SBML Model Report

Model name: "Smallbone2013 - Serine biosynthesis"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah[1] and Kieran Smallbone[2] at March 20th 2012 at no o' clock in the morning. and last time modified at June tenth 2013 at 1:56 p. m. Table 1 shows an overview of the quantities of all components of this model.

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

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	7
events	0	constraints	0
reactions	3	function definitions	0
global parameters	0	unit definitions	3
rules	0	initial assignments	0

Model Notes

Smallbone2013 - Serine biosynthesis

Kinetic modelling of metabolic pathways in application to Serine biosynthesis.

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This model is described in the article:Kinetic Modeling of Metabolic Pathways: Application to Serine BiosynthesisKieran Smallbone, Natalie J. StanfordMethods in Molecular Biology. 2013; 985:113-121

Abstract:

In this chapter, we describe the steps needed to create a kinetic model of a metabolic pathway using kinetic data from both experimental measurements and literature review. Our methodology is presented by using the example of serine biosynthesis in E. coli.

As there are no plots to be reproduced as curation figure, table 6 and 7 that corresponds to steady state concentration of metabolite and steady state fluxes of reactions has been reproduced.

This model is hosted on BioModels Database and identifiedby: BIOMD0000000458 .

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

2 Unit Definitions

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

2.1 Unit `substance`

Name mmol

Definition mmol

2.2 Unit `mM`

Name mM

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

2.3 Unit `per_s`

Name per s

Definition s^{-1}

2.4 Unit `volume`

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

Definition l

2.5 Unit area

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

Definition m^2

2.6 Unit length

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

Definition m

2.7 Unit time

Notes Second is the predefined SBML unit for time.

Definition s

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
cell	cell	0000290	3	1	litre	☑	

3.1 Compartment cell

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

Name cell

SBO:0000290 physical compartment

4 Species

This model contains seven species. The boundary condition of five 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
p3g	3-phosphoglycerate	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
php	phosphohydroxypyruvate	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
pser	phosphoserine	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
ser	serine	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
serA	serA	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
serC	serC	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
serB	serB	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑

5 Reactions

This model contains three 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	PDH	phosphoglycerate dehydrogenase	p3g $\xrightleftharpoons{\text{serA, ser, serA, p3g, php, ser}}$ php	0000176
2	PSA	phosphoserine aminotransferase	php $\xrightleftharpoons{\text{serC, serC, php, pser}}$ pser	0000176
3	PSP	phosphoserine phosphatase	pser $\xrightleftharpoons{\text{serB, serB, pser, ser}}$ ser	0000176

5.1 Reaction PDH

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

Name phosphoglycerate dehydrogenase

SBO:0000176 biochemical reaction

Reaction equation

$$\text{p3g} \xrightleftharpoons{\text{serA, ser, serA, p3g, php, ser}} \text{php} \tag{1}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
p3g	3-phosphoglycerate	

Modifiers

Table 6: Properties of each modifier.

Id	Name	SBO
serA	serA	
ser	serine	
serA	serA	
p3g	3-phosphoglycerate	
php	phosphohydroxypyruvate	
ser	serine	

Product

Table 7: Properties of each product.

Id	Name	SBO
php	phosphohydroxypyruvate	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{\frac{\mathrm{vol(cell)} \cdot [\mathrm{serA}] \cdot \mathrm{kcatA} \cdot \frac{[\mathrm{p3g}]}{\mathrm{KAp3g}}}{1 + \frac{[\mathrm{p3g}]}{\mathrm{KAp3g}} + \frac{[\mathrm{php}]}{\mathrm{KAphp}}}}{1 + \frac{[\mathrm{ser}]}{\mathrm{KiAser}}} \tag{2}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcatA			0.550	s^{-1}	☑
KAp3g			1.200	$mmol \cdot l^{-1}$	☑
KAphp			0.003	$mmol \cdot l^{-1}$	☑
KiAser			0.004	$mmol \cdot l^{-1}$	☑

5.2 Reaction PSA

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

Name phosphoserine aminotransferase

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{php} \xrightleftharpoons{\mathrm{serC,\ serC,\ php,\ pser}} \mathrm{pser} \tag{3}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
php	phosphohydroxypyruvate	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
serC	serC	
serC	serC	
php	phosphohydroxypyruvate	
pser	phosphoserine	

Product

Table 11: Properties of each product.

Id	Name	SBO
pser	phosphoserine	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\mathrm{vol}\,(\mathrm{cell}) \cdot [\mathrm{serC}] \cdot \mathrm{kcatC} \cdot \frac{[\mathrm{php}]}{\mathrm{KCphp}}}{1 + \frac{[\mathrm{php}]}{\mathrm{KCphp}} + \frac{[\mathrm{pser}]}{\mathrm{KCpser}}} \tag{4}$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcatC			1.750	s^{-1}	☑
KCphp			0.002	$mmol \cdot l^{-1}$	☑
KCpser			0.002	$mmol \cdot l^{-1}$	☑

5.3 Reaction PSP

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

Name phosphoserine phosphatase

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{pser} \xrightleftharpoons{\mathrm{serB},\ \mathrm{serB},\ \mathrm{pser},\ \mathrm{ser}} \mathrm{ser} \tag{5}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
pser	phosphoserine	

Modifiers

Table 14: Properties of each modifier.

Id	Name	SBO
serB	serB	
serB	serB	
pser	phosphoserine	
ser	serine	

Product

Table 15: Properties of each product.

Id	Name	SBO
ser	serine	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \frac{\mathrm{vol}\,(\mathrm{cell}) \cdot [\mathrm{serB}] \cdot \mathrm{kcatB} \cdot \frac{[\mathrm{pser}]}{\mathrm{KBpser}}}{1 + \frac{[\mathrm{pser}]}{\mathrm{KBpser}} + \frac{[\mathrm{ser}]}{\mathrm{KBser}}} \tag{6}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kcatB			1.430	s^{-1}	☑
KBpser			0.002	$mmol \cdot l^{-1}$	☑
KBser			0.150	$mmol \cdot l^{-1}$	☑

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 p3g

Name 3-phosphoglycerate

SBO:0000247 simple chemical

Initial concentration $2.36\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{p3g} = 0 \tag{7}$$

6.2 Species php

Name phosphohydroxypyruvate

SBO:0000247 simple chemical

Initial concentration $0.6\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in PSA and as a product in PDH and as a modifier in PDH, PSA).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{php} = v_1 - v_2 \tag{8}$$

6.3 Species pser

Name phosphoserine

SBO:0000247 simple chemical

Initial concentration $0.09\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in PSP and as a product in PSA and as a modifier in PSA, PSP).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{pser} = v_2 - v_3 \tag{9}$$

6.4 Species ser

Name serine

SBO:0000247 simple chemical

Initial concentration $4.9\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ser} = 0 \tag{10}$$

6.5 Species serA

Name serA

SBO:0000252 polypeptide chain

Initial concentration $1.15\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{serA} = 0 \tag{11}$$

6.6 Species serC

Name serC

SBO:0000252 polypeptide chain

Initial concentration $0.1\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{serC} = 0 \tag{12}$$

6.7 Species serB

Name serB

SBO:0000252 polypeptide chain

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{serB} = 0 \tag{13}$$

A Glossary of Systems Biology Ontology Terms

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

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

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

SBO:0000290 physical compartment: Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

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.

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