SBML Model Report

Model name: “Edelstein1996 - EPSP ACh event”

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Nicolas Le Novre[1] at February second 2005 at 2:56 p. m. and last time modified at October 31st 2014 at 5:17 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	12
events	1	constraints	0
reactions	17	function definitions	0
global parameters	35	unit definitions	0
rules	0	initial assignments	0

Model Notes

Edelstein1996 - EPSP ACh event

Model of a nicotinic Excitatory Post-Synaptic Potential in a Torpedo electric organ. Acetylcholine is not represented explicitely, but by an event that changes the constants of transition from unliganded to liganded.

This model has initially been encoded using StochSim.

[1]EMBL-EBI, lenov@ebi.ac.uk

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: BIOMD0000000001 .

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

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
comp1	compartment1	0000290	3	10^{-16}	l	☑	

3.1 Compartment comp1

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

Name compartment1

SBO:0000290 physical compartment

4 Species

This model contains twelve species. 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
BLL	BasalACh2	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
IL	IntermediateACh	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
AL	ActiveACh	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
A	Active	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
BL	BasalACh	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
B	Basal	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DLL	DesensitisedACh2	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
D	Desensitised	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ILL	IntermediateACh2	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DL	DesensitisedACh	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
I	Intermediate	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ALL	ActiveACh2	comp1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 35 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kf_0		0000035	3000.000		☐
kr_0		0000038	8000.000		☑
kf_1		0000035	1500.000		☐
kr_1		0000038	16000.000		☑
kf_2		0000035	30000.000		☑
kr_2		0000038	700.000		☑
kf_3		0000035	3000.000		☐
kr_3		0000038	8.640		☑
kf_4		0000035	1500.000		☐
kr_4		0000038	17.280		☑
kf_5		0000035	0.540		☑
kr_5		0000038	10800.000		☑
kf_6		0000035	130.000		☑
kr_6		0000038	2740.000		☑
kf_7		0000035	3000.000		☐
kr_7		0000038	4.000		☑
kf_8		0000035	1500.000		☐
kr_8		0000038	8.000		☑
kf_9		0000035	19.700		☑
kr_9		0000038	3.740		☑
kf_10		0000035	19.850		☑
kr_10		0000038	1.740		☑
kf_11		0000035	20.000		☑
kr_11		0000038	0.810		☑
kf_12		0000035	3000.000		☐
kr_12		0000038	4.000		☑
kf_13		0000035	1500.000		☐
kr_13		0000038	8.000		☑
kf_14		0000035	0.050		☑
kr_14		0000038	0.001		☑
kf_15		0000035	0.050		☑
kr_15		0000038	0.001		☑
kf_16		0000035	0.050		☑
kr_16		0000038	0.001		☑
t2			20.000		☑

6 Event

This is an overview of one event. Each event is initiated whenever its trigger condition switches from `false` to `true`. A delay function postpones the effects of an event to a later time point. At the time of execution, an event can assign values to species, parameters or compartments if these are not set to constant.

6.1 Event `RemovalACh`

Name removal of ACh

Trigger condition

$$\text{time} > \text{t2} \tag{1}$$

Assignments

$$\text{kf\_0} = 0 \tag{2}$$
$$\text{kf\_3} = 0 \tag{3}$$
$$\text{kf\_7} = 0 \tag{4}$$
$$\text{kf\_12} = 0 \tag{5}$$
$$\text{kf\_1} = 0 \tag{6}$$
$$\text{kf\_4} = 0 \tag{7}$$
$$\text{kf\_8} = 0 \tag{8}$$
$$\text{kf\_13} = 0 \tag{9}$$

7 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.

Table 5: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	React0	React0	B $\rightleftharpoons$ BL	0000177
2	React1	React1	BL $\rightleftharpoons$ BLL	0000177
3	React2	React2	BLL $\rightleftharpoons$ ALL	0000181
4	React3	React3	A $\rightleftharpoons$ AL	0000177
5	React4	React4	AL $\rightleftharpoons$ ALL	0000177
6	React5	React5	B $\rightleftharpoons$ A	0000181
7	React6	React6	BL $\rightleftharpoons$ AL	0000181
8	React7	React7	I $\rightleftharpoons$ IL	0000177
9	React8	React8	IL $\rightleftharpoons$ ILL	0000177
10	React9	React9	A $\rightleftharpoons$ I	0000181
11	React10	React10	AL $\rightleftharpoons$ IL	0000181
12	React11	React11	ALL $\rightleftharpoons$ ILL	0000181
13	React12	React12	D $\rightleftharpoons$ DL	0000177
14	React13	React13	DL $\rightleftharpoons$ DLL	0000177
15	React14	React14	I $\rightleftharpoons$ D	0000181
16	React15	React15	IL $\rightleftharpoons$ DL	0000181
17	React16	React16	ILL $\rightleftharpoons$ DLL	0000181

7.1 Reaction React0

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

Name React0

SBO:0000177 non-covalent binding

Notes first ligand on basal

Reaction equation

$$\mathrm{B} \rightleftharpoons \mathrm{BL} \tag{10}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
B	Basal	0000010

Product

Table 7: Properties of each product.

Id	Name	SBO
BL	BasalACh	0000011

Kinetic Law

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme

Notes kf_0 * B - kr_0 * BL

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{comp1}) \cdot (\mathrm{kf\_0} \cdot [\mathrm{B}] - \mathrm{kr\_0} \cdot [\mathrm{BL}]) \tag{11}$$

7.2 Reaction React1

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

Name React1

SBO:0000177 non-covalent binding

Notes second ligand on basal

Reaction equation

$$\mathrm{BL} \rightleftharpoons \mathrm{BLL} \tag{12}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
BL	BasalACh	0000010

Product

Table 9: Properties of each product.

Id	Name	SBO
BLL	BasalACh2	0000011

Kinetic Law

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme

Notes kf_1 * BL - kr_1 * BLL

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}(\mathrm{comp1}) \cdot (\mathrm{kf\_1} \cdot [\mathrm{BL}] - \mathrm{kr\_1} \cdot [\mathrm{BLL}]) \tag{13}$$

7.3 Reaction React2

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

Name React2

SBO:0000181 conformational transition

Notes opening of biliganded

Reaction equation

$$\mathrm{BLL} \rightleftharpoons \mathrm{ALL} \tag{14}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
BLL	BasalACh2	0000010

Product

Table 11: Properties of each product.

Id	Name	SBO
ALL	ActiveACh2	0000011

Kinetic Law

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme

Notes kf_2 * BLL - kr_2 * ALL

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{comp1}) \cdot (\mathrm{kf\_2} \cdot [\mathrm{BLL}] - \mathrm{kr\_2} \cdot [\mathrm{ALL}]) \tag{15}$$

7.4 Reaction React3

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

Name React3

SBO:0000177 non-covalent binding

Notes first ligand on active

Reaction equation

$$\mathrm{A} \rightleftharpoons \mathrm{AL} \tag{16}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
A	Active	0000010

Product

Table 13: Properties of each product.

Id	Name	SBO
AL	ActiveACh	0000011

Kinetic Law

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme

Notes kf_3 * A - kr_3 * AL

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}(\mathrm{comp1}) \cdot (\mathrm{kf\_3} \cdot [\mathrm{A}] - \mathrm{kr\_3} \cdot [\mathrm{AL}]) \tag{17}$$

7.5 Reaction React4

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

Name React4

SBO:0000177 non-covalent binding

Notes second ligand on active

Reaction equation

$$\mathrm{AL} \rightleftharpoons \mathrm{ALL} \tag{18}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
AL	ActiveACh	0000010

Product

Table 15: Properties of each product.

Id	Name	SBO
ALL	ActiveACh2	0000011

Kinetic Law

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme

Notes kf_4 * AL - kr_4 * ALL

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}(\mathrm{comp1}) \cdot (\mathrm{kf\_4} \cdot [\mathrm{AL}] - \mathrm{kr\_4} \cdot [\mathrm{ALL}]) \tag{19}$$

7.6 Reaction React5

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

Name React5

SBO:0000181 conformational transition

Notes opening of unliganded

Reaction equation

$$\mathrm{B} \rightleftharpoons \mathrm{A} \tag{20}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
B	Basal	0000010

Product

Table 17: Properties of each product.

Id	Name	SBO
A	Active	0000011

Kinetic Law

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme

Notes kf_5 * B - kr_5 * A

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{comp1}) \cdot (\mathrm{kf\_5} \cdot [\mathrm{B}] - \mathrm{kr\_5} \cdot [\mathrm{A}]) \tag{21}$$

7.7 Reaction React6

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

Name React6

SBO:0000181 conformational transition

Notes opening of monoliganded

Reaction equation

$$\mathrm{BL} \rightleftharpoons \mathrm{AL} \tag{22}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
BL	BasalACh	0000010

Product

Table 19: Properties of each product.

Id	Name	SBO
AL	ActiveACh	0000011

Kinetic Law

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme

Notes kf_6 * BL - kr_6 * AL

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}(\mathrm{comp1}) \cdot (\mathrm{kf\_6} \cdot [\mathrm{BL}] - \mathrm{kr\_6} \cdot [\mathrm{AL}]) \tag{23}$$

7.8 Reaction React7

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

Name React7

SBO:0000177 non-covalent binding

Notes first ligand on intermediate

Reaction equation

$$\mathrm{I} \rightleftharpoons \mathrm{IL} \tag{24}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
I	Intermediate	0000010

Product

Table 21: Properties of each product.

Id	Name	SBO
IL	IntermediateACh	0000011

Kinetic Law

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme

Notes kf_7 * I - kr_7 * IL

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}(\mathrm{comp1}) \cdot (\mathrm{kf\_7} \cdot [\mathrm{I}] - \mathrm{kr\_7} \cdot [\mathrm{IL}]) \tag{25}$$

7.9 Reaction React8

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

Name React8

SBO:0000177 non-covalent binding

Notes second ligand on intermediate

Reaction equation

$$\mathrm{IL} \rightleftharpoons \mathrm{ILL} \tag{26}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
IL	IntermediateACh	0000010

Product

Table 23: Properties of each product.

Id	Name	SBO
ILL	IntermediateACh2	0000011

Kinetic Law

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme

Notes kf_8 * IL - kr_8 * ILL

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}(\mathrm{comp1}) \cdot (\mathrm{kf\_8} \cdot [\mathrm{IL}] - \mathrm{kr\_8} \cdot [\mathrm{ILL}]) \tag{27}$$

7.10 Reaction React9

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

Name React9

SBO:0000181 conformational transition

Notes unliganded active <=> unliganded intermediate

Reaction equation

$$\mathrm{A} \rightleftharpoons \mathrm{I} \tag{28}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
A	Active	0000010

Product

Table 25: Properties of each product.

Id	Name	SBO
I	Intermediate	0000011

Kinetic Law

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme

Notes kf_9 * A - kr_9 * I

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}(\mathrm{comp1}) \cdot (\mathrm{kf\_9} \cdot [\mathrm{A}] - \mathrm{kr\_9} \cdot [\mathrm{I}]) \tag{29}$$

7.11 Reaction React10

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

Name React10

SBO:0000181 conformational transition

Notes monoliganded active <=> monoliganded intermediate

Reaction equation

$$\mathrm{AL} \rightleftharpoons \mathrm{IL} \tag{30}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
AL	ActiveACh	0000010

Product

Table 27: Properties of each product.

Id	Name	SBO
IL	IntermediateACh	0000011

Kinetic Law

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme

Notes kf_10 * AL - kr_10 * IL

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}(\mathrm{comp1}) \cdot (\mathrm{kf\_10} \cdot [\mathrm{AL}] - \mathrm{kr\_10} \cdot [\mathrm{IL}]) \tag{31}$$

7.12 Reaction React11

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

Name React11

SBO:0000181 conformational transition

Notes biliganded active <=> biliganded intermediate

Reaction equation

$$\mathrm{ALL} \rightleftharpoons \mathrm{ILL} \tag{32}$$

Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
ALL	ActiveACh2	0000010

Product

Table 29: Properties of each product.

Id	Name	SBO
ILL	IntermediateACh2	0000011

Kinetic Law

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme

Notes kf_11 * ALL - kr_11 * ILL

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}(\mathrm{comp1}) \cdot (\mathrm{kf\_11} \cdot [\mathrm{ALL}] - \mathrm{kr\_11} \cdot [\mathrm{ILL}]) \tag{33}$$

7.13 Reaction React12

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

Name React12

SBO:0000177 non-covalent binding

Notes first ligand on desensitised

Reaction equation

$$\mathrm{D} \rightleftharpoons \mathrm{DL} \tag{34}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
D	Desensitised	0000010

Product

Table 31: Properties of each product.

Id	Name	SBO
DL	DesensitisedACh	0000011

Kinetic Law

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme

Notes kf_12 * D - kr_12 * DL

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}(\mathrm{comp1}) \cdot (\mathrm{kf\_12} \cdot [\mathrm{D}] - \mathrm{kr\_12} \cdot [\mathrm{DL}]) \tag{35}$$

7.14 Reaction React13

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

Name React13

SBO:0000177 non-covalent binding

Notes second ligand on desensitised

Reaction equation

$$\mathrm{DL} \rightleftharpoons \mathrm{DLL} \tag{36}$$

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
DL	DesensitisedACh	0000010

Product

Table 33: Properties of each product.

Id	Name	SBO
DLL	DesensitisedACh2	0000011

Kinetic Law

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme

Notes kf_13 * DL - kr_13 * DLL

Derived unit contains undeclared units

$$v_{14} = \mathrm{vol}\,(\mathrm{comp1}) \cdot (\mathrm{kf\_13} \cdot [\mathrm{DL}] - \mathrm{kr\_13} \cdot [\mathrm{DLL}]) \tag{37}$$

7.15 Reaction React14

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

Name React14

SBO:0000181 conformational transition

Notes unliganded intermediate <=> unliganded desensitised

Reaction equation

$$\mathrm{I} \rightleftharpoons \mathrm{D} \tag{38}$$

Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
I	Intermediate	0000010

Product

Table 35: Properties of each product.

Id	Name	SBO
D	Desensitised	0000011

Kinetic Law

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme

Notes kf_14 * I - kr_14 * D

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}(\mathrm{comp1}) \cdot (\mathrm{kf\_14} \cdot [\mathrm{I}] - \mathrm{kr\_14} \cdot [\mathrm{D}]) \tag{39}$$

7.16 Reaction React15

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

Name React15

SBO:0000181 conformational transition

Notes monoliganded intermediate <=> monoliganded desensitised

Reaction equation

$$\mathrm{IL} \rightleftharpoons \mathrm{DL} \tag{40}$$

Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
IL	IntermediateACh	0000010

Product

Table 37: Properties of each product.

Id	Name	SBO
DL	DesensitisedACh	0000011

Kinetic Law

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme

Notes kf_15 * IL - kr_15 * DL

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}(\mathrm{comp1}) \cdot (\mathrm{kf\_15} \cdot [\mathrm{IL}] - \mathrm{kr\_15} \cdot [\mathrm{DL}]) \tag{41}$$

7.17 Reaction React16

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

Name React16

SBO:0000181 conformational transition

Notes biliganded intermediate <=> biliganded desensitised

Reaction equation

$$\mathrm{ILL} \rightleftharpoons \mathrm{DLL} \tag{42}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
ILL	IntermediateACh2	0000010

Product

Table 39: Properties of each product.

Id	Name	SBO
DLL	DesensitisedACh2	0000011

Kinetic Law

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme

Notes kf_16 * ILL - kr_16 * DLL

Derived unit contains undeclared units

$$v_{17} = \mathrm{vol}\,(\mathrm{comp1}) \cdot (\mathrm{kf\_16} \cdot [\mathrm{ILL}] - \mathrm{kr\_16} \cdot [\mathrm{DLL}]) \tag{43}$$

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.

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.

8.1 Species BLL

Name BasalACh2

SBO:0000297 protein complex

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{BLL} = v_2 - v_3 \tag{44}$$

8.2 Species IL

Name IntermediateACh

SBO:0000297 protein complex

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IL} = v_8 + v_{11} - v_9 - v_{16} \tag{45}$$

8.3 Species AL

Name ActiveACh

SBO:0000297 protein complex

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AL} = v_4 + v_7 - v_5 - v_{11} \tag{46}$$

8.4 Species A

Name Active

SBO:0000420 multimer of macromolecules

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A} = v_6 - v_4 - v_{10} \tag{47}$$

8.5 Species BL

Name BasalACh

SBO:0000297 protein complex

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{BL} = v_1 - v_2 - v_7 \tag{48}$$

8.6 Species B

Name Basal

SBO:0000420 multimer of macromolecules

Notes unliganded basal state

Initial amount $1.66057788110262 \cdot 10^{-21}$ mol

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{B} = -v_1 - v_6 \tag{49}$$

8.7 Species DLL

Name DesensitisedACh2

SBO:0000297 protein complex

Notes biliganded desensitised state

Initial amount 0 mol

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DLL} = v_{14} + v_{17} \tag{50}$$

8.8 Species D

Name Desensitised

SBO:0000420 multimer of macromolecules

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{D} = v_{15} - v_{13} \tag{51}$$

8.9 Species ILL

Name IntermediateACh2

SBO:0000297 protein complex

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ILL} = v_{9} + v_{12} - v_{17} \tag{52}$$

8.10 Species DL

Name DesensitisedACh

SBO:0000297 protein complex

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DL} = v_{13} + v_{16} - v_{14} \tag{53}$$

8.11 Species I

Name Intermediate

SBO:0000420 multimer of macromolecules

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{I} = v_{10} - v_{8} - v_{15} \tag{54}$$

8.12 Species ALL

Name ActiveACh2

SBO:0000297 protein complex

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ALL} = v_{3} + v_{5} - v_{12} \tag{55}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000010 reactant: Substance consumed by a chemical reaction. Reactants react with each other to form the products of a chemical reaction. In a chemical equation the Reactants are the elements or compounds on the left hand side of the reaction equation. A reactant can be consumed and produced by the same reaction, its global quantity remaining unchanged

SBO:0000011 product: Substance that is produced in a reaction. In a chemical equation the Products are the elements or compounds on the right hand side of the reaction equation. A product can be produced and consumed by the same reaction, its global quantity remaining unchanged

SBO:0000035 forward unimolecular rate constant, continuous case: Numerical parameter that quantifies the forward velocity of a chemical reaction involving only one reactant. This parameter encompasses all the contributions to the velocity except the quantity of the reactant. It is to be used in a reaction modelled using a continuous framework

SBO:0000038 reverse unimolecular rate constant, continuous case: Numerical parameter that quantifies the reverse velocity of a chemical reaction involving only one product. This parameter encompasses all the contributions to the velocity except the quantity of the product. It is to be used in a reaction modelled using a continuous framework

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme: Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does include a reverse process that creates the reactants from the products. The rate of the forward process is proportional to the quantity of one reactant. The rate of the reverse process is proportional to the quantity of one product. It is to be used in a reaction modelled using a continuous framework.

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

SBO:0000181 conformational transition: Biochemical reaction that does not result in the modification of covalent bonds of reactants, but rather modifies the conformation of some reactants, that is the relative position of their atoms in space

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

SBO:0000297 protein complex: Macromolecular complex containing one or more polypeptide chains possibly associated with simple chemicals. CHEBI:3608

SBO:0000420 multimer of macromolecules: Non-covalent association between several macromolecule

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