

SBML Model Report

Model name: “Hermansen2015 - denovo biosynthesis of pyrimidines in yeast”



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: Brian Mannakee¹ and Ryan Gutenkunst² at December tenth 2015 at 1:40 p.m. and last time modified at December tenth 2015 at 1:40 p.m. Table 1 gives an overview of the quantities of all components of this model.

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

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	9
events	0	constraints	0
reactions	20	function definitions	20
global parameters	30	unit definitions	2
rules	0	initial assignments	0

Model Notes

Hermansen2015 - denovo biosynthesis of pyrimidines in yeast

This model is described in the article:[Characterizing selective pressures on the pathway for de novo biosynthesis of pyrimidines in yeast](#). Hermansen RA , Mannakee BK , Knecht W , Liberles DA , Gutenkunst RNBMC Evolutionary Biology. 2015, 15:232

¹University of Arizona, mannakee@email.arizona.edu

²University of Arizona, rgutenk@email.arizona.edu

Abstract:

Selection on proteins is typically measured with the assumption that each protein acts independently. However, selection more likely acts at higher levels of biological organization, requiring an integrative view of protein function. Here, we built a kinetic model for de novo pyrimidine biosynthesis in the yeast *Saccharomyces cerevisiae* to relate pathway function to selective pressures on individual protein-encoding genes. Gene families across yeast were constructed for each member of the pathway and the ratio of nonsynonymous to synonymous nucleotide substitution rates (dN/dS) was estimated for each enzyme from *S. cerevisiae* and closely related species. We found a positive relationship between the influence that each enzyme has on pathway function and its selective constraint. We expect this trend to be locally present for enzymes that have pathway control, but over longer evolutionary timescales we expect that mutation-selection balance may change the enzymes that have pathway control.

This model is hosted on [BioModels Database](#) and identified by: [MODEL1512160000](#).

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

To the extent possible under law, all copyright and related or neighbouring rights to this encoded model have been dedicated to the public domain worldwide. Please refer to [CC0 Public Domain Dedication](#) for more information.

2 Unit Definitions

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

2.1 Unit `time`

Name `time`

Definition 3600 s

2.2 Unit `substance`

Name `substance`

Definition mmol

2.3 Unit `volume`

Notes Litre is the predefined SBML unit for volume.

Definition 1

2.4 Unit `area`

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

Definition m^2

2.5 Unit `length`

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

Definition m

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

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

3.1 Compartment `compartment`

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

Name `compartment`

4 Species

This model contains nine species. 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 Condi- tion
cp	cp	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square
ca	ca	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square
dho	dho	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square
oro	oro	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square
omp	omp	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square
ump	ump	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square
udp	udp	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square
utp	utp	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square
ctp	ctp	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square

5 Parameters

This model contains 30 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vmax1	vmax1		3.616		✓
bc	[bc]		1.523		✓
glu	[glu]		0.546		✓
K_utp	K_utp		1.414		✓
K_q	K_q		0.058		✓
K_bc	K_bc		2.372		✓
vmax2	vmax2		2.446		✓
asp	[asp]		0.097		✓
atp	[atp]		0.151		✓
K_atp	K_atp		1.289		✓
K_m2	K_m2		2.005		✓
vmax3	vmax3		28.661		✓
K_m3	K_m3		1.272		✓
vmax4	vmax4		91.780		✓
K_m4	K_m4		0.016		✓
vmax5	vmax5		5227.497		✓
K_m5	K_m5		0.020		✓
prpp	[prpp]		0.182		✓
vmax6	vmax6		34.972		✓
K_m6	K_m6		20.341		✓
vmax10	vmax10		6.555		✓
K_m10	K_m10		0.027		✓
vmax7	vmax7		5.831		✓
K_m7	K_m7		0.166		✓
g_pyr	g_pyr		0.198		✓
K_Mp	K_Mp		5.487		✓
vmax8	vmax8		0.163		✓
K_m8	K_m8		0.004		✓
K_asp	K_asp		0.168		✓
d	d		0.100		✓

6 Function definitions

This is an overview of 20 function definitions.

6.1 Function definition `Function_for_r2`

Name Function for r2

Arguments `K_asp`, `K_m2`, `K_utp`, `asp`, `vol (compartment)`, `[cp]`, `[utp]`, `vmax2`

Mathematical Expression

$$\frac{\frac{vmax2 \cdot [cp] \cdot asp}{\left(1 + \frac{[utp]}{K_{utp}}\right) \cdot (K_{m2} + [cp]) \cdot (K_{asp} + asp)}}{vol (compartment)} \quad (1)$$

6.2 Function definition `Function_for_r1`

Name Function for r1

Arguments `K_atp`, `K_bc`, `K_q`, `K_utp`, `atp`, `bc`, `vol (compartment)`, `glu`, `[utp]`, `vmax1`

Mathematical Expression

$$\frac{\frac{vmax1 \cdot bc \cdot glu \cdot atp}{\left(1 + \frac{[utp]}{K_{utp}}\right) \cdot (K_{atp} + atp) \cdot (K_{bc} + bc) \cdot (K_q + glu)}}{vol (compartment)} \quad (2)$$

6.3 Function definition `Function_for_r3`

Name Function for r3

Arguments `K_m3`, `[ca]`, `vol (compartment)`, `vmax3`

Mathematical Expression

$$\frac{\frac{vmax3 \cdot [ca]}{K_{m3} + [ca]}}{vol (compartment)} \quad (3)$$

6.4 Function definition `Function_for_r4`

Name Function for r4

Arguments `K_m4`, `vol (compartment)`, `[dho]`, `vmax4`

Mathematical Expression

$$\frac{\frac{vmax4 \cdot [dho]}{K_{m4} + [dho]}}{vol (compartment)} \quad (4)$$

6.5 Function definition [Function_for_r5](#)

Name Function for r5

Arguments K_m5, vol (compartment), [oro], prpp, vmax5

Mathematical Expression

$$\frac{\frac{vmax5 \cdot [oro] \cdot prpp}{K_m5 + [oro] \cdot prpp}}{vol (compartment)} \quad (5)$$

6.6 Function definition [Function_for_r6](#)

Name Function for r6

Arguments K_m6, vol (compartment), [omp], vmax6

Mathematical Expression

$$\frac{\frac{vmax6 \cdot [omp]}{K_m6 + [omp]}}{vol (compartment)} \quad (6)$$

6.7 Function definition [Function_for_r10](#)

Name Function for r10

Arguments K_m10, vol (compartment), [ump], vmax10

Mathematical Expression

$$\frac{\frac{vmax10 \cdot [ump]}{K_m10 + [ump]}}{vol (compartment)} \quad (7)$$

6.8 Function definition [Function_for_r7](#)

Name Function for r7

Arguments K_m7, vol (compartment), [udp], vmax7

Mathematical Expression

$$\frac{\frac{vmax7 \cdot [udp]}{K_m7 + [udp]}}{vol (compartment)} \quad (8)$$

6.9 Function definition [Function_for_utp_degradation](#)

Name Function for utp_degradation

Arguments K_Mp, vol (compartment), g_pyr, [utp]

Mathematical Expression

$$\frac{\frac{g_pyr \cdot [utp]}{K_Mp + [utp]}}{vol (compartment)} \quad (9)$$

6.10 Function definition [Function_for_r8](#)

Name Function for r8

Arguments K_m8, vol (compartment), [utp], vmax8

Mathematical Expression

$$\frac{\frac{vmax8 \cdot [utp]}{K_m8 + [utp]}}{vol (compartment)} \quad (10)$$

6.11 Function definition [Function_for_ctp_degradation](#)

Name Function for ctp_degradation

Arguments K_Mp, vol (compartment), [ctp], g_pyr

Mathematical Expression

$$\frac{\frac{g_pyr \cdot [ctp]}{K_Mp + [ctp]}}{vol (compartment)} \quad (11)$$

6.12 Function definition [Function_for_cp_dilution](#)

Name Function for cp_dilution

Arguments vol (compartment), [cp], d

Mathematical Expression

$$\frac{d \cdot [cp]}{vol (compartment)} \quad (12)$$

6.13 Function definition [Function_for_ca_dilution](#)

Name Function for ca_dilution

Arguments [ca], vol (compartment), d

Mathematical Expression

$$\frac{d \cdot [\text{ca}]}{\text{vol}(\text{compartment})} \quad (13)$$

6.14 Function definition [Function_for_dho_dilution](#)

Name Function for dho_dilution

Arguments vol (compartment), d, [dho]

Mathematical Expression

$$\frac{d \cdot [\text{dho}]}{\text{vol}(\text{compartment})} \quad (14)$$

6.15 Function definition [Function_for_oro_dilution](#)

Name Function for oro_dilution

Arguments vol (compartment), d, [oro]

Mathematical Expression

$$\frac{d \cdot [\text{oro}]}{\text{vol}(\text{compartment})} \quad (15)$$

6.16 Function definition [Function_for_omp_dilution](#)

Name Function for omp_dilution

Arguments vol (compartment), d, [omp]

Mathematical Expression

$$\frac{d \cdot [\text{omp}]}{\text{vol}(\text{compartment})} \quad (16)$$

6.17 Function definition [Function_for_ump_dilution](#)

Name Function for ump_dilution

Arguments vol (compartment), d, [ump]

Mathematical Expression

$$\frac{d \cdot [\text{ump}]}{\text{vol}(\text{compartment})} \quad (17)$$

6.18 Function definition [Function_for_udp_dilution](#)

Name Function for udp_dilution

Arguments $\text{vol}(\text{compartment})$, d , $[\text{udp}]$

Mathematical Expression

$$\frac{d \cdot [\text{udp}]}{\text{vol}(\text{compartment})} \quad (18)$$

6.19 Function definition [Function_for_utp_dilution](#)

Name Function for utp_dilution

Arguments $\text{vol}(\text{compartment})$, d , $[\text{utp}]$

Mathematical Expression

$$\frac{d \cdot [\text{utp}]}{\text{vol}(\text{compartment})} \quad (19)$$

6.20 Function definition [Function_for_ctp_dilution](#)

Name Function for ctp_dilution

Arguments $\text{vol}(\text{compartment})$, $[\text{ctp}]$, d

Mathematical Expression

$$\frac{d \cdot [\text{ctp}]}{\text{vol}(\text{compartment})} \quad (20)$$

7 Reactions

This model contains 20 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

Nº	Id	Name	Reaction Equation	SBO
1	r1	r1	$\emptyset \xrightleftharpoons{\text{utp, utp}} \text{cp}$	
2	r2	r2	$\text{cp} \xrightleftharpoons{\text{utp, cp, utp}} \text{ca}$	
3	r3	r3	$\text{ca} \xrightleftharpoons{\text{ca}} \text{dho}$	
4	r4	r4	$\text{dho} \xrightleftharpoons{\text{dho}} \text{oro}$	
5	r5	r5	$\text{oro} \xrightleftharpoons{\text{oro}} \text{omp}$	
6	r6	r6	$\text{omp} \xrightleftharpoons{\text{omp}} \text{ump}$	
7	r10	r10	$\text{ump} \xrightleftharpoons{\text{ump}} \text{udp}$	
8	r7	r7	$\text{udp} \xrightleftharpoons{\text{udp}} \text{utp}$	
9	utp_degradation	utp_degradation	$\text{utp} \xrightleftharpoons{\text{utp}} \emptyset$	
10	r8	r8	$\text{utp} \xrightleftharpoons{\text{utp}} \text{ctp}$	
11	ctp_degradation	ctp_degradation	$\text{ctp} \xrightleftharpoons{\text{ctp}} \emptyset$	
12	cp_dilution	cp_dilution	$\text{cp} \xrightleftharpoons{\text{cp}} \emptyset$	
13	ca_dilution	ca_dilution	$\text{ca} \xrightleftharpoons{\text{ca}} \emptyset$	
14	dho_dilution	dho_dilution	$\text{dho} \xrightleftharpoons{\text{dho}} \emptyset$	
15	oro_dilution	oro_dilution	$\text{oro} \xrightleftharpoons{\text{oro}} \emptyset$	
16	omp_dilution	omp_dilution	$\text{omp} \xrightleftharpoons{\text{omp}} \emptyset$	

Nº	Id	Name	Reaction Equation	SBO
17	ump_dilution	ump_dilution	$\text{ump} \xrightleftharpoons{\text{ump}} \emptyset$	
18	udp_dilution	udp_dilution	$\text{udp} \xrightleftharpoons{\text{udp}} \emptyset$	
19	utp_dilution	utp_dilution	$\text{utp} \xrightleftharpoons{\text{utp}} \emptyset$	
20	ctp_dilution	ctp_dilution	$\text{ctp} \xrightleftharpoons{\text{ctp}} \emptyset$	

7.1 Reaction r1

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

Name r1

Reaction equation



Modifiers

Table 6: Properties of each modifier.

Id	Name	SBO
utp	utp	
utp	utp	

Product

Table 7: Properties of each product.

Id	Name	SBO
cp	cp	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}(\text{compartment}) \cdot \text{Function_for_r1}(\text{K_atp}, \text{K_bc}, \text{K_q}, \text{K_utp}, \text{atp}, \text{bc}, \text{vol}(\text{compartment}), \text{glu}, [\text{utp}], \text{vmax1}) \quad (22)$$

$$\begin{aligned} & \text{Function_for_r1}(\text{K_atp}, \text{K_bc}, \text{K_q}, \text{K_utp}, \text{atp}, \text{bc}, \text{vol}(\text{compartment}), \text{glu}, [\text{utp}], \text{vmax1}) \\ &= \frac{\text{vmax1} \cdot \text{bc} \cdot \text{glu} \cdot \text{atp}}{\left(1 + \frac{[\text{utp}]}{\text{K_utp}}\right) \cdot (\text{K_atp} + \text{atp}) \cdot (\text{K_bc} + \text{bc}) \cdot (\text{K_q} + \text{glu})} \cdot \text{vol}(\text{compartment}) \end{aligned} \quad (23)$$

$$\begin{aligned} & \text{Function_for_r1}(\text{K_atp}, \text{K_bc}, \text{K_q}, \text{K_utp}, \text{atp}, \text{bc}, \text{vol}(\text{compartment}), \text{glu}, [\text{utp}], \text{vmax1}) \\ &= \frac{\text{vmax1} \cdot \text{bc} \cdot \text{glu} \cdot \text{atp}}{\left(1 + \frac{[\text{utp}]}{\text{K_utp}}\right) \cdot (\text{K_atp} + \text{atp}) \cdot (\text{K_bc} + \text{bc}) \cdot (\text{K_q} + \text{glu})} \cdot \text{vol}(\text{compartment}) \end{aligned} \quad (24)$$

7.2 Reaction r_2

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

Name r_2

Reaction equation



Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
cp	cp	

Modifiers

Table 9: Properties of each modifier.

Id	Name	SBO
utp	utp	
cp	cp	
utp	utp	

Product

Table 10: Properties of each product.

Id	Name	SBO
ca	ca	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol}(\text{compartment}) \cdot \text{Function_for_}r_2(K_{\text{asp}}, K_{\text{m2}}, K_{\text{utp}}, \text{asp}, \text{vol}(\text{compartment}), [\text{cp}], [\text{utp}], v_{\text{max2}}) \quad (26)$$

$$\begin{aligned} & \text{Function_for_r2}(\text{K_asp}, \text{K_m2}, \text{K_utp}, \text{asp}, \text{vol}(\text{compartment}), [\text{cp}], [\text{utp}], \text{vmax2}) \\ &= \frac{\text{vmax2} \cdot [\text{cp}] \cdot \text{asp}}{\left(1 + \frac{[\text{utp}]}{\text{K_utp}}\right) \cdot (\text{K_m2} + [\text{cp}]) \cdot (\text{K_asp} + \text{asp})} \cdot \text{vol}(\text{compartment}) \end{aligned} \quad (27)$$

$$\begin{aligned} & \text{Function_for_r2}(\text{K_asp}, \text{K_m2}, \text{K_utp}, \text{asp}, \text{vol}(\text{compartment}), [\text{cp}], [\text{utp}], \text{vmax2}) \\ &= \frac{\text{vmax2} \cdot [\text{cp}] \cdot \text{asp}}{\left(1 + \frac{[\text{utp}]}{\text{K_utp}}\right) \cdot (\text{K_m2} + [\text{cp}]) \cdot (\text{K_asp} + \text{asp})} \cdot \text{vol}(\text{compartment}) \end{aligned} \quad (28)$$

7.3 Reaction r3

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

Name r3

Reaction equation



Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
ca	ca	

Modifier

Table 12: Properties of each modifier.

Id	Name	SBO
ca	ca	

Product

Table 13: Properties of each product.

Id	Name	SBO
dho	dho	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}(\text{compartment}) \cdot \text{Function_for_r3}(\text{K_m3}, [\text{ca}], \text{vol}(\text{compartment}), \text{vmax3}) \quad (30)$$

$$\text{Function_for_r3}(\text{K_m3}, [\text{ca}], \text{vol}(\text{compartment}), \text{vmax3}) = \frac{\frac{\text{vmax3} \cdot [\text{ca}]}{\text{K_m3} + [\text{ca}]}}{\text{vol}(\text{compartment})} \quad (31)$$

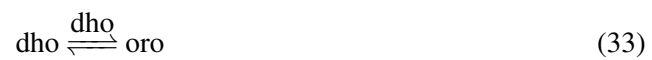
$$\text{Function_for_r3}(\text{K_m3}, [\text{ca}], \text{vol}(\text{compartment}), \text{vmax3}) = \frac{\frac{\text{vmax3} \cdot [\text{ca}]}{\text{K_m3} + [\text{ca}]}}{\text{vol}(\text{compartment})} \quad (32)$$

7.4 Reaction r4

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

Name r4

Reaction equation



Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
dho	dho	

Modifier

Table 15: Properties of each modifier.

Id	Name	SBO
dho	dho	

Product

Table 16: Properties of each product.

Id	Name	SBO
oro	oro	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{vol}(\text{compartment}) \cdot \text{Function_for_r4}(K_{m4}, \text{vol}(\text{compartment}), [\text{dho}], v_{\max4}) \quad (34)$$

$$\text{Function_for_r4}(K_{m4}, \text{vol}(\text{compartment}), [\text{dho}], v_{\max4}) = \frac{\frac{v_{\max4} \cdot [\text{dho}]}{K_{m4} + [\text{dho}]}}{\text{vol}(\text{compartment})} \quad (35)$$

$$\text{Function_for_r4}(K_{m4}, \text{vol}(\text{compartment}), [\text{dho}], v_{\max4}) = \frac{\frac{v_{\max4} \cdot [\text{dho}]}{K_{m4} + [\text{dho}]}}{\text{vol}(\text{compartment})} \quad (36)$$

7.5 Reaction r5

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

Name r5

Reaction equation



Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
oro	oro	

Modifier

Table 18: Properties of each modifier.

Id	Name	SBO
oro	oro	

Product

Table 19: Properties of each product.

Id	Name	SBO
omp	omp	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{vol}(\text{compartment}) \cdot \text{Function_for_r5}(\text{K_m5}, \text{vol}(\text{compartment}), [\text{oro}], \text{prpp}, \text{vmax5}) \quad (38)$$

$$\text{Function_for_r5}(\text{K_m5}, \text{vol}(\text{compartment}), [\text{oro}], \text{prpp}, \text{vmax5}) = \frac{\frac{\text{vmax5} \cdot [\text{oro}] \cdot \text{prpp}}{\text{K_m5} + [\text{oro}] \cdot \text{prpp}}}{\text{vol}(\text{compartment})} \quad (39)$$

$$\text{Function_for_r5}(\text{K_m5}, \text{vol}(\text{compartment}), [\text{oro}], \text{prpp}, \text{vmax5}) = \frac{\frac{\text{vmax5} \cdot [\text{oro}] \cdot \text{prpp}}{\text{K_m5} + [\text{oro}] \cdot \text{prpp}}}{\text{vol}(\text{compartment})} \quad (40)$$

7.6 Reaction r6

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

Name r6

Reaction equation



Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
omp	omp	

Modifier

Table 21: Properties of each modifier.

Id	Name	SBO
omp	omp	

Product

Table 22: Properties of each product.

Id	Name	SBO
ump	ump	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{vol}(\text{compartment}) \cdot \text{Function_for_r6}(K_m6, \text{vol}(\text{compartment}), [\text{omp}], v_{\text{max}6}) \quad (42)$$

$$\text{Function_for_r6}(K_m6, \text{vol}(\text{compartment}), [\text{omp}], v_{\text{max}6}) = \frac{\frac{v_{\text{max}6} \cdot [\text{omp}]}{K_m6 + [\text{omp}]}}{\text{vol}(\text{compartment})} \quad (43)$$

$$\text{Function_for_r6}(K_m6, \text{vol}(\text{compartment}), [\text{omp}], v_{\text{max}6}) = \frac{\frac{v_{\text{max}6} \cdot [\text{omp}]}{K_m6 + [\text{omp}]}}{\text{vol}(\text{compartment})} \quad (44)$$

7.7 Reaction r10

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

Name r10

Reaction equation



Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
ump	ump	

Modifier

Table 24: Properties of each modifier.

Id	Name	SBO
ump	ump	

Product

Table 25: Properties of each product.

Id	Name	SBO
udp	udp	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{vol}(\text{compartment}) \cdot \text{Function_for_r10}(\text{K_m10}, \text{vol}(\text{compartment}), [\text{ump}], \text{vmax10}) \quad (46)$$

$$\text{Function_for_r10}(\text{K_m10}, \text{vol}(\text{compartment}), [\text{ump}], \text{vmax10}) = \frac{\frac{\text{vmax10} \cdot [\text{ump}]}{\text{K_m10} + [\text{ump}]}}{\text{vol}(\text{compartment})} \quad (47)$$

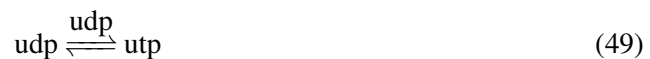
$$\text{Function_for_r10}(\text{K_m10}, \text{vol}(\text{compartment}), [\text{ump}], \text{vmax10}) = \frac{\frac{\text{vmax10} \cdot [\text{ump}]}{\text{K_m10} + [\text{ump}]}}{\text{vol}(\text{compartment})} \quad (48)$$

7.8 Reaction r7

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

Name r7

Reaction equation



Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
udp	udp	

Modifier

Table 27: Properties of each modifier.

Id	Name	SBO
udp	udp	

Product

Table 28: Properties of each product.

Id	Name	SBO
utp	utp	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{vol}(\text{compartment}) \cdot \text{Function_for_r7}(K_{m7}, \text{vol}(\text{compartment}), [\text{udp}], v_{\max 7}) \quad (50)$$

$$\text{Function_for_r7}(K_{m7}, \text{vol}(\text{compartment}), [\text{udp}], v_{\max 7}) = \frac{\frac{v_{\max 7} \cdot [\text{udp}]}{K_{m7} + [\text{udp}]}}{\text{vol}(\text{compartment})} \quad (51)$$

$$\text{Function_for_r7}(K_{m7}, \text{vol}(\text{compartment}), [\text{udp}], v_{\max 7}) = \frac{\frac{v_{\max 7} \cdot [\text{udp}]}{K_{m7} + [\text{udp}]}}{\text{vol}(\text{compartment})} \quad (52)$$

7.9 Reaction `utp_degradation`

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

Name `utp_degradation`

Reaction equation



Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
utp	utp	

Modifier

Table 30: Properties of each modifier.

Id	Name	SBO
utp	utp	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{vol}(\text{compartment}) \cdot \text{Function_for_utp_degradation}(\text{K_Mp}, \text{vol}(\text{compartment}), \text{g_pyr}, [\text{utp}]) \quad (54)$$

$$\text{Function_for_utp_degradation}(\text{K_Mp}, \text{vol}(\text{compartment}), \text{g_pyr}, [\text{utp}]) = \frac{\frac{\text{g_pyr} \cdot [\text{utp}]}{\text{K_Mp} + [\text{utp}]}}{\text{vol}(\text{compartment})} \quad (55)$$

$$\text{Function_for_utp_degradation}(\text{K_Mp}, \text{vol}(\text{compartment}), \text{g_pyr}, [\text{utp}]) = \frac{\frac{\text{g_pyr} \cdot [\text{utp}]}{\text{K_Mp} + [\text{utp}]}}{\text{vol}(\text{compartment})} \quad (56)$$

7.10 Reaction r8

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

Name r8

Reaction equation



Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
utp	utp	

Modifier

Table 32: Properties of each modifier.

Id	Name	SBO
utp	utp	

Product

Table 33: Properties of each product.

Id	Name	SBO
ctp	ctp	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{vol}(\text{compartment}) \cdot \text{Function_for_r8}(K_{m8}, \text{vol}(\text{compartment}), [\text{utp}], v_{\max 8}) \quad (58)$$

$$\text{Function_for_r8}(K_{m8}, \text{vol}(\text{compartment}), [\text{utp}], v_{\max 8}) = \frac{\frac{v_{\max 8} \cdot [\text{utp}]}{K_{m8} + [\text{utp}]}}{\text{vol}(\text{compartment})} \quad (59)$$

$$\text{Function_for_r8}(K_{m8}, \text{vol}(\text{compartment}), [\text{utp}], v_{\max 8}) = \frac{\frac{v_{\max 8} \cdot [\text{utp}]}{K_{m8} + [\text{utp}]}}{\text{vol}(\text{compartment})} \quad (60)$$

7.11 Reaction `ctp_degradation`

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

Name `ctp_degradation`

Reaction equation



Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
ctp	ctp	

Modifier

Table 35: Properties of each modifier.

Id	Name	SBO
ctp	ctp	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \text{vol}(\text{compartment}) \cdot \text{Function_for_ctp_degradation}(\text{K_Mp}, \text{vol}(\text{compartment}), [\text{ctp}], \text{g_pyr}) \quad (62)$$

$$\text{Function_for_ctp_degradation}(\text{K_Mp}, \text{vol}(\text{compartment}), [\text{ctp}], \text{g_pyr}) = \frac{\frac{\text{g_pyr} \cdot [\text{ctp}]}{\text{K_Mp} + [\text{ctp}]}}{\text{vol}(\text{compartment})} \quad (63)$$

$$\text{Function_for_ctp_degradation}(\text{K_Mp}, \text{vol}(\text{compartment}), [\text{ctp}], \text{g_pyr}) = \frac{\frac{\text{g_pyr} \cdot [\text{ctp}]}{\text{K_Mp} + [\text{ctp}]}}{\text{vol}(\text{compartment})} \quad (64)$$

7.12 Reaction cp_dilution

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

Name cp_dilution

Reaction equation



Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
cp	cp	

Modifier

Table 37: Properties of each modifier.

Id	Name	SBO
cp	cp	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \text{vol}(\text{compartment}) \cdot \text{Function_for_cp_dilution}(\text{vol}(\text{compartment}), [\text{cp}], d) \quad (66)$$

$$\text{Function_for_cp_dilution}(\text{vol}(\text{compartment}), [\text{cp}], d) = \frac{d \cdot [\text{cp}]}{\text{vol}(\text{compartment})} \quad (67)$$

$$\text{Function_for_cp_dilution}(\text{vol}(\text{compartment}), [\text{cp}], d) = \frac{d \cdot [\text{cp}]}{\text{vol}(\text{compartment})} \quad (68)$$

7.13 Reaction `ca_dilution`

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

Name `ca_dilution`

Reaction equation



Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
ca	ca	

Modifier

Table 39: Properties of each modifier.

Id	Name	SBO
ca	ca	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \text{vol}(\text{compartment}) \cdot \text{Function_for_ca_dilution}([ca], \text{vol}(\text{compartment}), d) \quad (70)$$

$$\text{Function_for_ca_dilution}([ca], \text{vol}(\text{compartment}), d) = \frac{d \cdot [ca]}{\text{vol}(\text{compartment})} \quad (71)$$

$$\text{Function_for_ca_dilution}([ca], \text{vol}(\text{compartment}), d) = \frac{d \cdot [ca]}{\text{vol}(\text{compartment})} \quad (72)$$

7.14 Reaction dho_dilution

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

Name dho_dilution

Reaction equation



Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
dho	dho	

Modifier

Table 41: Properties of each modifier.

Id	Name	SBO
dho	dho	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \text{vol}(\text{compartment}) \cdot \text{Function_for_dho_dilution}(\text{vol}(\text{compartment}), d, [\text{dho}]) \quad (74)$$

$$\text{Function_for_dho_dilution}(\text{vol}(\text{compartment}), d, [\text{dho}]) = \frac{d \cdot [\text{dho}]}{\text{vol}(\text{compartment})} \quad (75)$$

$$\text{Function_for_dho_dilution}(\text{vol}(\text{compartment}), d, [\text{dho}]) = \frac{d \cdot [\text{dho}]}{\text{vol}(\text{compartment})} \quad (76)$$

7.15 Reaction oro_dilution

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

Name oro_dilution

Reaction equation



Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
oro	oro	

Modifier

Table 43: Properties of each modifier.

Id	Name	SBO
oro	oro	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{vol}(\text{compartment}) \cdot \text{Function_for_oro_dilution}(\text{vol}(\text{compartment}), d, [\text{oro}]) \quad (78)$$

$$\text{Function_for_oro_dilution}(\text{vol}(\text{compartment}), d, [\text{oro}]) = \frac{d \cdot [\text{oro}]}{\text{vol}(\text{compartment})} \quad (79)$$

$$\text{Function_for_oro_dilution}(\text{vol}(\text{compartment}), d, [\text{oro}]) = \frac{d \cdot [\text{oro}]}{\text{vol}(\text{compartment})} \quad (80)$$

7.16 Reaction omp_dilution

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

Name omp_dilution

Reaction equation



Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
omp	omp	

Modifier

Table 45: Properties of each modifier.

Id	Name	SBO
omp	omp	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \text{vol}(\text{compartment}) \cdot \text{Function_for_omp_dilution}(\text{vol}(\text{compartment}), d, [\text{omp}]) \quad (82)$$

$$\text{Function_for_omp_dilution}(\text{vol}(\text{compartment}), d, [\text{omp}]) = \frac{d \cdot [\text{omp}]}{\text{vol}(\text{compartment})} \quad (83)$$

$$\text{Function_for_omp_dilution}(\text{vol}(\text{compartment}), d, [\text{omp}]) = \frac{d \cdot [\text{omp}]}{\text{vol}(\text{compartment})} \quad (84)$$

7.17 Reaction `ump_dilution`

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

Name `ump_dilution`

Reaction equation



Reactant

Table 46: Properties of each reactant.

Id	Name	SBO
ump	ump	

Modifier

Table 47: Properties of each modifier.

Id	Name	SBO
ump	ump	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \text{vol}(\text{compartment}) \cdot \text{Function_for_ump_dilution}(\text{vol}(\text{compartment}), d, [\text{ump}]) \quad (86)$$

$$\text{Function_for_ump_dilution}(\text{vol}(\text{compartment}), d, [\text{ump}]) = \frac{d \cdot [\text{ump}]}{\text{vol}(\text{compartment})} \quad (87)$$

$$\text{Function_for_ump_dilution}(\text{vol}(\text{compartment}), d, [\text{ump}]) = \frac{d \cdot [\text{ump}]}{\text{vol}(\text{compartment})} \quad (88)$$

7.18 Reaction `udp_dilution`

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

Name `udp_dilution`

Reaction equation



Reactant

Table 48: Properties of each reactant.

Id	Name	SBO
udp	udp	

Modifier

Table 49: Properties of each modifier.

Id	Name	SBO
udp	udp	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \text{vol}(\text{compartment}) \cdot \text{Function_for_udp_dilution}(\text{vol}(\text{compartment}), d, [\text{udp}]) \quad (90)$$

$$\text{Function_for_udp_dilution}(\text{vol}(\text{compartment}), d, [\text{udp}]) = \frac{d \cdot [\text{udp}]}{\text{vol}(\text{compartment})} \quad (91)$$

$$\text{Function_for_udp_dilution}(\text{vol}(\text{compartment}), d, [\text{udp}]) = \frac{d \cdot [\text{udp}]}{\text{vol}(\text{compartment})} \quad (92)$$

7.19 Reaction `utp_dilution`

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

Name `utp_dilution`

Reaction equation



Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
utp	utp	

Modifier

Table 51: Properties of each modifier.

Id	Name	SBO
utp	utp	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \text{vol}(\text{compartment}) \cdot \text{Function_for_utp_dilution}(\text{vol}(\text{compartment}), d, [\text{utp}]) \quad (94)$$

$$\text{Function_for_utp_dilution}(\text{vol}(\text{compartment}), d, [\text{utp}]) = \frac{d \cdot [\text{utp}]}{\text{vol}(\text{compartment})} \quad (95)$$

$$\text{Function_for_utp_dilution}(\text{vol}(\text{compartment}), d, [\text{utp}]) = \frac{d \cdot [\text{utp}]}{\text{vol}(\text{compartment})} \quad (96)$$

7.20 Reaction ctp_dilution

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

Name ctp_dilution

Reaction equation



Reactant

Table 52: Properties of each reactant.

Id	Name	SBO
ctp	ctp	

Modifier

Table 53: Properties of each modifier.

Id	Name	SBO
ctp	ctp	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \text{vol}(\text{compartment}) \cdot \text{Function_for_ctp_dilution}(\text{vol}(\text{compartment}), [\text{ctp}], d) \quad (98)$$

$$\text{Function_for_ctp_dilution}(\text{vol}(\text{compartment}), [\text{ctp}], d) = \frac{d \cdot [\text{ctp}]}{\text{vol}(\text{compartment})} \quad (99)$$

$$\text{Function_for_ctp_dilution}(\text{vol}(\text{compartment}), [\text{ctp}], d) = \frac{d \cdot [\text{ctp}]}{\text{vol}(\text{compartment})} \quad (100)$$

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 cp

Name cp

Initial concentration $3.7 \cdot 10^{-4} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in [r2](#), [cp_dilution](#) and as a product in [r1](#) and as a modifier in [r2](#), [cp_dilution](#)).

$$\frac{d}{dt}cp = v_1 - v_2 - v_{12} \quad (101)$$

8.2 Species [ca](#)

Name [ca](#)

Initial concentration $3.7 \cdot 10^{-4} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in [r3](#), [ca_dilution](#) and as a product in [r2](#) and as a modifier in [r3](#), [ca_dilution](#)).

$$\frac{d}{dt}ca = v_2 - v_3 - v_{13} \quad (102)$$

8.3 Species [dho](#)

Name [dho](#)

Initial concentration $3.7 \cdot 10^{-4} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in [r4](#), [dho_dilution](#) and as a product in [r3](#) and as a modifier in [r4](#), [dho_dilution](#)).

$$\frac{d}{dt}dho = v_3 - v_4 - v_{14} \quad (103)$$

8.4 Species [oro](#)

Name [oro](#)

Initial concentration $3.7 \cdot 10^{-4} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in [r5](#), [oro_dilution](#) and as a product in [r4](#) and as a modifier in [r5](#), [oro_dilution](#)).

$$\frac{d}{dt}oro = v_4 - v_5 - v_{15} \quad (104)$$

8.5 Species [omp](#)

Name [omp](#)

Initial concentration $3.7 \cdot 10^{-4} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in [r6](#), [omp_dilution](#) and as a product in [r5](#) and as a modifier in [r6](#), [omp_dilution](#)).

$$\frac{d}{dt}omp = v_5 - v_6 - v_{16} \quad (105)$$

8.6 Species ump

Name ump

Initial concentration $3.7 \cdot 10^{-4} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in [r10](#), [ump_dilution](#) and as a product in [r6](#) and as a modifier in [r10](#), [ump_dilution](#)).

$$\frac{d}{dt}\text{ump} = v_6 - v_7 - v_{17} \quad (106)$$

8.7 Species udp

Name udp

Initial concentration $0.002886 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in [r7](#), [udp_dilution](#) and as a product in [r10](#) and as a modifier in [r7](#), [udp_dilution](#)).

$$\frac{d}{dt}\text{udp} = v_7 - v_8 - v_{18} \quad (107)$$

8.8 Species utp

Name utp

Initial concentration $0.00666 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in eleven reactions (as a reactant in [utp_degradation](#), [r8](#), [utp_dilution](#) and as a product in [r7](#) and as a modifier in [r1](#), [r1](#), [r2](#), [r2](#), [utp_degradation](#), [r8](#), [utp_dilution](#)).

$$\frac{d}{dt}\text{utp} = v_8 - v_9 - v_{10} - v_{19} \quad (108)$$

8.9 Species ctp

Name ctp

Initial concentration $3.7 \cdot 10^{-4} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in [ctp_degradation](#), [ctp_dilution](#) and as a product in [r8](#) and as a modifier in [ctp_degradation](#), [ctp_dilution](#)).

$$\frac{d}{dt}\text{ctp} = v_{10} - v_{11} - v_{20} \quad (109)$$

SBML²LaTeX was developed by Andreas Dräger^a, Hannes Planatscher^a, Dieudonné M Wouamba^a, Adrian Schröder^a, Michael Hucka^b, Lukas Endler^c, Martin Golebiewski^d and Andreas Zell^a. Please see <http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX> for more information.

^aCenter for Bioinformatics Tübingen (ZBIT), Germany

^bCalifornia Institute of Technology, Beckman Institute BNMC, Pasadena, United States

^cEuropean Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom

^dEML Research gGmbH, Heidelberg, Germany