SBML Model Report

Model name: "Clancy2002_CardiacSodiumChannel_WT"

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1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Enuo He[1] at July 15th 2007 at 1:35 p. m. and last time modified at October tenth 2014 at 10:23 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	9
events	2	constraints	0
reactions	11	function definitions	0
global parameters	24	unit definitions	2
rules	16	initial assignments	0

Model Notes

The model is according to the paper *Na+ Channel Mutation That Causes Both Brugada and Long-QT Syndrome Phenotypes: A Simulation Study of Mechanism* Original model comes from ModelDB with accession number: 62661. This is the wide type model. All the values and reactions obtained from Data Supplement6: Appendix of the paper. Figure3 has been reproduced by MathSBML. The stimulus v=-30mV during the time from 5ms to 20 ms displayed in the event.

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The meaning for the keyword, C: Close states; O: Open states; IF: Fast inactivation states; IC: Closed-Inactivation states; IM: Intermediat Inactivation states.

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

2.1 Unit `unitDefinition_0000001`

Name time(ms)

Definition ms

2.2 Unit `unitDefinition_0000002`

Name voltage(mV)

Definition mV

2.3 Unit `substance`

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

Definition mol

2.4 Unit `volume`

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

Definition l

2.5 Unit area

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

Definition m^2

2.6 Unit length

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

Definition m

2.7 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
cell			3	1	litre	☑	

3.1 Compartment cell

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

4 Species

This model contains nine species. Section 9 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
C1		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C2		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C3		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
IC3		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
IC2		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
IM1		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
IM2		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
O	open states	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
IF		cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 24 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
nao	[Na]out		140.0		☑
nai	[Na]in		15.0		☑
scale			1000.0		☑
v			−80.0		☐
Ena			0.0		☐
a11			0.0		☐
a12			0.0		☐
a13			0.0		☐
b11			0.0		☐
b12			0.0		☐
b13			0.0		☐
a2			0.0		☐
b2			0.0		☐
a3			0.0		☐
b3			0.0		☐
a4			0.0		☐
b4			0.0		☐
a5			0.0		☐
b5			0.0		☐
Gna			23.5		☑
Rk			8314.0		☑
Fara			96485.0		☑
Temp			310.0		☑
Ina	I_Na		0.0		☐

6 Rules

This is an overview of 16 rules.

6.1 Rule a11

Rule a11 is an assignment rule for parameter a11:

$$\mathrm{a11} = \frac{3.802}{0.1027 \cdot \exp\left(\frac{\mathrm{v}}{17}\right) + 0.2 \cdot \exp\left(\frac{\mathrm{v}}{150}\right)} \tag{1}$$

6.2 Rule a12

Rule a12 is an assignment rule for parameter a12:

$$\mathrm{a12} = \frac{3.802}{0.1027 \cdot \exp\left(\frac{\mathrm{v}}{15}\right) + 0.23 \cdot \exp\left(\frac{\mathrm{v}}{150}\right)} \tag{2}$$

6.3 Rule a13

Rule a13 is an assignment rule for parameter a13:

$$\mathrm{a13} = \frac{3.802}{0.1027 \cdot \exp\left(\frac{\mathrm{v}}{12}\right) + 0.25 \cdot \exp\left(\frac{\mathrm{v}}{150}\right)} \tag{3}$$

6.4 Rule a2

Rule a2 is an assignment rule for parameter a2:

$$\mathrm{a2} = 9.178 \cdot \exp\left(\frac{\mathrm{v}}{29.68}\right) \tag{4}$$

6.5 Rule a3

Rule a3 is an assignment rule for parameter a3:

$$\mathrm{a3} = 3.7933 \cdot 1.0E-7 \cdot \exp\left(\frac{\mathrm{v}}{7.7}\right) \tag{5}$$

6.6 Rule b3

Rule b3 is an assignment rule for parameter b3:

$$\mathrm{b3} = 0.0084 + 2.0E-5 \cdot \mathrm{v} \tag{6}$$

6.7 Rule a4

Rule a4 is an assignment rule for parameter a4:

$$\mathrm{a4} = \frac{\mathrm{a2}}{100} \tag{7}$$

6.8 Rule b4

Rule b4 is an assignment rule for parameter b4:

$$\mathrm{b4} = \mathrm{a3} \tag{8}$$

6.9 Rule a5

Rule a5 is an assignment rule for parameter a5:

$$\mathrm{a5} = \frac{\mathrm{a2}}{9.5 \cdot 10000} \tag{9}$$

6.10 Rule b5

Rule b5 is an assignment rule for parameter b5:

$$\mathrm{b5} = \frac{\mathrm{a3}}{50} \tag{10}$$

6.11 Rule Ena

Rule Ena is an assignment rule for parameter Ena:

$$\mathrm{Ena} = \frac{\mathrm{Rk} \cdot \mathrm{Temp}}{\mathrm{Fara}} \cdot \left(\frac{\mathrm{nao}}{\mathrm{nai}}\right) \tag{11}$$

6.12 Rule Ina

Rule Ina is an assignment rule for parameter Ina:

$$\mathrm{Ina} = \frac{\mathrm{Gna} \cdot \frac{[\mathrm{O}]}{[\mathrm{IC3}]+[\mathrm{IC2}]+[\mathrm{IF}]+[\mathrm{IM1}]+[\mathrm{IM2}]+[\mathrm{C3}]+[\mathrm{C2}]+[\mathrm{C1}]+[\mathrm{O}]} \cdot (\mathrm{v} - \mathrm{Ena})}{\mathrm{scale}} \tag{12}$$

6.13 Rule b11

Rule b11 is an assignment rule for parameter b11:

$$\mathrm{b11} = 0.1917 \cdot \exp\left(\frac{\mathrm{v}}{20.3}\right) \tag{13}$$

6.14 Rule b12

Rule b12 is an assignment rule for parameter b12:

$$\mathrm{b12} = 0.2 \cdot \exp\left(\frac{(\mathrm{v} - 5)}{20.3}\right) \tag{14}$$

6.15 Rule b13

Rule b13 is an assignment rule for parameter b13:

$$\mathrm{b13} = 0.22 \cdot \exp\left(\frac{(\mathrm{v} - 10)}{20.3}\right) \tag{15}$$

6.16 Rule b2

Rule b2 is an assignment rule for parameter b2:

$$\mathrm{b2} = \frac{\mathrm{a13} \cdot \mathrm{a2} \cdot \mathrm{a3}}{\mathrm{b13} \cdot \mathrm{b3}} \tag{16}$$

7 Events

This is an overview of two events. 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.

7.1 Event `event_0000001`

Trigger condition

$$(\text{time} \geq 5) \wedge (\text{time} \leq 20) \tag{17}$$

Assignment

$$\text{v} = -30 \tag{18}$$

7.2 Event `event_0000002`

Trigger condition

$$\text{time} > 20 \tag{19}$$

Assignment

$$\text{v} = -80 \tag{20}$$

8 Reactions

This model contains eleven 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_0000001	IC3=IC2	IC3 $\rightleftharpoons$ IC2	
2	reaction_0000002	IC2=IF	IC2 $\rightleftharpoons$ IF	
3	reaction_0000003	IF=IM1	IF $\rightleftharpoons$ IM1	
4	reaction_0000004	IM1=IM2	IM1 $\rightleftharpoons$ IM2	
5	reaction_0000005	C3=IC3	C3 $\rightleftharpoons$ IC3	
6	reaction_0000006	C2=C3	C2 $\rightleftharpoons$ C3	
7	reaction_0000007	C2=IC2	C2 $\rightleftharpoons$ IC2	
8	reaction_0000008	C1=C2	C1 $\rightleftharpoons$ C2	
9	reaction_0000009	C1=IF	C1 $\rightleftharpoons$ IF	
10	reaction_0000010	IF=O	IF $\rightleftharpoons$ O	
11	reaction_0000011	O=C1	O $\rightleftharpoons$ C1	

8.1 Reaction reaction_0000001

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

Name IC3=IC2

Reaction equation

$$\mathrm{IC3} \rightleftharpoons \mathrm{IC2} \tag{21}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
IC3		

Product

Table 7: Properties of each product.

Id	Name	SBO
IC2		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{IC3}] \cdot \mathrm{a11} - [\mathrm{IC2}] \cdot \mathrm{b11}) \tag{22}$$

8.2 Reaction reaction_0000002

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

Name IC2=IF

Reaction equation

$$\mathrm{IC2} \rightleftharpoons \mathrm{IF} \tag{23}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
IC2		

Product

Table 9: Properties of each product.

Id	Name	SBO
IF		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{IC2}] \cdot \mathrm{a12} - [\mathrm{IF}] \cdot \mathrm{b12}) \tag{24}$$

8.3 Reaction reaction_0000003

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

Name IF=IM1

Reaction equation

$$\mathrm{IF} \rightleftharpoons \mathrm{IM1} \tag{25}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
IF		

Product

Table 11: Properties of each product.

Id	Name	SBO
IM1		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{IF}] \cdot \mathrm{a4} - [\mathrm{IM1}] \cdot \mathrm{b4}) \tag{26}$$

8.4 Reaction `reaction_0000004`

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

Name IM1=IM2

Reaction equation

$$\mathrm{IM1} \rightleftharpoons \mathrm{IM2} \tag{27}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
`IM1`		

Product

Table 13: Properties of each product.

Id	Name	SBO
`IM2`		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{IM1}] \cdot \mathrm{a5} - [\mathrm{IM2}] \cdot \mathrm{b5}) \tag{28}$$

8.5 Reaction `reaction_0000005`

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

Name C3=IC3

Reaction equation

$$\mathrm{C3} \rightleftharpoons \mathrm{IC3} \tag{29}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
C3		

Product

Table 15: Properties of each product.

Id	Name	SBO
IC3		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{C3}] \cdot \mathrm{b3} - [\mathrm{IC3}] \cdot \mathrm{a3}) \tag{30}$$

8.6 Reaction reaction_0000006

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

Name C2=C3

Reaction equation

$$\mathrm{C2} \rightleftharpoons \mathrm{C3} \tag{31}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
C2		

Product

Table 17: Properties of each product.

Id	Name	SBO
C3		

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{C2}] \cdot \mathrm{b11} - [\mathrm{C3}] \cdot \mathrm{a11}) \tag{32}$$

8.7 Reaction reaction_0000007

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

Name C2=IC2

Reaction equation

$$\mathrm{C2} \rightleftharpoons \mathrm{IC2} \tag{33}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
C2		

Product

Table 19: Properties of each product.

Id	Name	SBO
IC2		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{C2}] \cdot \mathrm{b3} - [\mathrm{IC2}] \cdot \mathrm{a3}) \tag{34}$$

8.8 Reaction reaction_0000008

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

Name C1=C2

Reaction equation

$$\mathrm{C1} \rightleftharpoons \mathrm{C2} \tag{35}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
C1		

Product

Table 21: Properties of each product.

Id	Name	SBO
C2		

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}(\mathrm{cell}) \cdot ([\mathrm{C1}] \cdot \mathrm{b12} - [\mathrm{C2}] \cdot \mathrm{a12}) \tag{36}$$

8.9 Reaction reaction_0000009

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

Name C1=IF

Reaction equation

$$\mathrm{C1} \rightleftharpoons \mathrm{IF} \tag{37}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
C1		

Product

Table 23: Properties of each product.

Id	Name	SBO
IF		

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{C1}] \cdot \mathrm{b3} - [\mathrm{IF}] \cdot \mathrm{a3}) \tag{38}$$

8.10 Reaction reaction_0000010

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

Name IF=O

Reaction equation

$$\mathrm{IF} \rightleftharpoons \mathrm{O} \tag{39}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
IF		

Product

Table 25: Properties of each product.

Id	Name	SBO
O	open states	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{IF}] \cdot \mathrm{b2} - \mathrm{a2} \cdot [\mathrm{O}]) \tag{40}$$

8.11 Reaction `reaction_0000011`

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

Name O=C1

Reaction equation

$$\mathrm{O} \rightleftharpoons \mathrm{C1} \tag{41}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
O	open states	

Product

Table 27: Properties of each product.

Id	Name	SBO
C1		

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{cell}) \cdot ([\mathrm{C1}] \cdot \mathrm{a13} + [\mathrm{O}] \cdot \mathrm{b13}) \tag{42}$$

9 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.

9.1 Species `C1`

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

This species takes part in three reactions (as a reactant in `reaction_0000008`, `reaction_0000009` and as a product in `reaction_0000011`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C1} = v_{11} - v_8 - v_9 \tag{43}$$

9.2 Species `C2`

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

This species takes part in three reactions (as a reactant in `reaction_0000006`, `reaction_0000007` and as a product in `reaction_0000008`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C2} = v_8 - v_6 - v_7 \tag{44}$$

9.3 Species `C3`

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

This species takes part in two reactions (as a reactant in `reaction_0000005` and as a product in `reaction_0000006`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C3} = v_6 - v_5 \tag{45}$$

9.4 Species `IC3`

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

This species takes part in two reactions (as a reactant in `reaction_0000001` and as a product in `reaction_0000005`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IC3} = v_5 - v_1 \tag{46}$$

9.5 Species IC2

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

This species takes part in three reactions (as a reactant in reaction_0000002 and as a product in reaction_0000001, reaction_0000007).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IC2} = v_1 + v_7 - v_2 \tag{47}$$

9.6 Species IM1

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

This species takes part in two reactions (as a reactant in reaction_0000004 and as a product in reaction_0000003).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IM1} = v_3 - v_4 \tag{48}$$

9.7 Species IM2

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

This species takes part in one reaction (as a product in reaction_0000004).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IM2} = v_4 \tag{49}$$

9.8 Species O

Name open states

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

This species takes part in two reactions (as a reactant in reaction_0000011 and as a product in reaction_0000010).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{O} = v_{10} - v_{11} \tag{50}$$

9.9 Species IF

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

This species takes part in four reactions (as a reactant in reaction_0000003, reaction_0000010 and as a product in reaction_0000002, reaction_0000009).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IF} = v_2 + v_9 - v_3 - v_{10} \tag{51}$$

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.

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