# **SBML Model Report**

# Model name: "Edelstein1996 - EPSP ACh species"



May 5, 2016

# **1 General Overview**

This is a document in SBML Level 2 Version 4 format. This model was created by Nicolas Le Novre<sup>1</sup> at February second 2005 at 2:41 p.m. and last time modified at April first 2014 at 5:42 p.m. Table 1 provides 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	13
events	0	constraints	0
reactions	17	function definitions	0
global parameters	34	unit definitions	0
rules	0	initial assignments	0

# **Model Notes**

Edelstein1996 - EPSP ACh species

Model of a nicotinic Excitatory Post-Synaptic Potential in a Torpedo electric organ. Acetylcholine is represented explicitely as a molecular species.

This model has initially been encoded using StochSim.

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This model is described in the article: A kinetic mechanism for nicotinic acetylcholine receptors based on multiple allosteric transitions. Edelstein SJ, Schaad O, Henry E, Bertrand D, Changeux JP.Biol. Cybern. 1996 Nov; 75(5):361-79

#### Abstract:

Nicotinic acetylcholine receptors are transmembrane oligomeric proteins that mediate interconversions between open and closed channel states under the control of neurotransmitters. Fast in vitro chemical kinetics and in vivo electrophysiological recordings are consistent with the following multi-step scheme. Upon binding of agonists, receptor molecules in the closed but activatable resting state (the Basal state, B) undergo rapid transitions to states of higher affinities with either open channels (the Active state, A) or closed channels (the initial Inactivatable and fully Desensitized states, I and D). In order to represent the functional properties of such receptors, we have developed a kinetic model that links conformational interconversion rates to agonist binding and extends the general principles of the Monod-Wyman-Changeux model of allosteric transitions. The crucial assumption is that the linkage is controlled by the position of the interconversion transition states on a hypothetical linear reaction coordinate. Application of the model to the peripheral nicotine acetylcholine receptor (nAChR) accounts for the main properties of ligand-gating, including single-channel events, and several new relationships are predicted. Kinetic simulations reveal errors inherent in using the dose-response analysis, but justify its application under defined conditions. The model predicts that (in order to overcome the intrinsic stability of the B state and to produce the appropriate cooperativity) channel activation is driven by an A state with a Kd in the 50 nM range, hence some 140-fold stronger than the apparent affinity of the open state deduced previously. According to the model, recovery from the desensitized states may occur via rapid transit through the A state with minimal channel opening, thus without necessarily undergoing a distinct recovery pathway, as assumed in the standard 'cycle' model. Transitions to the desensitized states by low concentration 'pre-pulses' are predicted to occur without significant channel opening, but equilibrium values of IC50 can be obtained only with long pre-pulse times. Predictions are also made concerning allosteric effectors and their possible role in coincidence detection. In terms of future developments, the analysis presented here provides a physical basis for constructing more biologically realistic models of synaptic modulation that may be applied to artificial neural networks.

This model is hosted on BioModels Database and identified by: BIOMD000000002.

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

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# 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 1

# 2.3 Unit area

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

 $\text{Definition} \ m^2$ 

# 2.4 Unit length

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

 $\textbf{Definition} \ m$ 

# 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
comp1	compartment1		3	$10^{-16}$	1		

# 3.1 Compartment comp1

This is a three dimensional compartment with a constant size of  $10^{-16}$  litre.

Name compartment1

# 4 Species

This model contains 13 species. Section 7 provides further details and the derived rates of change of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary
					Condi-
					tion
BLL	BasalACh2	comp1	$mol \cdot l^{-1}$		Β
IL	IntermediateACh	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$		$\square$
AL	ActiveACh	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$		
A	Active	comp1	$mol \cdot l^{-1}$		
BL	BasalACh	comp1	$mol \cdot l^{-1}$		
В	Basal	comp1	$mol \cdot l^{-1}$		
DLL	DesensitisedACh2	comp1	$\operatorname{mol} \cdot l^{-1}$		
D	Desensitised	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$		$\square$
ILL	IntermediateACh2	comp1	$\operatorname{mol} \cdot l^{-1}$		
DL	DesensitisedACh	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$		
I	Intermediate	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$		
ALL	ActiveACh2	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$		
L	ACh	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$		

Table 3: Properties of each species

# **5** Parameters

This model contains 34 global parameters.

	Taul	e 4. I Toperties of each para		
Id	Name	SBO Value	Unit	Constant
kf_0		$3 \cdot 10^{8}$		
kr_0		8000.000	)	$\checkmark$
kf_1		$1.5 \cdot 10^{8}$		$\checkmark$
kr_1		16000.000	)	$\checkmark$
kf_2		30000.000	)	$\checkmark$
kr_2		700.000	)	$\checkmark$
kf_3		$3 \cdot 10^{8}$		$\checkmark$
kr_3		8.640	)	$\checkmark$
kf_4		$1.5 \cdot 10^{8}$		$\checkmark$
kr_4		17.280	)	$\checkmark$
kf_5		0.540	)	$\checkmark$
kr_5		10800.000	)	$\checkmark$
kf_6		130.000	)	$\checkmark$
kr_6		2740.000	)	$\checkmark$
$kf_7$		$3 \cdot 10^{8}$		
kr_7		4.000	)	
kf_8		$1.5 \cdot 10^{8}$		$\checkmark$
kr_8		8.000	)	$\checkmark$
kf_9		19.700	)	$\checkmark$
kr_9		3.740	)	$\checkmark$
$kf_10$		19.850	)	$\checkmark$
$kr_10$		1.740		$\checkmark$
$kf_11$		20.000		$\checkmark$
$kr_11$		0.810		
$kf_12$		$3 \cdot 10^{8}$	•	
kr_12		4.000		$\checkmark$
$kf_13$		$1.5 \cdot 10^{8}$	•	
kr_13		8.000		
$kf_14$		0.050		
kr_14		0.001		
$kf_15$		0.050		
$kr_15$		0.001		
$kf_16$		0.050		$\checkmark$
$kr_{-}16$		0.001		$\checkmark$

Table 4: Properties of each parameter.

# • 6 Reactions

This model contains 17 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.

N⁰	Id	Name	Reaction Equation	SBO
1	React0	React0	$B + L \rightleftharpoons BL$	
2	React1	React1	$BL + L \Longrightarrow BLL$	
3	React2	React2	$BLL \rightleftharpoons ALL$	
4	React3	React3	$A + L \rightleftharpoons AL$	
5	React4	React4	$AL + L \Longrightarrow ALL$	
6	React5	React5	$B \rightleftharpoons A$	
7	React6	React6	$BL \rightleftharpoons AL$	
8	React7	React7	$I + L \rightleftharpoons IL$	
9	React8	React8	$IL + L \rightleftharpoons ILL$	
10	React9	React9	$A \rightleftharpoons I$	
11	React10	React10	$AL \rightleftharpoons IL$	
12	React11	React11	$ALL \rightleftharpoons ILL$	
13	React12	React12	$D + L \rightleftharpoons DL$	
14	React13	React13	$DL + L \rightleftharpoons DLL$	
15	React14	React14	$I \rightleftharpoons D$	
16	React15	React15	$IL \rightleftharpoons DL$	
17	React16	React16	$ILL \Longrightarrow DLL$	

Table 5: Overview of all reactions

### 6.1 Reaction React0

This is a reversible reaction of two reactants forming one product.

Name React0

**Notes** first ligand on basal

#### **Reaction equation**

$$\mathbf{B} + \mathbf{L} \rightleftharpoons \mathbf{B} \mathbf{L} \tag{1}$$

#### **Reactants**

Table 6	: Pro	perties of	f each r	eactant.
	Id	Name	SBO	-
	В	Basal		
	L	ACh		

#### Product

Table	e 7: P	roperties of e	ach pro	duct.
	Id	Name	SBO	
	BL	BasalACh		

#### **Kinetic Law**

Notes  $kf_0 * B * L - kr_0 * BL$ 

Derived unit contains undeclared units

$$v_1 = \operatorname{vol}(\operatorname{comp1}) \cdot (\operatorname{kf_0} \cdot [\mathbf{B}] \cdot [\mathbf{L}] - \operatorname{kr_0} \cdot [\mathbf{BL}])$$
(2)

# 6.2 Reaction React1

This is a reversible reaction of two reactants forming one product.

Name React1

Notes second ligand on basal

**Reaction equation** 

$$BL + L \rightleftharpoons BLL$$
 (3)

Produced by SBML2ATEX

#### Reactants

Table 8: Properties of each reactant.
---------------------------------------

Id	Name	SBO
BL	BasalACh	
L	ACh	

# Product

Tab	le 9: P	roperties of ea	ch product.
	Id	Name	SBO
	BLL	BasalACh2	

# **Kinetic Law**

**Notes**  $kf_1 * BL * L - kr_1 * BLL$ 

Derived unit contains undeclared units

$$v_2 = \operatorname{vol}(\operatorname{comp1}) \cdot (\operatorname{kf_-1} \cdot [\operatorname{BL}] \cdot [\operatorname{L}] - \operatorname{kr_-1} \cdot [\operatorname{BLL}])$$
(4)

#### 6.3 Reaction React2

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

Name React2

**Notes** opening of biliganded

**Reaction equation** 

$$BLL \rightleftharpoons ALL \tag{5}$$

Reactant

Table	10:	Properties	of each	reactant.
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Id	Name	SBO
BLL	BasalACh2	

# Product

Tab	le 11: ]	Properties of ea	ch product.
	Id	Name	SBO
	ALL	ActiveACh2	

**Kinetic Law** 

Notes kf\_2 \* BLL - kr\_2 \* ALL

Derived unit contains undeclared units

$$v_3 = \operatorname{vol}(\operatorname{comp1}) \cdot (\operatorname{kf}_2 \cdot [\operatorname{BLL}] - \operatorname{kr}_2 \cdot [\operatorname{ALL}])$$
(6)

# 6.4 Reaction React3

This is a reversible reaction of two reactants forming one product.

Name React3

**Notes** first ligand on active

**Reaction equation** 

$$A + L \rightleftharpoons AL \tag{7}$$

Reactants

Table	12:	Properties	of	each	reactant.

Id	Name	SBO
A	Active	
L	ACh	

# Product

Table	13:	Prope	erties	of	each	product.
						1

Id	Name	SBO
AL	ActiveACh	

#### **Kinetic Law**

Notes  $kf_3 * A * L - kr_3 * AL$ 

Derived unit contains undeclared units

$$v_4 = \operatorname{vol}(\operatorname{comp1}) \cdot (\operatorname{kf}_3 \cdot [A] \cdot [L] - \operatorname{kr}_3 \cdot [AL])$$
(8)

#### 6.5 Reaction React4

This is a reversible reaction of two reactants forming one product.

Name React4

Notes second ligand on active

## **Reaction equation**

$$AL + L \rightleftharpoons ALL$$
 (9)

#### **Reactants**

Table	: 14: 1	Properties of e	each read	ctant.
	Id	Name	SBO	
	AL	ActiveACh		
	L	ACh		

#### Product

Tab	le 15: l	Properties of ea	ch product.
	Id	Name	SBO
	ALL	ActiveACh2	

#### **Kinetic Law**

**Notes**  $kf_4 * AL * L - kr_4 * ALL$ 

Derived unit contains undeclared units

$$v_5 = \operatorname{vol}(\operatorname{comp1}) \cdot (\operatorname{kf}_4 \cdot [\operatorname{AL}] \cdot [\operatorname{L}] - \operatorname{kr}_4 \cdot [\operatorname{ALL}])$$
(10)

### 6.6 Reaction React5

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

Name React5

Notes opening of unliganded

#### **Reaction equation**

$$B \rightleftharpoons A$$
 (11)

#### Reactant

Table 16	6: Pro	operties c	of each 1	reactant
	Id	Name	SBO	
	В	Basal		

Product

 Table 17: Properties of each product.

 Id
 Name
 SBO

 A
 Active

#### **Kinetic Law**

**Notes**  $kf_5 * B - kr_5 * A$ 

Derived unit contains undeclared units

$$v_6 = \operatorname{vol}(\operatorname{comp1}) \cdot (\operatorname{kf}_5 \cdot [B] - \operatorname{kr}_5 \cdot [A])$$
(12)

# 6.7 Reaction React6

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

Name React6

Notes opening of monoliganded

**Reaction equation** 

$$BL \rightleftharpoons AL$$
 (13)

Produced by SBML2ATEX

# Reactant

Table	18: F	: Properties of each reactant.				
	Id	Name	SBO			
	BL	BasalACh				

#### Product

Table	19: Properties of each product				
	Id	Name	SBO		
	AL	ActiveACh			

# **Kinetic Law**

**Notes**  $kf_6 * BL - kr_6 * AL$ 

Derived unit contains undeclared units

$$v_7 = \operatorname{vol}(\operatorname{comp1}) \cdot (\operatorname{kf_-6} \cdot [\operatorname{BL}] - \operatorname{kr_-6} \cdot [\operatorname{AL}])$$
(14)

## 6.8 Reaction React7

This is a reversible reaction of two reactants forming one product.

Name React7

Notes first ligand on intermediate

**Reaction equation** 

$$I + L \rightleftharpoons IL$$
 (15)

#### **Reactants**

Id	Name	SBO
Ι	Intermediate	
L	ACh	

# Product

Ta	Cable 21: Properties of each product				
	Id	Name	SBO		
	IL	IntermediateACh			

**Kinetic Law** 

Notes  $kf_7 * I * L - kr_7 * IL$ 

**Derived unit** contains undeclared units

$$v_8 = \operatorname{vol}(\operatorname{comp1}) \cdot (\operatorname{kf}_7 \cdot [I] \cdot [L] - \operatorname{kr}_7 \cdot [IL])$$
(16)

#### 6.9 Reaction React8

This is a reversible reaction of two reactants forming one product.

Name React8

**Notes** second ligand on intermediate

**Reaction equation** 

$$IL + L \rightleftharpoons ILL \tag{17}$$

# Reactants

Та	Table 22: Properties of each reactant.				
	Id	Name	SBO		
	IL	IntermediateACh			
	L	ACh			

#### Product

Table 23: Properties of each product.					
	Id	Name	SBO		
	ILL	IntermediateACh2			

#### **Kinetic Law**

Notes  $kf_8 * IL * L - kr_8 * ILL$ 

Derived unit contains undeclared units

$$v_9 = \operatorname{vol}(\operatorname{comp1}) \cdot (\operatorname{kf}_{-8} \cdot [\operatorname{IL}] \cdot [\operatorname{L}] - \operatorname{kr}_{-8} \cdot [\operatorname{ILL}])$$
(18)

#### 6.10 Reaction React9

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

Name React9

**Notes** unlig act <=> unlig interm

**Reaction equation** 

$$A \rightleftharpoons I \tag{19}$$

Reactant

 Table 24: Properties of each reactant.

 Id
 Name
 SBO

 A
 Active

Product

Tabl	ble 25: Properties of each prod		
	Id	Name	SBO
	I	Intermediate	

**Kinetic Law** 

Notes  $kf_9 * A - kr_9 * I$ 

Derived unit contains undeclared units

$$v_{10} = \operatorname{vol}\left(\operatorname{comp1}\right) \cdot \left(\operatorname{kf_9} \cdot [A] - \operatorname{kr_9} \cdot [I]\right)$$
(20)

#### 6.11 Reaction React10

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

Produced by SBML2ATEX

Name React10

**Notes** monolig act <=> monolig interm

#### **Reaction equation**

$$AL \rightleftharpoons IL$$
 (21)

# Reactant

Table 26: Properties of each reactant.				
	Id	Name	SBO	
	AL	ActiveACh		

#### Product

Та	ıble	27: Properties of eac	h product.
	Id	Name	SBO
	IL	IntermediateACh	

#### **Kinetic Law**

Notes  $kf_10 * AL - kr_10 * IL$ 

**Derived unit** contains undeclared units

$$v_{11} = \operatorname{vol}(\operatorname{comp1}) \cdot (\operatorname{kf}_{-}10 \cdot [\operatorname{AL}] - \operatorname{kr}_{-}10 \cdot [\operatorname{IL}])$$
(22)

#### 6.12 Reaction React11

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

Name React11

**Notes** bilig act <=> bilig interm

#### **Reaction equation**

$$ALL \rightleftharpoons ILL$$
 (23)

Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
ALL	ActiveACh2	

# Product

1	Table 29: Properties of each product.				
	Id	Name	SBO		
	ILL	IntermediateACh2			

# **Kinetic Law**

**Notes**  $kf_11 * ALL - kr_11 * ILL$ 

**Derived unit** contains undeclared units

$$v_{12} = \operatorname{vol}(\operatorname{comp1}) \cdot (\operatorname{kf}_{-}11 \cdot [\operatorname{ALL}] - \operatorname{kr}_{-}11 \cdot [\operatorname{ILL}])$$
(24)

## 6.13 Reaction React12

This is a reversible reaction of two reactants forming one product.

Name React12

Notes first ligand on desensitised

#### **Reaction equation**

$$D + L \Longrightarrow DL$$
 (25)

# Reactants

Table 30: Properties of each reactant.			
	Id	Name	SBO
	D	Desensitised	
	L	ACh	

# Product

Table 31: Properties of each product.

Id	Name	SBO
DL	DesensitisedACh	

# **Kinetic Law**

**Notes**  $kf_12 * D * L - kr_12 * DL$ 

Derived unit contains undeclared units

$$v_{13} = \operatorname{vol}(\operatorname{comp1}) \cdot (\operatorname{kf}_{-12} \cdot [D] \cdot [L] - \operatorname{kr}_{-12} \cdot [DL])$$
(26)

# 6.14 Reaction React13

This is a reversible reaction of two reactants forming one product.

Name React13

Notes second ligand on desensitised

#### **Reaction equation**

$$DL + L \rightleftharpoons DLL$$
 (27)

**Reactants** 

Та	Cable 32: Properties of each reactant.				
	Id	Name	SBO		
	DL	DesensitisedACh			
	L	ACh			

#### Product

Table 33: Properties of each product.			
	Id	Name	SBO
	DLL	L DesensitisedACh2	

#### **Kinetic Law**

Notes  $kf_13 * DL * L - kr_13 * DLL$ 

Derived unit contains undeclared units

$$v_{14} = \operatorname{vol}(\operatorname{comp1}) \cdot (\operatorname{kf}_{-13} \cdot [\operatorname{DL}] \cdot [\operatorname{L}] - \operatorname{kr}_{-13} \cdot [\operatorname{DLL}])$$

$$(28)$$

#### 6.15 Reaction React14

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

Name React14

**Notes** unlig interm <=> unlig desen

**Reaction equation** 

$$I \rightleftharpoons D \tag{29}$$

#### Reactant

Table 34: Properties of each reactant. Id Name SBO I Intermediate

**Product** 

Table 35: Properties of each product.			
·	Id	Name	SBO
	D	Desensitised	

**Kinetic Law** 

**Notes**  $kf_{-}14 * I - kr_{-}14 * D$ 

Derived unit contains undeclared units

$$v_{15} = \operatorname{vol}(\operatorname{comp1}) \cdot (\operatorname{kf}_{-}14 \cdot [\mathrm{I}] - \operatorname{kr}_{-}14 \cdot [\mathrm{D}])$$
(30)

#### 6.16 Reaction React15

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

Name React15

**Notes** monolig interm <=> monolig desen

# **Reaction equation**

$$IL \rightleftharpoons DL$$
 (31)

# Reactant

Та	Table 36: Properties of each reactant.		
	Id	Name	SBO
	IL	IntermediateACh	

# Product

Table 37: Properties of each product.			
	Id	Name	SBO
	DL	DesensitisedACh	

#### **Kinetic Law**

**Notes** kf\_15 \* IL - kr\_15 \* DL

**Derived unit** contains undeclared units

$$v_{16} = \operatorname{vol}(\operatorname{comp1}) \cdot (\operatorname{kf}_{-15} \cdot [\operatorname{IL}] - \operatorname{kr}_{-15} \cdot [\operatorname{DL}])$$
(32)

# 6.17 Reaction React16

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

Name React16

**Notes** bilig interm <=> bilig desen

# **Reaction equation**

$$ILL \Longrightarrow DLL$$
 (33)

#### Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
ILL	IntermediateACh2	

## Product

Table 39: Properties of each product.			
Id	Name	SBO	
DLL DesensitisedACh2		ACh2	

## **Kinetic Law**

Notes  $kf_16 * ILL - kr_16 * DLL$ 

Derived unit contains undeclared units

$$v_{17} = \operatorname{vol}(\operatorname{comp1}) \cdot (\operatorname{kf_16} \cdot [\operatorname{ILL}] - \operatorname{kr_16} \cdot [\operatorname{DLL}])$$
(34)

# 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 BLL

Name BasalACh2

Notes biliganded basal state

Initial amount 0 mol

This species takes part in two reactions (as a reactant in React2 and as a product in React1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{BLL} = v_2 - v_3 \tag{35}$$

#### 7.2 Species IL

Name IntermediateACh

Notes monoliganded intermediate

#### Initial amount 0 mol

This species takes part in four reactions (as a reactant in React8, React15 and as a product in React7, React10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IL} = v_8 + v_{11} - v_9 - v_{16} \tag{36}$$

#### 7.3 Species AL

Name ActiveACh

Notes monoliganded active state

#### Initial amount 0 mol

This species takes part in four reactions (as a reactant in React4, React10 and as a product in React3, React6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AL} = v_4 + v_7 - v_5 - v_{11} \tag{37}$$

#### 7.4 Species A

Name Active

Notes unkiganded active state

#### Initial amount 0 mol

This species takes part in three reactions (as a reactant in React3, React9 and as a product in React5).

$$\frac{d}{dt}A = v_6 - v_4 - v_{10}$$
(38)

#### 7.5 Species BL

Name BasalACh

Notes monoliganded basal state

#### Initial amount 0 mol

This species takes part in three reactions (as a reactant in React1, React6 and as a product in React0).

$$\frac{d}{dt}BL = v_1 - v_2 - v_7$$
(39)

### 7.6 Species B

Name Basal

Notes unliganded basal state

Initial amount  $10^{-22}$  mol

This species takes part in two reactions (as a reactant in React0, React5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{B} = -v_1 - v_6 \tag{40}$$

#### 7.7 Species DLL

Name DesensitisedACh2

Notes biliganded desensitised state

Initial amount 0 mol

This species takes part in two reactions (as a product in React13, React16).

$$\frac{d}{dt}DLL = v_{14} + v_{17}$$
(41)

#### 7.8 Species D

Name Desensitised

**Notes** fully desensitised state

**Initial amount** 0 mol

This species takes part in two reactions (as a reactant in React12 and as a product in React14).

$$\frac{d}{dt}D = v_{15} - v_{13}$$
(42)

#### 7.9 Species ILL

Name IntermediateACh2

Notes biliganded intermediate

Initial amount 0 mol

This species takes part in three reactions (as a reactant in React16 and as a product in React8, React11).

$$\frac{d}{dt}ILL = v_9 + v_{12} - v_{17}$$
(43)

# 7.10 Species DL

Name DesensitisedACh

Notes monoliganded desensitised state

#### Initial amount 0 mol

This species takes part in three reactions (as a reactant in React13 and as a product in React12, React15).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DL} = v_{13} + v_{16} - v_{14} \tag{44}$$

#### 7.11 Species I

Name Intermediate

Notes unliganted intermediate

#### Initial amount 0 mol

This species takes part in three reactions (as a reactant in React7, React14 and as a product in React9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{I} = v_{10} - v_8 - v_{15} \tag{45}$$

## 7.12 Species ALL

Name ActiveACh2

Notes biliganted active state

Initial amount 0 mol

This species takes part in three reactions (as a reactant in React11 and as a product in React2, React4).

$$\frac{d}{dt}ALL = v_3 + v_5 - v_{12}$$
(46)

#### 7.13 Species L

Name ACh

Notes ligand

Initial amount  $10^{-21}$  mol

This species takes part in eight reactions (as a reactant in React0, React1, React3, React4, React7, React8, React12, React13).

$$\frac{d}{dt}L = -v_1 - v_2 - v_4 - v_5 - v_8 - v_9 - v_{13} - v_{14}$$
(47)

Produced by SBML2ATEX

**BML2**<sup>AT</sup>EX 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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