SBML Model Report

Model name: "Bartholome2007_MDCKII"

SBML2LATEX

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by the following two authors: Kilian Bartholom[1] and Lukas Endler[2] at September 25th 2008 at 4:51 p. m. and last time modified at April eighth 2016 at 3:52 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	3
species types	0	species	7
events	0	constraints	0
reactions	10	function definitions	0
global parameters	12	unit definitions	6
rules	2	initial assignments	0

Model Notes

SBML model exported from PottersWheel on 2007-09-19 15:35:47.

The values for parameters and the inital concentrations of this model where directly provided by the main author:

Parameter values —p0.3—p0.3—p0.3—

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parameter	value	unit
p1	0.0025	1/min
p2	0.0784	1/min
p3	0.0013	1/min
p4	0.0827	1/min
p5	0.0091	1/min
p6	0.000064	1/(nmole*min)
p7	0.0397	1/min
p8	1000	nmole
p9	0.0098	1/(nmole*min)
p10	1.6	1/min
p11	1000	nmole
p12	0.0003	ml/min

The basal chamber volume was taken as 1 ml, the apical as 1.5. As starting values x1 was set to 88 nmole, all other species to 0.

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

2 Unit Definitions

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

2.1 Unit `substance`

Name nmole

Definition nmol

2.2 Unit `volume`

Name ml

Definition ml

2.3 Unit `time`

Name min

Definition $60\,\text{s}$

2.4 Unit `permin`

Name permin

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

2.5 Unit `ml_per_min`

Name ml_per_min

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

2.6 Unit `per_nmole_per_ml`

Name per_nmole_per_ml

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

2.7 Unit `area`

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

Definition m^2

2.8 Unit `length`

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

Definition m

3 Compartments

This model contains three compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
basolat	basolateral extrocellular space	0000290	3	1	litre	☑	
cell	intracellular	0000290	3	1	litre	☑	
apical	apical extracellular space	0000290	3	1.5	ml	☑	

3.1 Compartment `basolat`

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

Name basolateral extrocellular space

SBO:0000290 physical compartment

3.2 Compartment `cell`

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

Name intracellular

SBO:0000290 physical compartment

3.3 Compartment `apical`

This is a three dimensional compartment with a constant size of 1.5 ml.

Name apical extracellular space

SBO:0000290 physical compartment

4 Species

This model contains seven 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 8 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
x1	free basolateral BSP	basolat	nmol	⊟	⊟
x2	basolateral bound BSP	basolat	nmol	⊟	⊟
x3	free intracellular BSP	cell	nmol	⊟	⊟
x4	bound intracellular BSP	cell	nmol	⊟	⊟
x5	apical BSP	apical	nmol	⊟	⊟
BSP_tot	total BSP	apical	nmol	⊟	☑
BSP_cell	intracellular BSP	cell	nmol	⊟	☑

5 Parameters

This model contains twelve global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
p1			0.003	$(60\,\mathrm{s})^{-1}$	☑
p2			0.078	$(60\,\mathrm{s})^{-1}$	☑
p3			0.001	$(60\,\mathrm{s})^{-1}$	☑
p4			0.083	$(60\,\mathrm{s})^{-1}$	☑
p5			0.009	$(60\,\mathrm{s})^{-1}$	☑
p6			$6.4\cdot 10^{-5}$	$\mathrm{nmol}^{-1}\cdot(60\,\mathrm{s})^{-1}$	☑
p7			0.040	$(60\,\mathrm{s})^{-1}$	☑
p8			1000.000	nmol	☑
p9			0.010	$\mathrm{nmol}^{-1}\cdot(60\,\mathrm{s})^{-1}$	☑
p10			1.600	$(60\,\mathrm{s})^{-1}$	☑
p11			1000.000	nmol	☑
p12			$3\cdot 10^{-4}$	$\mathrm{ml}\cdot(60\,\mathrm{s})^{-1}$	☑

6 Rules

This is an overview of two rules.

6.1 Rule `BSP_tot`

Rule `BSP_tot` is an assignment rule for species `BSP_tot`:

$$[\mathrm{BSP\_tot}] = \mathrm{x1} + \mathrm{x2} + \mathrm{x3} + \mathrm{x4} + \mathrm{x5} \tag{1}$$

Derived unit nmol

6.2 Rule `BSP_cell`

Rule `BSP_cell` is an assignment rule for species `BSP_cell`:

$$[\mathrm{BSP\_cell}] = \mathrm{x3} + \mathrm{x4} \tag{2}$$

Derived unit nmol

Produced by SBML2LATEX

7 Reactions

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

Table 5: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	OATP1B3	OATP1B3 mediated import	$x1 \longrightarrow x3$	0000185
2	ABCC2	ABCC2 mediated export	$x3 \longrightarrow x5$	0000185
3	endo_in_bl	endogenous basolateral import	$x1 \longrightarrow x3$	0000185
4	endo_ex_bl	endogenous basolateral export	$x3 \longrightarrow x1$	0000185
5	endo_ex_ap	endogenous apical export	$x3 \longrightarrow x5$	0000185
6	bl_BSP_binding	basolateral BSP binding	$x1 \longrightarrow x2$	0000177
7	bl_BSP_dissoc	basolateral BSP dissoc	$x2 \longrightarrow x1$	0000180
8	cellular_BSP-_binding	cellular BSP binding	$x3 \longrightarrow x4$	0000177
9	cellular_BSP-_dissoc	cellular BSP dissoc	$x4 \longrightarrow x3$	0000180
10	paracell_transp	paracellular transport	$x1 \rightleftharpoons x5$	0000185

7.1 Reaction `OATP1B3`

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

Name OATP1B3 mediated import

SBO:0000185 transport reaction

Reaction equation

$$x1 \longrightarrow x3 \tag{3}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
x1	free basolateral BSP	

Product

Table 7: Properties of each product.

Id	Name	SBO
x3	free intracellular BSP	

Kinetic Law

Derived unit $(60\,\mathrm{s})^{-1} \cdot \mathrm{nmol}$

$$v_1 = p1 \cdot x1 \tag{4}$$

7.2 Reaction `ABCC2`

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

Name ABCC2 mediated export

SBO:0000185 transport reaction

Reaction equation

$$x3 \longrightarrow x5 \tag{5}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
x3	free intracellular BSP	

Product

Table 9: Properties of each product.

Id	Name	SBO
x5	apical BSP	

Kinetic Law

Derived unit $(60\,\mathrm{s})^{-1} \cdot \mathrm{nmol}$

$$v_2 = \mathrm{p2} \cdot \mathrm{x3} \tag{6}$$

7.3 Reaction `endo_in_bl`

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

Name endogenous basolateral import

SBO:0000185 transport reaction

Reaction equation

$$\mathrm{x1} \longrightarrow \mathrm{x3} \tag{7}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
x1	free basolateral BSP	

Product

Table 11: Properties of each product.

Id	Name	SBO
x3	free intracellular BSP	

Kinetic Law

Derived unit $(60\,\mathrm{s})^{-1} \cdot \mathrm{nmol}$

$$v_3 = \mathrm{p3} \cdot \mathrm{x1} \tag{8}$$

7.4 Reaction `endo_ex_bl`

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

Name endogenous basolateral export

SBO:0000185 transport reaction

Reaction equation

$$\mathrm{x3} \longrightarrow \mathrm{x1} \tag{9}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
x3	free intracellular BSP	

Product

Table 13: Properties of each product.

Id	Name	SBO
x1	free basolateral BSP	

Kinetic Law

Derived unit $(60\,\mathrm{s})^{-1} \cdot \mathrm{nmol}$

$$v_4 = \mathrm{p4} \cdot \mathrm{x3} \tag{10}$$

Produced by SBML2LATEX

7.5 Reaction `endo_ex_ap`

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

Name endogenous apical export

SBO:0000185 transport reaction

Reaction equation

$$\text{x3} \longrightarrow \text{x5} \tag{11}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
x3	free intracellular BSP	

Product

Table 15: Properties of each product.

Id	Name	SBO
x5	apical BSP	

Kinetic Law

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

$$v_5 = \text{p5} \cdot \text{x3} \tag{12}$$

7.6 Reaction `bl_BSP_binding`

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

Name basolateral BSP binding

SBO:0000177 non-covalent binding

Reaction equation

$$\text{x1} \longrightarrow \text{x2} \tag{13}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
x1	free basolateral BSP	

Product

Table 17: Properties of each product.

Id	Name	SBO
x2	basolateral bound BSP	

Kinetic Law

Derived unit $(60\,\mathrm{s})^{-1} \cdot \mathrm{nmol}$

$$v_6 = \mathrm{p6} \cdot \mathrm{x1} \cdot (\mathrm{p8} - \mathrm{x2}) \tag{14}$$

7.7 Reaction `bl_BSP_dissoc`

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

Name basolateral BSP dissoc

SBO:0000180 dissociation

Reaction equation

$$\mathrm{x2} \longrightarrow \mathrm{x1} \tag{15}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
x2	basolateral bound BSP	

Product

Table 19: Properties of each product.

Id	Name	SBO
x1	free basolateral BSP	

Kinetic Law

Derived unit $(60\,\mathrm{s})^{-1} \cdot \mathrm{nmol}$

$$v_7 = \mathrm{p7} \cdot \mathrm{x2} \tag{16}$$

7.8 Reaction `cellular_BSP_binding`

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

Name cellular BSP binding

SBO:0000177 non-covalent binding

Reaction equation

$$\mathrm{x3} \longrightarrow \mathrm{x4} \tag{17}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
x3	free intracellular BSP	

Product

Table 21: Properties of each product.

Id	Name	SBO
x4	bound intracellular BSP	

Kinetic Law

Derived unit $(60\,\mathrm{s})^{-1} \cdot \mathrm{nmol}$

$$v_8 = \mathrm{p9} \cdot \mathrm{x3} \cdot (\mathrm{p11} - \mathrm{x4}) \tag{18}$$

7.9 Reaction `cellular_BSP_dissoc`

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

Name cellular BSP dissoc

SBO:0000180 dissociation

Reaction equation

$$x4 \longrightarrow x3 \tag{19}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
x4	bound intracellular BSP	

Product

Table 23: Properties of each product.

Id	Name	SBO
x3	free intracellular BSP	

Kinetic Law

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

$$v_9 = \text{p10} \cdot \text{x4} \tag{20}$$

7.10 Reaction `paracell_transp`

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

Name paracellular transport

SBO:0000185 transport reaction

Reaction equation

$$x1 \rightleftharpoons x5 \tag{21}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
x1	free basolateral BSP	

Product

Table 25: Properties of each product.

Id	Name	SBO
x5	apical BSP	

Kinetic Law

Derived unit $(60\,\mathrm{s})^{-1} \cdot \mathrm{nmol}$

$$v_{10} = \mathrm{p12} \cdot \left(\frac{\mathrm{x1}}{\mathrm{vol\,(basolat)}} - \frac{\mathrm{x5}}{\mathrm{vol\,(apical)}} \right) \tag{22}$$

8 Derived Rate Equations

When interpreted as an ordinary differential equation framework, this model implies the following set of equations for the rates of change of each species.

8.1 Species x1

Name free basolateral BSP

SBO:0000247 simple chemical

Initial amount 88 nmol

This species takes part in six reactions (as a reactant in `OATP1B3`, `endo_in_bl`, `bl_BSP_binding`, `paracell_transp` and as a product in `endo_ex_bl`, `bl_BSP_dissoc`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x1} = v_4 + v_7 - v_1 - v_3 - v_6 - v_{10} \tag{23}$$

8.2 Species x2

Name basolateral bound BSP

SBO:0000247 simple chemical

Initial amount 0 nmol

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

$$\frac{\mathrm{d}}{\mathrm{d}t}x2 = v_6 - v_7 \tag{24}$$

8.3 Species $x3$

Name free intracellular BSP

SBO:0000247 simple chemical

Initial amount 0 nmol

This species takes part in seven reactions (as a reactant in `ABCC2`, `endo_ex_bl`, `endo_ex_ap`, `cellular_BSP_binding` and as a product in `OATP1B3`, `endo_in_bl`, `cellular_BSP_dissoc`).

$$\frac{\mathrm{d}}{\mathrm{d}t}x3 = v_1 + v_3 + v_9 - v_2 - v_4 - v_5 - v_8 \tag{25}$$

8.4 Species $x4$

Name bound intracellular BSP

SBO:0000247 simple chemical

Initial amount 0 nmol

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

$$\frac{\mathrm{d}}{\mathrm{d}t}x4 = v_8 - v_9 \tag{26}$$

8.5 Species $x5$

Name apical BSP

SBO:0000247 simple chemical

Initial amount 0 nmol

This species takes part in three reactions (as a product in `ABCC2`, `endo_ex_ap`, `paracell-_transp`).

$$\frac{\mathrm{d}}{\mathrm{d}t}x5 = v_2 + v_5 + v_{10} \tag{27}$$

8.6 Species `BSP_tot`

Name total BSP

SBO:0000247 simple chemical

Involved in rule `BSP_tot`

One rule determines the species' quantity.

8.7 Species `BSP_cell`

Name intracellular BSP

SBO:0000247 simple chemical

Involved in rule `BSP_cell`

One rule determines the species' quantity.

A Glossary of Systems Biology Ontology Terms

SBO:0000177 non-covalent binding: Interaction between several biochemical entities that results in the formation of a non-covalent comple

SBO:0000180 dissociation: Transformation of a non-covalent complex that results in the formation of several independent biochemical entitie

SBO:0000185 transport reaction: Movement of a physical entity without modification of the structure of the entity

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

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