fgmps4}} \cdot \text{XMP}^{\text{fgmps7}} \tag{36}$$

Table 69: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
agmps			0.374		✓
fgmps4			0.120		✓
fgmps7			0.160		✓

5.19 Reaction gnuc

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

Reaction equation

$$\text{GTP} \xrightarrow{\text{Pi}} \text{Gua} \tag{37}$$

Reactant

Table 70: Properties of each reactant.

Id	Name	SBO
GTP	GTP_GDP_GMP	

Modifier

Table 71: Properties of each modifier.

Id	Name	SBO
Pi	phosphate	

Product

Table 72: Properties of each product.

Id	Name	SBO
Gua	guanine	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \text{agnuc} \cdot \text{GTP}^{\text{fgnuc8}} \cdot \text{Pi}^{\text{fgnuc18}} \tag{38}$$

Table 73: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
agnuc			0.251		☑
fgnuc8			0.900		☑
fgnuc18			-0.340		☑

5.20 Reaction `gprt`

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

Reaction equation

$$\text{Gua} + \text{PRPP} \xrightarrow{\text{GTP}} \text{GTP} \tag{39}$$

Reactants

Table 74: Properties of each reactant.

Id	Name	SBO
Gua	guanine	
PRPP	phosphoribosylpyrophosphate	

Modifier

Table 75: Properties of each modifier.

Id	Name	SBO
GTP	GTP_GDP_GMP	

Product

Table 76: Properties of each product.

Id	Name	SBO
GTP	GTP_GDP_GMP	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \text{agprt} \cdot \text{PRPP}^{\text{fgprt1}} \cdot \text{GTP}^{\text{fgprt8}} \cdot \text{Gua}^{\text{fgprt15}} \tag{40}$$

Table 77: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
agprt			361.69		☑
fgprt1			1.20		☑
fgprt8			-1.20		☑
fgprt15			0.42		☑

5.21 Reaction `grna`

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

Reaction equation

$$\text{GTP} \xrightarrow{\text{ATP}} \text{RNA} \tag{41}$$

Reactant

Table 78: Properties of each reactant.

Id	Name	SBO
GTP	GTP_GDP_GMP	

Modifier

Table 79: Properties of each modifier.

Id	Name	SBO
ATP	ATP_ADP_AMP_Ado	

Product

Table 80: Properties of each product.

Id	Name	SBO
RNA		

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \text{agrna} \cdot \text{ATP}^{\text{frnap4}} \cdot \text{GTP}^{\text{frnap8}} \tag{42}$$

Table 81: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
agrna			409.60		☑
frnap4			0.05		☑
frnap8			0.13		☑

5.22 Reaction gua

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

Reaction equation

$$\text{Gua} \longrightarrow \text{Xa} \tag{43}$$

Reactant

Table 82: Properties of each reactant.

Id	Name	SBO
Gua	guanine	

Product

Table 83: Properties of each product.

Id	Name	SBO
Xa	xanthine	

Kinetic Law

Derived unit contains undeclared units

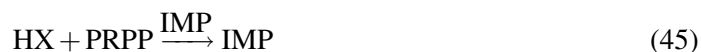$$v_{22} = \text{agua} \cdot \text{Gua}^{\text{fgua15}} \tag{44}$$

Table 84: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
agua			0.492		☑
fgua15			0.500		☑

5.23 Reaction `hprt`

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

Reaction equation

$$HX + PRPP \xrightarrow{IMP} IMP \tag{45}$$

Reactants

Table 85: Properties of each reactant.

Id	Name	SBO
HX	dIno_Ino_HX	
PRPP	phosphoribosylpyrophosphate	

Modifier

Table 86: Properties of each modifier.

Id	Name	SBO
IMP	inosine monophosphate	

Product

Table 87: Properties of each product.

Id	Name	SBO
IMP	inosine monophosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \text{ahprt} \cdot \text{PRPP}^{\text{fhprt1}} \cdot \text{IMP}^{\text{fhprt2}} \cdot \text{HX}^{\text{fhprt13}} \tag{46}$$

Table 88: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ahprt			12.569		✓
fhprt1			1.100		✓
fhprt2			−0.890		✓
fhprt13			0.480		✓

5.24 Reaction `hx`

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

Reaction equation

$$\text{HX} \longrightarrow \emptyset \tag{47}$$

Reactant

Table 89: Properties of each reactant.

Id	Name	SBO
HX	dIno_Ino_HX	

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \text{ahx} \cdot \text{HX}^{\text{fhx13}} \tag{48}$$

Table 90: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ahx			0.004		✓
fhx13			1.120		✓

5.25 Reaction `hxd`

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

Reaction equation

$$HX \longrightarrow Xa \tag{49}$$

Reactant

Table 91: Properties of each reactant.

Id	Name	SBO
HX	dIno_Ino_HX	

Product

Table 92: Properties of each product.

Id	Name	SBO
Xa	xanthine	

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \text{ahxd} \cdot HX^{\text{fhxd13}} \tag{50}$$

Table 93: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ahxd			0.275		☑
fhxd13			0.650		☑

5.26 Reaction `impd`

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

Reaction equation

$$IMP \xrightarrow{\text{GTP, XMP}} XMP \tag{51}$$

Reactant

Table 94: Properties of each reactant.

Id	Name	SBO
IMP	inosine monophosphate	

Modifiers

Table 95: Properties of each modifier.

Id	Name	SBO
GTP	GTP_GDP_GMP	
XMP	xanthosine monophosphate	

Product

Table 96: Properties of each product.

Id	Name	SBO
XMP	xanthosine monophosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = \text{aimpd} \cdot \text{IMP}^{\text{fimpd2}} \cdot \text{XMP}^{\text{fimpd7}} \cdot \text{GTP}^{\text{fimpd8}} \tag{52}$$

Table 97: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
aimpd			1.282		☑
fimpd2			0.150		☑
fimpd7			-0.090		☑
fimpd8			-0.030		☑

5.27 Reaction `inuc`

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

Reaction equation

$$\mathrm{IMP} \xrightarrow{\mathrm{Pi}} \mathrm{HX} \tag{53}$$

Reactant

Table 98: Properties of each reactant.

Id	Name	SBO
IMP	inosine monophosphate	

Modifier

Table 99: Properties of each modifier.

Id	Name	SBO
Pi	phosphate	

Product

Table 100: Properties of each product.

Id	Name	SBO
HX	dIno_Ino_HX	

Kinetic Law

Derived unit contains undeclared units

$$v_{27} = \mathrm{ainuc} \cdot \mathrm{IMP}^{\mathrm{finuc2}} \cdot \mathrm{Pi}^{\mathrm{finuc18}} \tag{54}$$

Table 101: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ainuc			0.914		✓
finuc2			0.800		✓
finuc18			-0.360		✓

5.28 Reaction `mat`

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

Reaction equation

$$\text{ATP} \xrightarrow{\text{SAM}} \text{SAM} \tag{55}$$

Reactant

Table 102: Properties of each reactant.

Id	Name	SBO
ATP	ATP_ADP_AMP_Ado	

Modifier

Table 103: Properties of each modifier.

Id	Name	SBO
SAM	s-adenosyl-L-methionine	

Product

Table 104: Properties of each product.

Id	Name	SBO
SAM	s-adenosyl-L-methionine	

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \text{amat} \cdot \text{ATP}^{\text{fmat4}} \cdot \text{SAM}^{\text{fmat5}} \tag{56}$$

Table 105: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
amat			7.207		☑
fmat4			0.200		☑
fmat5			-0.600		☑

5.29 Reaction `polyam`

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

Reaction equation

$$\text{SAM} \longrightarrow \text{Ade} \tag{57}$$

Reactant

Table 106: Properties of each reactant.

Id	Name	SBO
SAM	s-adenosyl-L-methionine	

Product

Table 107: Properties of each product.

Id	Name	SBO
Ade	adenine	

Kinetic Law

Derived unit contains undeclared units

$$v_{29} = \text{apolyam} \cdot \text{SAM}^{\text{fpolyam5}} \tag{58}$$

Table 108: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
apolyam			0.29		☑
fpolyam5			0.90		☑

5.30 Reaction `prpps`

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

Reaction equation

$$\text{R5P} \xrightarrow{\text{ATP, GTP, Pi, PRPP}} \text{PRPP} \tag{59}$$

Reactant

Table 109: Properties of each reactant.

Id	Name	SBO
R5P	ribose-5-phosphate	

Modifiers

Table 110: Properties of each modifier.

Id	Name	SBO
ATP	ATP_ADP_AMP_Ado	
GTP	GTP_GDP_GMP	
Pi	phosphate	
PRPP	phosphoribosylpyrophosphate	

Product

Table 111: Properties of each product.

Id	Name	SBO
PRPP	phosphoribosylpyrophosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{30} = \text{aprpps} \cdot \text{PRPP}^{\text{fprpps1}} \cdot \text{ATP}^{\text{fprpps4}} \cdot \text{GTP}^{\text{fprpps8}} \cdot \text{R5P}^{\text{fprpps17}} \cdot \text{Pi}^{\text{fprpps18}} \qquad (60)$$

Table 112: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
aprpps			0.90		✓
fprpps1			−0.03		✓
fprpps4			−0.45		✓
fprpps8			−0.04		✓
fprpps17			0.65		✓
fprpps18			0.70		✓

5.31 Reaction pyr

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

Reaction equation

$$PRPP \longrightarrow \emptyset \qquad (61)$$

Reactant

Table 113: Properties of each reactant.

Id	Name	SBO
PRPP	phosphoribosylpyrophosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{31} = \text{apyr} \cdot \text{PRPP}^{\text{fpyr1}} \qquad (62)$$

Table 114: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
apyr			1.295		☑
fpyr1			1.270		☑

5.32 Reaction rnaa

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

Reaction equation

$$RNA \longrightarrow ATP \qquad (63)$$

Reactant

Table 115: Properties of each reactant.

Id	Name	SBO
RNA		

Product

Table 116: Properties of each product.

Id	Name	SBO
ATP	ATP_ADP_AMP_Ado	

Kinetic Law

Derived unit contains undeclared units

$$v_{32} = \text{arnaa} \cdot \text{RNA}^{\text{frnan11}} \tag{64}$$

Table 117: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
arnaa			0.069		☑
frnan11			1.000		☑

5.33 Reaction rnag

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

Reaction equation

$$\text{RNA} \longrightarrow \text{GTP} \tag{65}$$

Reactant

Table 118: Properties of each reactant.

Id	Name	SBO
RNA		

Product

Table 119: Properties of each product.

Id	Name	SBO
GTP	GTP_GDP_GMP	

Kinetic Law

Derived unit contains undeclared units

$$v_{33} = \text{arnag} \cdot \text{RNA}^{\text{frnan11}} \qquad (66)$$

Table 120: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
arnag			0.046		☑
frnan11			1.000		☑

5.34 Reaction `trans`

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

Reaction equation

$$\text{SAM} \longrightarrow \text{ATP} \qquad (67)$$
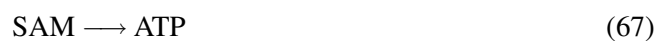
Reactant

Table 121: Properties of each reactant.

Id	Name	SBO
SAM	s-adenosyl-L-methionine	

Product

Table 122: Properties of each product.

Id	Name	SBO
ATP	ATP_ADP_AMP_Ado	

Kinetic Law

Derived unit contains undeclared units

$$v_{34} = \text{atrans} \cdot \text{SAM}^{\text{ftrans5}} \qquad (68)$$

Table 123: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
atrans			8.854		☑
ftrans5			0.330		☑

5.35 Reaction `ua`

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

Reaction equation

$$UA \longrightarrow \emptyset \tag{69}$$

Reactant

Table 124: Properties of each reactant.

Id	Name	SBO
UA	uric acid	

Kinetic Law

Derived unit contains undeclared units

$$v_{35} = \text{aua} \cdot \text{UA}^{\text{fua16}} \tag{70}$$

Table 125: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
aua			$8.744 \cdot 10^{-5}$		☑
fua16			2.210		☑

5.36 Reaction `x`

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

Reaction equation

$$Xa \longrightarrow \emptyset \tag{71}$$
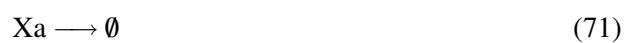
Reactant

Table 126: Properties of each reactant.

Id	Name	SBO
Xa	xanthine	

Kinetic Law

Derived unit contains undeclared units

$$v_{36} = \mathrm{ax} \cdot \mathrm{Xa}^{\mathrm{fx14}} \tag{72}$$

Table 127: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ax			0.001		☑
fx14			2.000		☑

5.37 Reaction xd

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

Reaction equation

$$\mathrm{Xa} \longrightarrow \mathrm{UA} \tag{73}$$

Reactant

Table 128: Properties of each reactant.

Id	Name	SBO
Xa	xanthine	

Product

Table 129: Properties of each product.

Id	Name	SBO
UA	uric acid	

Kinetic Law

Derived unit contains undeclared units

$$v_{37} = \text{axd} \cdot \text{Xa}^{\text{fxd14}} \tag{74}$$

Table 130: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
axd			0.949		☑
fxd14			0.550		☑

6 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.

6.1 Species PRPP

Name phosphoribosylpyrophosphate

Initial amount 5.01742 µmol

This species takes part in seven reactions (as a reactant in aprt, den, gprt, hprt, pyr and as a product in prpps and as a modifier in prpps).

$$\frac{\text{d}}{\text{d}t}\text{PRPP} = v_{30} - v_6 - v_{11} - v_{20} - v_{23} - v_{31} \tag{75}$$

6.2 Species IMP

Name inosine monophosphate

Initial amount 98.2634 µmol

This species takes part in ten reactions (as a reactant in `asuc`, `impd`, `inuc` and as a product in `ampd`, `den`, `gmpr`, `hprt` and as a modifier in `den`, `gmpr`, `hprt`).

$$\frac{d}{dt}\text{IMP} = v_5 + v_{11} + v_{17} + v_{23} - v_8 - v_{26} - v_{27} \tag{76}$$

6.3 Species `SAMP`

Name adenylosuccinate

Initial amount 0.198189 µmol

This species takes part in two reactions (as a reactant in `asli` and as a product in `asuc`).

$$\frac{d}{dt}\text{SAMP} = v_8 - v_9 \tag{77}$$

6.4 Species `ATP`

Name ATP_ADP_AMP_Ado

Initial amount 2475.35 µmol

This species takes part in 17 reactions (as a reactant in `ada`, `adrnr`, `ampd`, `arna`, `mat` and as a product in `aprt`, `asli`, `rnaa`, `trans` and as a modifier in `aprt`, `asuc`, `asli`, `den`, `gmpr`, `gmps`, `grna`, `prpps`).

$$\frac{d}{dt}\text{ATP} = v_6 + v_9 + v_{32} + v_{34} - v_1 - v_4 - v_5 - v_7 - v_{28} \tag{78}$$

6.5 Species `SAM`

Name s-adenosyl-L-methionine

Initial amount 3.99187 µmol

This species takes part in four reactions (as a reactant in `polyam`, `trans` and as a product in `mat` and as a modifier in `mat`).

$$\frac{d}{dt}\text{SAM} = v_{28} - v_{29} - v_{34} \tag{79}$$

6.6 Species `Ade`

Name adenine

Initial amount 0.98473 µmol

This species takes part in three reactions (as a reactant in `ade`, `aprt` and as a product in `polyam`).

$$\frac{d}{dt}\text{Ade} = v_{29} - v_2 - v_6 \tag{80}$$

6.7 Species `XMP`

Name xanthosine monophosphate

Initial amount 24.793 μmol

This species takes part in four reactions (as a reactant in `gmps` and as a product in `impd` and as a modifier in `gmpr`, `impd`).

$$\frac{d}{dt}\text{XMP} = v_{26} - v_{18} \tag{81}$$

6.8 Species `GTP`

Name GTP_GDP_GMP

Initial amount 410.223 μmol

This species takes part in 14 reactions (as a reactant in `gdrnr`, `gmpr`, `gnuc`, `grna` and as a product in `gmps`, `gprt`, `rnag` and as a modifier in `ampd`, `arna`, `asuc`, `den`, `gprt`, `impd`, `prpps`).

$$\frac{d}{dt}\text{GTP} = v_{18} + v_{20} + v_{33} - v_{16} - v_{17} - v_{19} - v_{21} \tag{82}$$

6.9 Species `dATP`

Name dATP_dADP_dAMP_dAdo

Initial amount 6.01413 μmol

This species takes part in seven reactions (as a reactant in `adna`, `dada` and as a product in `adrnr`, `dnaa` and as a modifier in `adrnr`, `gdna`, `gdrnr`).

$$\frac{d}{dt}\text{dATP} = v_4 + v_{13} - v_3 - v_{10} \tag{83}$$

6.10 Species `dGTP`

Name dGTP_dGDP_dGMP

Initial amount 3.02581 μmol

This species takes part in eight reactions (as a reactant in `dgnuc`, `gdna` and as a product in `dnag`, `gdrnr` and as a modifier in `adna`, `adrnr`, `den`, `gdrnr`).

$$\frac{d}{dt}\text{dGTP} = v_{14} + v_{16} - v_{12} - v_{15} \tag{84}$$

6.11 Species `RNA`

Initial amount 28680.5 μmol

This species takes part in four reactions (as a reactant in `rnaa`, `rnag` and as a product in `arna`, `grna`).

$$\frac{d}{dt}RNA = v_7 + v_{21} - v_{32} - v_{33} \tag{85}$$

6.12 Species `DNA`

Initial amount 5179.34 μmol

This species takes part in four reactions (as a reactant in `dnaa`, `dnag` and as a product in `adna`, `gdna`).

$$\frac{d}{dt}DNA = v_3 + v_{15} - v_{13} - v_{14} \tag{86}$$

6.13 Species `HX`

Name dIno_Ino_HX

Initial amount 9.51785 μmol

This species takes part in six reactions (as a reactant in `hprt`, `hx`, `hxd` and as a product in `ada`, `dada`, `inuc`).

$$\frac{d}{dt}HX = v_1 + v_{10} + v_{27} - v_{23} - v_{24} - v_{25} \tag{87}$$

6.14 Species `Xa`

Name xanthine

Initial amount 5.05941 μmol

This species takes part in four reactions (as a reactant in `x`, `xd` and as a product in `gua`, `hxd`).

$$\frac{d}{dt}Xa = v_{22} + v_{25} - v_{36} - v_{37} \tag{88}$$

6.15 Species `Gua`

Name guanine

Initial amount 5.50638 μmol

This species takes part in four reactions (as a reactant in `gprt`, `gua` and as a product in `dgnuc`, `gnuc`).

$$\frac{d}{dt}Gua = v_{12} + v_{19} - v_{20} - v_{22} \tag{89}$$

6.16 Species UA

Name uric acid

Initial amount 100.293 μmol

This species takes part in two reactions (as a reactant in `ua` and as a product in `xd`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{UA} = v_{37} - v_{35} \tag{90}$$

6.17 Species R5P

Name ribose-5-phosphate

Initial amount 18 μmol

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R5P} = 0 \tag{91}$$

6.18 Species Pi

Name phosphate

Initial amount 1400 μmol

This species takes part in six reactions (as a modifier in `ampd`, `asuc`, `den`, `gnuc`, `inuc`, `prpps`), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pi} = 0 \tag{92}$$