

SBML Model Report

Model name: “Chassagnole2001_Threonine Synthesis”



May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Jacky L Snoep¹ and Harish Dharuri² at August 29th 2006 at 10:11 a. m. and last time modified at May 16th 2012 at 10:20 a. 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	7	function definitions	0
global parameters	0	unit definitions	7
rules	0	initial assignments	0

Model Notes

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SBML level 2 code generated for the JWS Online project by Jacky Snoep using **PySCeS**
Run this model online at <http://jjj.biochem.sun.ac.za>

To cite JWS Online please refer to: Olivier, B.G. and Snoep, J.L. (2004) **Web-based modelling using JWS Online** , Bioinformatics, 20:2143-2144

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Biomodels Curation: The model reproduces Fig 2f of the paper. The Vmax values for different reactions are obtained by multiplying the specific activities given in Table 3 of the paper with the protein concentration and an assay correction factor that was provided by the authors. The protein concentration is 202 mg/litre. The specific activities that need to be taken into consideration are those given for „variable threonine,, in Table 3. The following are the assay correction factors provided by the authors: vak1=1.49; vak3=1.12; vasd=1.14; vhsd=1.42; vts=1.15; vkh=1.13. The model was successfully tested on MathSBML and Jarnac

2 Unit Definitions

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

2.1 Unit substance

Name millimole

Definition mmol

2.2 Unit time

Name min

Definition 60 s

2.3 Unit mM

Name mM

Definition $\text{mmol} \cdot \text{l}^{-1}$

2.4 Unit mM_per_min

Name mM_per_min

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

2.5 Unit litre_per_mg_per_min

Name litre_per_mg_per_min

Definition $1 \cdot \text{mg}^{-1} \cdot (60 \text{ s})^{-1}$

2.6 Unit millimole_per_mg_per_min

Name millimole_per_mg_per_min

Definition $\text{mmol} \cdot \text{mg}^{-1} \cdot (60 \text{ s})^{-1}$

2.7 Unit mg_per_litre

Name mg_per_litre

Definition $\text{mg} \cdot \text{l}^{-1}$

2.8 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

2.9 Unit area

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

Definition m^2

2.10 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			3	1	litre	<input checked="" type="checkbox"/>	

3.1 **Compartment** compartment

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

4 Species

This model contains eleven species. 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
aspp	Aspartyl phosphate	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square
asa	Aspartate beta-semialdehyde	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square
hs	Homoserine	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square
hsp	O-Phospho-homoserine	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square
phos	Phos	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square
thr	Threonine	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square
asp	Aspartate	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square
nadp	NADP	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square
nadph	NADPH	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square
adp	ADP	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square
atp	ATP	compartment	$\text{mmol} \cdot \text{l}^{-1}$	\square	\square

5 Reactions

This model contains seven 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

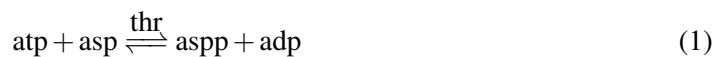
Nº	Id	Name	Reaction Equation	SBO
1	vak	Aspartate Kinase	$\text{atp} + \text{asp} \xrightleftharpoons{\text{thr}} \text{aspp} + \text{adp}$	
2	vasd	Aspartate semialdehyde dehydrogenase	$\text{nadph} + \text{aspp} \rightleftharpoons \text{nadp} + \text{phos} + \text{asa}$	
3	vhdh	Homoserine dehydrogenase	$\text{nadph} + \text{asa} \xrightleftharpoons{\text{asp, thr}} \text{hs} + \text{nadp}$	
4	vt sy	Threonine synthase	$\text{hsp} \rightleftharpoons \text{thr} + \text{phos}$	
5	vhk	Homoserine kinase	$\text{hs} + \text{atp} \xrightleftharpoons{\text{thr}} \text{hsp} + \text{adp}$	
6	vnadph_endo	Endogenous consumption of NADPH	$\text{nadph} \rightleftharpoons \text{nadp}$	
7	vatpase	ATPase	$\text{atp} \rightleftharpoons \text{adp} + \text{phos}$	

5.1 Reaction vak

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

Name Aspartate Kinase

Reaction equation



Reactants

Table 5: Properties of each reactant.

Id	Name	SBO
atp	ATP	
asp	Aspartate	

Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
thr	Threonine	

Products

Table 7: Properties of each product.

Id	Name	SBO
aspp	Aspartyl phosphate	
adp	ADP	

Kinetic Law

Derived unit contains undeclared units

$$\begin{aligned}
v_1 &= \text{vol}(\text{compartment}) \\
&\cdot \left(\frac{\text{vm11} \cdot \left([\text{asp}] \cdot [\text{atp}] - \frac{[\text{aspp}] \cdot [\text{adp}]}{\text{keqak}} \right)}{\left(\frac{k11 \cdot \left(1 + \left(\frac{[\text{thr}]}{k1\text{thr}} \right)^{\text{nak1}} \right)}{1 + \left(\frac{[\text{thr}]}{\alpha \cdot k1\text{thr}} \right)^{\text{nak1}}} + \frac{k11 \cdot [\text{aspp}]}{k1\text{aspp}} + [\text{asp}] \right) \cdot \left(k1\text{atp} \cdot \left(1 + \frac{[\text{adp}]}{k1\text{adp}} \right) + [\text{atp}] \right)} \right. \\
&\quad \left. + \frac{\text{vm13} \cdot \left([\text{asp}] \cdot [\text{atp}] - \frac{[\text{aspp}] \cdot [\text{adp}]}{\text{keqak}} \right)}{\left(1 + \left(\frac{\text{lys}}{k1\text{lys}} \right)^{\text{nak3}} \right) \cdot \left(k13 \cdot \left(1 + \frac{[\text{aspp}]}{k13\text{aspp}} \right) + [\text{asp}] \right) \cdot \left(k13\text{atp} \cdot \left(1 + \frac{[\text{adp}]}{k13\text{adp}} \right) + [\text{atp}] \right)} \right) \quad (2)
\end{aligned}$$

Table 8: Properties of each parameter.

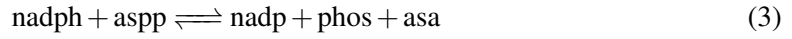
Id	Name	SBO	Value	Unit	Constant
vm11			0.150	$\text{mmol} \cdot \text{l}^{-1} \cdot (60 \text{ s})^{-1}$	✓
keqak			$6.4 \cdot 10^{-4}$	dimensionless	✓
k11			0.970	$\text{mmol} \cdot \text{l}^{-1}$	✓
k1thr			0.167	$\text{mmol} \cdot \text{l}^{-1}$	✓
nak1			4.090	dimensionless	✓
alpha			2.470	dimensionless	✓
k1aspp			0.017	$\text{mmol} \cdot \text{l}^{-1}$	✓
k1atp			0.980	$\text{mmol} \cdot \text{l}^{-1}$	✓
k1adp			0.250	$\text{mmol} \cdot \text{l}^{-1}$	✓
vm13			0.072	$\text{mmol} \cdot \text{l}^{-1} \cdot (60 \text{ s})^{-1}$	✓
lys			0.460	$\text{mmol} \cdot \text{l}^{-1}$	✓
k1lys			0.391	$\text{mmol} \cdot \text{l}^{-1}$	✓
nak3			2.800	dimensionless	✓
k13			0.320	$\text{mmol} \cdot \text{l}^{-1}$	✓
k13aspp			0.017	$\text{mmol} \cdot \text{l}^{-1}$	✓
k13atp			0.220	$\text{mmol} \cdot \text{l}^{-1}$	✓
k13adp			0.250	$\text{mmol} \cdot \text{l}^{-1}$	✓

5.2 Reaction `vasd`

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

Name Aspartate semialdehyde dehydrogenase

Reaction equation



Reactants

Table 9: Properties of each reactant.

Id	Name	SBO
nadph	NADPH	
aspp	Aspartyl phosphate	

Products

Table 10: Properties of each product.

Id	Name	SBO
nadp	NADP	
phos	Phos	
asa	Aspartate beta-semialdehyde	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol}(\text{compartment}) \cdot \frac{\text{vm2f} \cdot \left([\text{aspp}] \cdot [\text{nadph}] - \frac{[\text{asa}] \cdot [\text{nadp}] \cdot [\text{phos}]}{k_{2\text{eq}}} \right)}{\left(k_{2\text{aspp}} \cdot \left(1 + \frac{[\text{asa}]}{k_{2\text{asa}}} \right) \cdot \left(1 + \frac{[\text{phos}]}{k_{2\text{p}}} \right) + [\text{aspp}] \right) \cdot \left(k_{2\text{nadph}} \cdot \left(1 + \frac{[\text{nadp}]}{k_{2\text{nadp}}} \right) + [\text{nadph}] \right)} \quad (4)$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vm2f			0.181	$\text{mmol} \cdot \text{l}^{-1} \cdot (60 \text{ s})^{-1}$	✓
k2eq			56.415	dimensionless	✓
k2aspp			0.022	$\text{mmol} \cdot \text{l}^{-1}$	✓
k2asa			0.110	$\text{mmol} \cdot \text{l}^{-1}$	✓

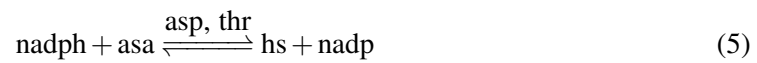
Id	Name	SBO	Value	Unit	Constant
k2p			10.000	mmol · l ⁻¹	<input checked="" type="checkbox"/>
k2nadph			0.029	mmol · l ⁻¹	<input checked="" type="checkbox"/>
k2nadp			0.144	mmol · l ⁻¹	<input checked="" type="checkbox"/>

5.3 Reaction vhdh

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

Name Homoserine dehydrogenase

Reaction equation



Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
nadph	NADPH	
asa	Aspartate beta-semialdehyde	

Modifiers

Table 13: Properties of each modifier.

Id	Name	SBO
asp	Aspartate	
thr	Threonine	

Products

Table 14: Properties of each product.

Id	Name	SBO
hs	Homoserine	
nadp	NADP	

Kinetic Law

Derived unit contains undeclared units

$v_3 = \text{vol}(\text{compartment})$

$$v_3 = \frac{\text{vm3f} \cdot \left([\text{asa}] \cdot [\text{nadph}] - \frac{[\text{hs}] \cdot [\text{nadp}]}{k_{3\text{eq}}} \right)}{\frac{1 + \left(\frac{[\text{thr}]}{k_{3\text{thr}}} \right)^{\text{nhdh1}}}{1 + \left(\frac{[\text{thr}]}{\alpha_{\text{pha3}} \cdot k_{3\text{thr}}} \right)^{\text{nhdh1}}} \cdot \left(k_{3\text{asa}} + [\text{asa}] + \frac{[\text{hs}] \cdot k_{3\text{asa}}}{k_{3\text{hs}}} \right) \cdot \left(k_{3\text{nadph}} \cdot \left(1 + \frac{[\text{nadp}]}{k_{3\text{nadp}}} \right) + [\text{nadph}] \right)}$$

(6)

Table 15: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vm3f			1.001	$\text{mmol} \cdot \text{l}^{-1} \cdot (60 \text{ s})^{-1}$	✓
k3eq			3162.278	dimensionless	✓
k3thr			0.097	$\text{mmol} \cdot \text{l}^{-1}$	✓
nhdh1			1.410	dimensionless	✓
alpha3			3.930	dimensionless	✓
k3asa			0.240	$\text{mmol} \cdot \text{l}^{-1}$	✓
k3hs			3.390	$\text{mmol} \cdot \text{l}^{-1}$	✓
k3nadph			0.037	$\text{mmol} \cdot \text{l}^{-1}$	✓
k3nadp			0.067	$\text{mmol} \cdot \text{l}^{-1}$	✓

5.4 Reaction vtsy

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

Name Threonine synthase

Reaction equation



Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
hsp	O-Phospho-homoserine	

Products

Table 17: Properties of each product.

Id	Name	SBO
thr	Threonine	
phos	Phos	

Kinetic Law

Derived unit $0.0010 \text{ mol} \cdot (60 \text{ s})^{-1}$

$$v_4 = \frac{\text{vol}(\text{compartment}) \cdot \text{vm5} \cdot [\text{hsp}]}{[\text{hsp}] + \text{k5hsp}} \quad (8)$$

Table 18: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vm5			0.043	$\text{mmol} \cdot \text{l}^{-1} \cdot (60 \text{ s})^{-1}$	<input checked="" type="checkbox"/>
k5hsp			0.310	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>

5.5 Reaction [v_{hk}](#)

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

Name Homoserine kinase

Reaction equation



Reactants

Table 19: Properties of each reactant.

Id	Name	SBO
hs	Homoserine	
atp	ATP	

Modifier

Table 20: Properties of each modifier.

Id	Name	SBO
thr	Threonine	

Products

Table 21: Properties of each product.

Id	Name	SBO
hsp	O-Phospho-homoserine	
adp	ADP	

Kinetic Law

Derived unit contains undeclared units

$v_5 = \text{vol}(\text{compartment})$

$$v_5 = \frac{vm4f \cdot [hs] \cdot [atp]}{\left(1 + \frac{lys}{k4lys}\right) \cdot \left([atp] + k4atp \cdot \left(1 + \frac{[hs]}{k4ihs}\right)\right) \cdot \left([hs] + k4hs \cdot \left(1 + \frac{[thr]}{k4thr}\right) \cdot \left(1 + \frac{[atp]}{k4iatp}\right)\right)} \quad (10)$$

Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vm4f			0.100	$\text{mmol} \cdot \text{l}^{-1} \cdot (60 \text{ s})^{-1}$	<input checked="" type="checkbox"/>
lys			0.460	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>
k4lys			9.450	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>
k4atp			0.072	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>
k4ihs			4.700	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>
k4hs			0.110	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>
k4thr			1.090	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>
k4iatp			4.350	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>

5.6 Reaction vnadph_endo

This is a reversible reaction of one reactant forming one product.

Name Endogenous consumption of NADPH

Reaction equation



Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
nadph	NADPH	

Product

Table 24: Properties of each product.

Id	Name	SBO
nadp	NADP	

Kinetic Law

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

$$v_6 = \text{vol}(\text{compartment}) \cdot \text{prot} \cdot \text{knadph} \cdot [\text{nadph}] \quad (12)$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
knadph			$5.4 \cdot 10^{-6}$	$1 \cdot \text{mg}^{-1} \cdot (60 \text{ s})^{-1}$	<input checked="" type="checkbox"/>
prot	Protein		202.000	$\text{mg} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>

5.7 Reaction `vatpase`

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

Name ATPase

Reaction equation



Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
atp	ATP	

Products

Table 27: Properties of each product.

Id	Name	SBO
adp	ADP	
phos	Phos	

Kinetic Law

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

$$v_7 = \text{vol}(\text{compartment}) \cdot \text{prot} \cdot \text{katpase} \quad (14)$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
katpase			$4.1 \cdot 10^{-5}$	$\text{mmol} \cdot \text{mg}^{-1} \cdot (60 \text{ s})^{-1}$	<input checked="" type="checkbox"/>
prot	Protein		202.000	$\text{mg} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>

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.

6.1 Species `aspp`

Name Aspartyl phosphate

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

This species takes part in two reactions (as a reactant in [vasd](#) and as a product in [vak](#)).

$$\frac{d}{dt}\text{aspp} = v_1 - v_2 \quad (15)$$

6.2 Species `asa`

Name Aspartate beta-semialdehyde

Initial concentration 0 mmol · l⁻¹

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

$$\frac{d}{dt}\text{asa} = v_2 - v_3 \quad (16)$$

6.3 Species `hs`

Name Homoserine

Initial concentration 0 mmol · l⁻¹

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

$$\frac{d}{dt}\text{hs} = v_3 - v_5 \quad (17)$$

6.4 Species `hsp`

Name O-Phospho-homoserine

Initial concentration 0 mmol · l⁻¹

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

$$\frac{d}{dt}\text{hsp} = v_5 - v_4 \quad (18)$$

6.5 Species `phos`

Name Phos

Initial concentration 0 mmol · l⁻¹

This species takes part in three reactions (as a product in `vasd`, `vtsty`, `vatpase`).

$$\frac{d}{dt}\text{phos} = v_2 + v_4 + v_7 \quad (19)$$

6.6 Species thr

Name Threonine

Initial concentration $2 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a product in [vtsy](#) and as a modifier in [vak](#), [vhdh](#), [vhk](#)).

$$\frac{d}{dt}\text{thr} = v_4 \quad (20)$$

6.7 Species asp

Name Aspartate

Initial concentration $2 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in [vak](#) and as a modifier in [vhdh](#)).

$$\frac{d}{dt}\text{asp} = -v_1 \quad (21)$$

6.8 Species nadp

Name NADP

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

This species takes part in three reactions (as a product in [vasd](#), [vhdh](#), [vnadph_endo](#)).

$$\frac{d}{dt}\text{nadp} = v_2 + v_3 + v_6 \quad (22)$$

6.9 Species nadph

Name NADPH

Initial concentration $2 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in [vasd](#), [vhdh](#), [vnadph_endo](#)).

$$\frac{d}{dt}\text{nadph} = -v_2 - v_3 - v_6 \quad (23)$$

6.10 Species adp

Name ADP

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

This species takes part in three reactions (as a product in [vak](#), [vhk](#), [vatpase](#)).

$$\frac{d}{dt}\text{adp} = v_1 + v_5 + v_7 \quad (24)$$

6.11 Species atp

Name ATP

Initial concentration 10 mmol · l⁻¹

This species takes part in three reactions (as a reactant in [vak](#), [vhk](#), [vatpase](#)).

$$\frac{d}{dt}\text{atp} = -v_1 - v_5 - v_7 \quad (25)$$

SBML2^{AT}EX 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.

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