SBML Model Report

Model name: "McClean2007_CrossTalk"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Enuo He[1] and Christian Waltermann[2] at May eighth 2007 at 9:29 a. m. and last time modified at July fifth 2012 at 4:32 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	6
events	0	constraints	0
reactions	10	function definitions	0
global parameters	20	unit definitions	0
rules	0	initial assignments	0

Model Notes

This model encoded according to the paper *Cross-talk and decision making in MAP kinase pathways.* Supplementary Figure 2 has been reproduced by COPASI4.0.20 (development) using parameter scan method. You probably need to uncheck „always use initial conditions„ in copasi when you simulate for the second run in order to get the figure. S1 scale from 0 to 12. Keep in mind that the y axis is the fractions of excited X3 and Y3, meaning that X3P and Y3P are normalized by total concentration X3T and Y3T.

[1]BNMC, enuo@caltech.edu
[2]Max Planck Institute For Molecular Genetics, christian.waltermann@molgen.mpg.de

The results from modeling the pathway in Supplementary Figure1a, including both activation and inhibition. According to the paper, the value of ka and kd should in the orange region (ka belongs [0,1], kd belongs [1,10]) so assigned ka=0, kd=1.

The author made the simplifying assumption that the interactions between the pathways are symmetric. Thus the k12xy=k12yx=ka, k33xy=k33yx=kd.

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_0	cell		3	1	litre	☑	

3.1 Compartment compartment_0

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

Name cell

4 Species

This model contains six 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
species_0	X1p	compartment_0	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
species_1	X2p	compartment_0	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
species_2	X3p	compartment_0	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
species_3	Y1p	compartment_0	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
species_4	Y2p	compartment_0	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
species_5	Y3p	compartment_0	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 20 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
parameter_0	X1T		10.0		☑
parameter_1	X2T		10.0		☑
parameter_2	X3T		10.0		☑
parameter_3	Y1T		10.0		☑
parameter_4	Y2T		10.0		☑
parameter_5	Y3T		10.0		☑
parameter_6	kx		1.0		☑
parameter_7	S1		8.5		☑
parameter_8	Kmx		1.0		☑
parameter_9	k12x		1.0		☑
parameter_10	k23x		1.0		☑
parameter_11	kd		1.0		☑
parameter_12	ka		0.0		☑
parameter_13	Kmyx		1.0		☑
parameter_14	S2		5.0		☑
parameter_15	ky		1.0		☑
parameter_16	Kmy		1.0		☑
parameter_17	k12y		1.0		☑
parameter_18	k23y		1.0		☑
parameter_19	Kmxy		1.0		☑

6 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	reaction_0	X1 activats X2	species_0 $\longrightarrow$ species_1	
2	reaction_1	S1 activates X1	$\emptyset \longrightarrow$ species_0	
3	reaction_2	X2 activates X3	species_1 $\longrightarrow$ species_2	
4	reaction_3	S2 activates Y1	$\emptyset \longrightarrow$ species_3	
5	reaction_4	Y1p activates Y2p	species_3 $\longrightarrow$ species_4	
6	reaction_5	Y2p activates Y3p	species_4 $\longrightarrow$ species_5	
7	reaction_6	X1p activates Y2p	species_0 $\longrightarrow$ species_4	
8	reaction_7	Y1p activates X2p	species_3 $\longrightarrow$ species_1	
9	reaction_8	X3p inhibited by Y3p	species_2 $\xrightarrow{\text{species\_5}} \emptyset$	
10	reaction_9	Y3p inhibited by X3p	species_5 $\xrightarrow{\text{species\_2}} \emptyset$	

6.1 Reaction reaction_0

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

Name X1 activats X2

Reaction equation

$$\text{species\_0} \longrightarrow \text{species\_1} \tag{1}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
species_0	X1p	

Product

Table 7: Properties of each product.

Id	Name	SBO
species_1	X2p	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}\left(\text{compartment\_0}\right) \cdot \text{parameter\_9} \cdot [\text{species\_0}] \cdot (\text{parameter\_1} - [\text{species\_1}]) \tag{2}$$

6.2 Reaction reaction_1

This is an irreversible reaction of no reactant forming one product.

Name S1 activates X1

Reaction equation

$$\emptyset \longrightarrow \text{species\_0} \tag{3}$$

Product

Table 8: Properties of each product.

Id	Name	SBO
species_0	X1p	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\mathrm{vol}\left(\mathrm{compartment\_0}\right) \cdot \mathrm{parameter\_6} \cdot \mathrm{parameter\_7}}{1 + \frac{\mathrm{parameter\_7}}{\mathrm{parameter\_8}}} \cdot \left(\mathrm{parameter\_0} - [\mathrm{species\_0}]\right) \quad (4)$$

6.3 Reaction reaction_2

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

Name X2 activates X3

Reaction equation

$$\mathrm{species\_1} \longrightarrow \mathrm{species\_2} \quad (5)$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
species_1	X2p	

Product

Table 10: Properties of each product.

Id	Name	SBO
species_2	X3p	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\left(\mathrm{compartment\_0}\right) \cdot \mathrm{parameter\_10} \cdot [\mathrm{species\_1}] \cdot \left(\mathrm{parameter\_2} - [\mathrm{species\_2}]\right) \quad (6)$$

6.4 Reaction reaction_3

This is an irreversible reaction of no reactant forming one product.

Name S2 activates Y1

Reaction equation

$$\emptyset \longrightarrow \text{species\_3} \tag{7}$$

Product

Table 11: Properties of each product.

Id	Name	SBO
species_3	Y1p	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \frac{\text{vol}\left(\text{compartment\_0}\right) \cdot \text{parameter\_15} \cdot \text{parameter\_14}}{1 + \frac{\text{parameter\_14}}{\text{parameter\_16}}} \cdot \left(\text{parameter\_3} - [\text{species\_3}]\right) \tag{8}$$

6.5 Reaction reaction_4

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

Name Y1p activates Y2p

Reaction equation

$$\text{species\_3} \longrightarrow \text{species\_4} \tag{9}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
species_3	Y1p	

Product

Table 13: Properties of each product.

Id	Name	SBO
species_4	Y2p	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\left(\mathrm{compartment\_0}\right) \cdot \mathrm{parameter\_17} \cdot [\mathrm{species\_3}] \cdot \left(\mathrm{parameter\_4} - [\mathrm{species\_4}]\right) \quad (10)$$

6.6 Reaction reaction_5

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

Name Y2p activates Y3p

Reaction equation

$$\mathrm{species\_4} \longrightarrow \mathrm{species\_5} \quad (11)$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
species_4	Y2p	

Product

Table 15: Properties of each product.

Id	Name	SBO
species_5	Y3p	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\left(\mathrm{compartment\_0}\right) \cdot \mathrm{parameter\_18} \cdot [\mathrm{species\_4}] \cdot \left(\mathrm{parameter\_5} - [\mathrm{species\_5}]\right) \quad (12)$$

6.7 Reaction reaction_6

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

Name X1p activates Y2p

Reaction equation

$$\text{species\_0} \longrightarrow \text{species\_4} \tag{13}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
species_0	X1p	

Product

Table 17: Properties of each product.

Id	Name	SBO
species_4	Y2p	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{vol}\left(\text{compartment\_0}\right) \cdot \text{parameter\_12} \cdot [\text{species\_0}] \cdot (\text{parameter\_4} - [\text{species\_4}]) \tag{14}$$

6.8 Reaction reaction_7

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

Name Y1p activates X2p

Reaction equation

$$\text{species\_3} \longrightarrow \text{species\_1} \tag{15}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
species_3	Y1p	

Product

Table 19: Properties of each product.

Id	Name	SBO
species_1	X2p	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{compartment\_0}) \cdot \mathrm{parameter\_12} \cdot [\mathrm{species\_3}] \cdot (\mathrm{parameter\_1} - [\mathrm{species\_1}]) \quad (16)$$

6.9 Reaction reaction_8

This is an irreversible reaction of one reactant forming no product influenced by one modifier.

Name X3p inhibited by Y3p

Reaction equation

$$\mathrm{species\_2} \xrightarrow{\mathrm{species\_5}} \emptyset \quad (17)$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
species_2	X3p	

Modifier

Table 21: Properties of each modifier.

Id	Name	SBO
species_5	Y3p	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \frac{\mathrm{vol}\left(\mathrm{compartment\_0}\right) \cdot \mathrm{parameter\_11} \cdot [\mathrm{species\_5}] \cdot [\mathrm{species\_2}]}{1 + \frac{[\mathrm{species\_2}]}{\mathrm{parameter\_13}}} \tag{18}$$

6.10 Reaction `reaction_9`

This is an irreversible reaction of one reactant forming no product influenced by one modifier.

Name Y3p inhibited by X3p

Reaction equation

$$\mathrm{species\_5} \xrightarrow{\mathrm{species\_2}} \emptyset \tag{19}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
`species_5`	Y3p	

Modifier

Table 23: Properties of each modifier.

Id	Name	SBO
`species_2`	X3p	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \frac{\mathrm{vol}\left(\mathrm{compartment\_0}\right) \cdot \mathrm{parameter\_11} \cdot [\mathrm{species\_5}] \cdot [\mathrm{species\_2}]}{1 + \frac{[\mathrm{species\_5}]}{\mathrm{parameter\_19}}} \tag{20}$$

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.

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.

7.1 Species species_0

Name X1p

Notes The initial value for each species taken from the original submitted model, they are the concentration of the species when arrived to the steady states.

Initial concentration $1.023667\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in reaction_0, reaction_6 and as a product in reaction_1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_0} = v_2 - v_1 - v_7 \tag{21}$$

7.2 Species species_1

Name X2p

Initial concentration $2.154231\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in reaction_2 and as a product in reaction_0, reaction_7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_1} = v_1 + v_8 - v_3 \tag{22}$$

7.3 Species species_2

Name X3p

Initial concentration $6.271793\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in reaction_8 and as a product in reaction_2 and as a modifier in reaction_9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_2} = v_3 - v_9 \tag{23}$$

7.4 Species species_3

Name Y1p

Initial concentration $3.203692\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in reaction_4, reaction_7 and as a product in reaction_3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_3} = v_4 - v_5 - v_8 \tag{24}$$

7.5 Species species_4

Name Y2p

Initial concentration $8.232192\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in reaction_5 and as a product in reaction_4, reaction_6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_4} = v_5 + v_7 - v_6 \tag{25}$$

7.6 Species species_5

Name Y3p

Initial concentration $9.312021\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in reaction_9 and as a product in reaction_5 and as a modifier in reaction_8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_5} = v_6 - v_{10} \tag{26}$$

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.

[a]Center for Bioinformatics Tübingen (ZBIT), Germany
[b]California Institute of Technology, Beckman Institute BNMC, Pasadena, United States
[c]European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom
[d]EML Research gGmbH, Heidelberg, Germany