# **SBML Model Report**

# Model name: "Marwan2003 - Genetics, regulatory hierarchy between genes"



May 5, 2016

# 1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Nicolas Le Novre<sup>1</sup> at July seventh 2005 at 4:16 p.m. and last time modified at July eleventh 2012 at 5:34 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	12
events	0	constraints	0
reactions	12	function definitions	0
global parameters	0	unit definitions	1
rules	0	initial assignments	0

#### **Model Notes**

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# 2 Unit Definitions

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

#### 2.1 Unit time

Name hour

**Definition** 3600 s

#### 2.2 Unit substance

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

**Definition** mol

#### 2.3 Unit volume

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

**Definition** 1

#### 2.4 Unit area

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

**Definition** m<sup>2</sup>

# 2.5 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	Ø	

# 3.1 Compartment compartment

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

# 4 Species

This model contains twelve species. The boundary condition of one of these species is set to true so that this 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 Condi- tion
Pfr		compartment	$\text{mol} \cdot l^{-1}$		
Pr		compartment	$\text{mol} \cdot l^{-1}$		
Xi		compartment	$\text{mol} \cdot l^{-1}$	$\Box$	$\Box$
Xa		compartment	$\text{mol} \cdot l^{-1}$	$\Box$	$\Box$
prepreS		compartment	$\text{mol} \cdot l^{-1}$		
preS		compartment	$\text{mol} \cdot l^{-1}$		
Ya		compartment	$\text{mol} \cdot l^{-1}$	$\Box$	$\Box$
S		compartment	$\text{mol} \cdot l^{-1}$	$\Box$	$\Box$
Gluc		compartment	$\text{mol} \cdot l^{-1}$	$\Box$	
Yi		compartment	$\text{mol} \cdot l^{-1}$	$\Box$	
V		compartment	$\text{mol} \cdot l^{-1}$		
Pi		compartment	$\text{mol} \cdot 1^{-1}$		

# **5 Reactions**

This model contains twelve 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

N₀	Id Name	Reaction Equation	SBO
1	Photoreceptor-	$Pfr \longrightarrow Pr$	
	$\_$ activation		
2	Photoreceptor-	$\Pr \longrightarrow Pfr$	
	$_{ extstyle }$ inactivation		
3	Transducer-	$\mathrm{Xi} \overset{\mathrm{Pr}}{\longrightarrow} \mathrm{Xa}$	
	$\_$ activation		
4	Transducer-	$Xa \longrightarrow Xi$	
	$_{ extstyle }$ inactivation		
5	preS_formation	$prepreS \xrightarrow{Xa} preS$	
6	$S_{\underline{\hspace{0.1cm}}}$ generation	$\operatorname{preS} \xrightarrow{\operatorname{Ya}} \operatorname{S}$	
7	Glucose_sensor-	$Ya + Gluc \longrightarrow Yi$	
	$\_$ inactivation		
8	$S_{-}$ formation	$\emptyset \xrightarrow{\mathbf{V}} \mathbf{S}$	
9	$V_{\perp}$ formation	$\emptyset \xrightarrow{S} V$	
10	$S_{-}$ degradation	$S \longrightarrow \emptyset$	
11	$V_{-}$ degradation	$V \longrightarrow \emptyset$	
12	Photoreceptor-	$Pr \longrightarrow Pi$	
	_decay		

# **5.1 Reaction** Photoreceptor\_activation

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

# **Reaction equation**

$$Pfr \longrightarrow Pr \tag{1}$$

#### Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
Pfr		

# **Product**

Table 6: Properties of each product.

Id	Name	SBO
Pr		

# **Kinetic Law**

**Derived unit** contains undeclared units

$$v_1 = \text{vol}\left(\text{compartment}\right) \cdot [\text{Pfr}] \cdot \text{IfrSfrPfr}$$
 (2)

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
IfrSfrPfr			0.1		

# **5.2 Reaction** Photoreceptor\_inactivation

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

# **Reaction equation**

$$Pr \longrightarrow Pfr$$
 (3)

# Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
Pr		

# **Product**

Table 9: Properties of each product.

Id	Name	SBO
Pfr		

# **Kinetic Law**

**Derived unit** contains undeclared units

$$v_2 = \text{IrSrPr} \cdot [\text{Pr}] \cdot \text{vol} (\text{compartment}) \tag{4}$$

Table 10: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
IrSrPr		0.0	

# **5.3 Reaction** Transducer\_activation

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

# **Reaction equation**

$$Xi \xrightarrow{Pr} Xa$$
 (5)

# Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
Xi		

# **Modifier**

Table 12: Properties of each modifier.

Id	Name	SBO
Pr		

# **Product**

Table 13: Properties of each product.

Id	Name	SBO
Хa		

# **Kinetic Law**

**Derived unit** contains undeclared units

$$v_3 = [Xi] \cdot kia \cdot [Pr] \cdot vol (compartment)$$
 (6)

Table 14: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
kia		0.1	

# **5.4 Reaction** Transducer\_inactivation

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

# **Reaction equation**

$$Xa \longrightarrow Xi$$
 (7)

# Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
Хa		

# **Product**

Table 16: Properties of each product.

# **Kinetic Law**

**Derived unit** contains undeclared units

$$v_4 = \text{kai} \cdot [\text{Xa}] \cdot \text{vol} (\text{compartment})$$
 (8)

Table 17: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
kai		0.8	

# **5.5 Reaction** preS\_formation

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

# **Reaction equation**

$$prepreS \xrightarrow{Xa} preS$$
 (9)

#### Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
prepreS		

# **Modifier**

Table 19: Properties of each modifier.

Id	Name	SBO
Хa		

# **Product**

Table 20: Properties of each product.

Id	Name	SBO
preS		

# **Kinetic Law**

**Derived unit** contains undeclared units

$$v_5 = [prepreS] \cdot kx \cdot [Xa] \cdot vol(compartment)$$
 (10)

Table 21: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
kx		0.2	

# **5.6 Reaction** S\_generation

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

# **Reaction equation**

$$\operatorname{preS} \xrightarrow{\mathbf{Ya}} \mathbf{S} \tag{11}$$

#### Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
preS		

#### **Modifier**

Table 23: Properties of each modifier.

Id	Name	SBO
Ya		

# **Product**

Table 24: Properties of each product.

Id	Name	SBO
S		

# **Kinetic Law**

**Derived unit** contains undeclared units

$$v_6 = [\text{preS}] \cdot \text{ky} \cdot [\text{Ya}] \cdot \text{vol} (\text{compartment})$$
 (12)

Table 25: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
ky		1.0	

# 5.7 Reaction Glucose\_sensor\_inactivation

This is an irreversible reaction of two reactants forming one product.

# **Reaction equation**

$$Ya + Gluc \longrightarrow Yi$$
 (13)

#### **Reactants**

Table 26: Properties of each reactant.

Id	Name	SBO
Ya		
${ t Gluc}$		

# **Product**

Table 27: Properties of each product.

Id	Name	SBO
Yi		

# **Kinetic Law**

Derived unit contains undeclared units

$$v_7 = kG \cdot [Ya] \cdot [Gluc] \cdot vol (compartment)$$
 (14)

Table 28: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
kG		0.1	

# 5.8 Reaction S\_formation

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

# **Reaction equation**

$$\emptyset \xrightarrow{\mathbf{V}} \mathbf{S} \tag{15}$$

#### **Modifier**

Table 29: Properties of each modifier.

Id	Name	SBO
V		

#### **Product**

Table 30: Properties of each product.

Id	Name	SBO
S		

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_8 = \text{vol}\left(\text{compartment}\right) \cdot \frac{\text{alpha1}}{1 + [V]^3}$$
 (16)

Table 31: Properties of each parameter.

Id	Name	SBO V	Value Unit	Constant
alpha1		3	30.0	

# **5.9 Reaction V\_formation**

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

# **Reaction equation**

$$\emptyset \xrightarrow{S} V \tag{17}$$

# **Modifier**

Table 32: Properties of each modifier.

Id	Name	SBO
S		

# **Product**

Table 33: Properties of each product.

Id	Name	SBO
V		

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_9 = \text{vol}\left(\text{compartment}\right) \cdot \frac{\text{alpha2}}{1 + [S]^3}$$
 (18)

Table 34: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
alpha2		50.0	$\square$

# **5.10 Reaction** S\_degradation

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

# **Reaction equation**

$$S \longrightarrow \emptyset$$
 (19)

#### Reactant

Table 35: Properties of each reactant.

Id	Name	SBO
S		

# **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{10} = \text{kd\_s} \cdot [S] \cdot \text{vol} (\text{compartment})$$
 (20)

Table 36: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
kd_s		1.0	

# **5.11 Reaction V\_degradation**

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

# **Reaction equation**

$$V \longrightarrow \emptyset$$
 (21)

# Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
V		

# **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{11} = \text{vol}\left(\text{compartment}\right) \cdot [V] \cdot \text{kd}_{-V}$$
 (22)

Table 38: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
kd_v		1.0	

# **5.12 Reaction** Photoreceptor\_decay

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

# **Reaction equation**

$$Pr \longrightarrow Pi$$
 (23)

#### Reactant

Table 39: Properties of each reactant.

# **Product**

Table 40: Properties of each product.

Id	Name	SBO
Pi		

# **Kinetic Law**

Derived unit contains undeclared units

$$v_{12} = \text{vol}\left(\text{compartment}\right) \cdot \text{kd} \cdot [\text{Pr}]$$
 (24)

Table 41: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kd			0.1		$\overline{Z}$

# **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.

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.

#### 6.1 Species Pfr

#### Initial amount 10 mol

This species takes part in two reactions (as a reactant in Photoreceptor\_activation and as a product in Photoreceptor\_inactivation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pfr} = |v_2| - |v_1| \tag{25}$$

#### 6.2 Species Pr

#### **Initial amount** 0 mol

This species takes part in four reactions (as a reactant in Photoreceptor\_inactivation, Photoreceptor\_decay and as a product in Photoreceptor\_activation and as a modifier in Transducer\_activation).

$$\frac{d}{dt} Pr = |v_1| - |v_2| - |v_{12}| \tag{26}$$

#### 6.3 Species Xi

#### Initial amount 6 mol

This species takes part in two reactions (as a reactant in Transducer\_activation and as a product in Transducer\_inactivation).

$$\frac{\mathrm{d}}{\mathrm{d}t}Xi = v_4 - v_3 \tag{27}$$

# 6.4 Species Xa

#### Initial amount 0 mol

This species takes part in three reactions (as a reactant in Transducer\_inactivation and as a product in Transducer\_activation and as a modifier in preS\_formation).

$$\frac{\mathrm{d}}{\mathrm{d}t} X \mathbf{a} = |v_3| - |v_4| \tag{28}$$

# 6.5 Species prepreS

#### Initial amount 200 mol

This species takes part in one reaction (as a reactant in preS\_formation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{prepreS} = -v_5 \tag{29}$$

# 6.6 Species preS

#### Initial amount 0 mol

This species takes part in two reactions (as a reactant in S\_generation and as a product in preS\_formation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{preS} = |v_5| - |v_6| \tag{30}$$

#### **6.7 Species** Ya

# Initial amount 0.9 mol

This species takes part in two reactions (as a reactant in Glucose\_sensor\_inactivation and as a modifier in S\_generation).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{Ya} = -v_7 \tag{31}$$

#### **6.8 Species** S

#### Initial amount 0 mol

This species takes part in four reactions (as a reactant in S\_degradation and as a product in S\_generation, S\_formation and as a modifier in V\_formation).

$$\frac{d}{dt}S = |v_6| + |v_8| - |v_{10}| \tag{32}$$

# 6.9 Species Gluc

#### Initial amount 0 mol

This species takes part in one reaction (as a reactant in Glucose\_sensor\_inactivation), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gluc} = 0\tag{33}$$

# 6.10 Species Yi

#### Initial amount 0 mol

This species takes part in one reaction (as a product in Glucose\_sensor\_inactivation).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{Yi} = v_7 \tag{34}$$

# 6.11 Species V

#### Initial amount 30 mol

This species takes part in three reactions (as a reactant in V\_degradation and as a product in V\_formation and as a modifier in S\_formation).

$$\frac{\mathrm{d}}{\mathrm{d}t}V = |v_9| - |v_{11}| \tag{35}$$

# 6.12 Species Pi

#### Initial amount 0 mol

This species takes part in one reaction (as a product in Photoreceptor\_decay).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pi} = |v_{12}| \tag{36}$$

 $\mathfrak{BML2}^{d}$  was developed by Andreas Dräger<sup>a</sup>, Hannes Planatscher<sup>a</sup>, Dieudonné M Wouamba<sup>a</sup>, Adrian Schröder<sup>a</sup>, Michael Hucka<sup>b</sup>, Lukas Endler<sup>c</sup>, Martin Golebiewski<sup>d</sup> and Andreas Zell<sup>a</sup>. Please see http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX for more information.

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