SBML Model Report

Model name: "Nikolaev2005_AlbuminBilirubinAdsorption"

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: Vijayalakshmi Chelliah[1] and Andrey V Nikolaev[2] at September 20th 2010 at 10:43 a. m. and last time modified at October tenth 2014 at 11:15 a. 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	10
events	0	constraints	0
reactions	0	function definitions	0
global parameters	13	unit definitions	0
rules	7	initial assignments	0

Model Notes

This a model from the article:
Mathematical model of binding of albumin-bilirubin complex to the surface of carbon pyropolymer.
Nikolaev AV, Rozhilo YA, Starozhilova TK, Sarnatskaya VV, Yushko LA, Mikhailovskii SV,

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Kholodov AS, Lobanov AI. Bull Exp Biol Med2005 Sep;140(3):365-9. 16307060,
Abstract:
We proposed a mathematical model and estimated the parameters of adsorption of albumin-bilirubin complex to the surface of carbon pyropolymer. Design data corresponded to the results of experimental studies. Our findings indicate that modeling of this process should take into account fractal properties of the surface of carbon pyropolymer.

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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 five unit definitions which are all predefined by SBML and not mentioned in the model.

2.1 Unit `substance`

Notes Mole is the predefined SBML unit for `substance`.

Definition mol

2.2 Unit `volume`

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

Definition l

2.3 Unit `area`

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

Definition m^2

2.4 Unit `length`

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

Definition m

2.5 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
`compartment`	compartment		3	1	litre	☑	

3.1 Compartment `compartment`

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

Name compartment

4 Species

This model contains ten species. Section 7 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	AlB	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
x2	BC	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
x3	AlCn	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
x4	AlB2	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
x5	Al	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
x6	B	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
x7	C	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
A0	A0	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☐
B0	B0	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☐
C0	C0	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☐

Produced by SBML2LaTeX

5 Parameters

This model contains 13 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	0.484		☑
k2	k2	0000009	0.080		☑
k3	k3	0000009	$5.095 \cdot 10^{-6}$		☑
k4	k4	0000009	$2.656 \cdot 10^{-5}$		☑
k5	k5	0000009	0.005		☑
k6	k6	0000009	$3.226 \cdot 10^{-7}$		☑
k7	k7	0000009	0.003		☑
k8	k8	0000009	$1.011 \cdot 10^{-7}$		☑
k9	k9	0000009	0.017		☑
k10	k10	0000009	0.133		☑
K_AlB	K_AlB	0000009	95000.000		☑
K_AlB2	K_AlB2	0000009	3000.000		☑
n	n	0000189	1.000		☑

6 Rules

This is an overview of seven rules.

6.1 Rule x5

Rule x5 is an assignment rule for species x5:

$$\mathrm{x5} = [\mathrm{A0}] - [\mathrm{x1}] - [\mathrm{x3}] - [\mathrm{x4}] \tag{1}$$

Derived unit $\mathrm{mol} \cdot \mathrm{l}^{-1}$

6.2 Rule x6

Rule x6 is an assignment rule for species x6:

$$\mathrm{x6} = [\mathrm{B0}] - [\mathrm{x1}] - [\mathrm{x2}] - 2 \cdot [\mathrm{x4}] \tag{2}$$

6.3 Rule x7

Rule x7 is an assignment rule for species x7:

$$\mathrm{x7} = [\mathrm{C0}] - [\mathrm{x2}] - \mathrm{n} \cdot [\mathrm{x3}] \tag{3}$$

6.4 Rule x1

Rule x1 is a rate rule for species x1:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x1} = \mathrm{K\_AlB} \cdot \mathrm{k3} \cdot [\mathrm{x5}] \cdot [\mathrm{x6}] - \mathrm{K\_AlB2} \cdot \mathrm{k4} \cdot [\mathrm{x1}] \cdot [\mathrm{x6}] - \mathrm{k3} \cdot [\mathrm{x1}] - \mathrm{k9} \cdot [\mathrm{x1}] \cdot [\mathrm{x7}]^{\mathrm{n}+1} + \mathrm{k4} \cdot [\mathrm{x4}] + \mathrm{k10} \cdot [\mathrm{x4}] \cdot [\mathrm{x7}] \tag{4}$$

6.5 Rule x2

Rule x2 is a rate rule for species x2:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x2} = \mathrm{k6} \cdot [\mathrm{x7}] \cdot [\mathrm{x6}] - \mathrm{k8} \cdot [\mathrm{x2}] + \mathrm{k9} \cdot [\mathrm{x1}] \cdot [\mathrm{x7}]^{\mathrm{n}+1} + \mathrm{k10} \cdot [\mathrm{x4}] \cdot [\mathrm{x7}] \tag{5}$$

6.6 Rule x3

Rule x3 is a rate rule for species x3:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x3} = \mathrm{k5} \cdot [\mathrm{x7}]^{\mathrm{n}} \cdot [\mathrm{x5}] - \mathrm{k7} \cdot [\mathrm{x3}] + \mathrm{k9} \cdot [\mathrm{x1}] \cdot [\mathrm{x7}]^{\mathrm{n}+1} \tag{6}$$

6.7 Rule x4

Rule x4 is a rate rule for species x4:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x4} = \mathrm{K\_AlB2} \cdot \mathrm{k4} \cdot [\mathrm{x1}] \cdot [\mathrm{x6}] - \mathrm{k4} \cdot [\mathrm{x4}] - \mathrm{k10} \cdot [\mathrm{x4}] \cdot [\mathrm{x7}] \tag{7}$$

7 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.

7.1 Species x1

Name AlB

SBO:0000296 macromolecular complex

Initial concentration $0\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

Involved in rule x1

One rule which determines this species' quantity.

7.2 Species x2

Name BC

SBO:0000296 macromolecular complex

Initial concentration $0\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

Involved in rule x2

One rule which determines this species' quantity.

7.3 Species x3

Name AlCn

SBO:0000296 macromolecular complex

Initial concentration $0\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

Involved in rule x3

One rule which determines this species' quantity.

7.4 Species x4

Name AlB2

SBO:0000296 macromolecular complex

Initial concentration $0\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

Involved in rule x4

One rule which determines this species' quantity.

7.5 Species x5

Name Al

SBO:0000245 macromolecule

Initial concentration $0.4615385\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

Involved in rule x5

One rule which determines this species' quantity.

7.6 Species x6

Name B

SBO:0000247 simple chemical

Initial concentration $0.1754386\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

Involved in rule x6

One rule which determines this species' quantity.

7.7 Species x7

Name C

SBO:0000421 multimer of simple chemicals

Initial concentration $1.174\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

Involved in rule x7

One rule which determines this species' quantity.

7.8 Species A0

Name A0

SBO:0000245 macromolecule

Initial concentration $0.4615385\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A0} = 0 \tag{8}$$

7.9 Species B0

Name B0

SBO:0000247 simple chemical

Initial concentration $0.1754386\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{B0} = 0 \tag{9}$$

7.10 Species C0

Name C0

SBO:0000421 multimer of simple chemicals

Initial concentration $1.174\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C0} = 0 \tag{10}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000009 kinetic constant: Numerical parameter that quantifies the velocity of a chemical reaction

SBO:0000189 number of binding sites: Number of regions on a reactant to which specific other reactants, in this context collectively called ligands, form a chemical bond

SBO:0000245 macromolecule: Molecular entity mainly built-up by the repetition of pseudo-identical units. CHEBI:3383

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

SBO:0000296 macromolecular complex: Non-covalent complex of one or more macromolecules and zero or more simple chemicals

SBO:0000421 multimer of simple chemicals: Non-covalent association between several simple chemical

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