SBML Model Report

Model name: "Abell2011_CalciumSignaling-_WithAdaptation"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah[1] and Mary N Teruel[2] at August 17th 2011 at 3:57 p. m. and last time modified at September eighth 2011 at 12:03 a. 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	4
species types	0	species	9
events	0	constraints	0
reactions	17	function definitions	0
global parameters	22	unit definitions	0
rules	0	initial assignments	0

Model Notes

This model is from the article:
Parallel adaptive feedback enhances reliability of the Ca2+ signaling system.
Abell E, Ahrends R, Bandara S, Park BO, Teruel MN. Proc Natl Acad Sci U S A. 2011 Aug 15.

[1]EMBL-EBI, viji@ebi.ac.uk
[2]Department of Chemical and Systems Biology, Stanford University, Stanford, CA 94305, mteruel@stanford.edu

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Abstract:
Despite large cell-to-cell variations in the concentrations of individual signaling proteins, cells transmit signals correctly. This phenomenon raises the question of what signaling systems do to prevent a predicted high failure rate. Here we combine quantitative modeling, RNA interference, and targeted selective reaction monitoring (SRM) mass spectrometry, and we show for the ubiquitous and fundamental calcium signaling system that cells monitor cytosolic and endoplasmic reticulum (ER) Ca(2+) levels and adjust in parallel the concentrations of the store-operated Ca(2+) influx mediator stromal interaction molecule (STIM), the plasma membrane Ca(2+) pump plasma membrane Ca-ATPase (PMCA), and the ER Ca(2+) pump sarco/ER Ca(2+)-ATPase (SERCA). Model calculations show that this combined parallel regulation in protein expression levels effectively stabilizes basal cytosolic and ER Ca(2+) levels and preserves receptor signaling. Our results demonstrate that, rather than directly controlling the relative level of signaling proteins in a forward regulation strategy, cells prevent transmission failure by sensing the state of the signaling pathway and using multiple parallel adaptive feedbacks.

Note:

There are two models described in the paper to simulate basal and receptor stimulated Ca $^{2+}$ signaling. 1) No adaptive feedback (MODEL1108050000) and 2) with three slow adaptive feedback loops (this model: MODEL1108050001).

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 Compartments

This model contains four compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
cytosol	cytosol	0000290	3	1	litre	☐	
outside	Outside	0000290	3	1	litre	☑	
mitochondria	mito	0000290	3	1	litre	☑	
ER_store	ER_store	0000290	3	1	litre	☐	cytosol

3.1 Compartment cytosol

This is a three dimensional compartment with a not constant size of one litre.

Name cytosol

SBO:0000290 physical compartment

3.2 Compartment outside

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

Name Outside

SBO:0000290 physical compartment

3.3 Compartment mitochondria

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

Name mito

SBO:0000290 physical compartment

3.4 Compartment ER_store

This is a three dimensional compartment with a not constant size of one litre, which is surrounded by cytosol (cytosol).

Name ER_store

SBO:0000290 physical compartment

4 Species

This model contains nine 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
CaI	CaI	cytosol	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
IP3	IP3	cytosol	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
g	g	cytosol	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
mwaf195932-_a72c_4552_8cf2-_b349b15d39c4	PMCA	cytosol	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
mw0ebc76ad-_49d7_4845_8f88-_04d443fbe7f3	SERCA	cytosol	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
mw7cb2644a-_384a_4bbb_93fd-_fd686e01d7cb	STIM	cytosol	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
mwd6b792d8-_c983_42c1_b3bc-_2494d6a3363e	CaO	outside	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
mw013a7c64-_a9ec_483c_b3b8-_ed658337ee95	CaM	mitochondria	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CaS	CaS	ER_store	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 22 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
A	IP3R		3.000		☑
B	SERCA0		0.266		☑
D	IP3degradation		2.000		☑
E	IP3Rinhibition		5.000		☑
F	IP3Rrecovery		0.018		☑
k2	kSERCA		0.175		☑
L	ERleak		0.010		☑
R	R		1.000		☑
mw92b257b7-_00af-_4fd6_a11b-_8e4655a4ba65	kIP3R		0.175		☑
mw0ad64e84-_bb75-_4be4_a9c3-_2d4741b0f45f	PMleak		0.035		☑
mwfe8e89cf-_3c67-_4dd5_939e-_b4cfee2e0778	kSTIM		1.000		☑
mw004dcb62-_da5f-_41c7_a7bd-_033574894f48	STIM0		0.020		☑
mw78dd80b8-_e003-_4c62_81d1-_547d001767af	kIP3Rca		0.130		☑
mw3a93c3a6-_623a-_44fe_84e9-_a47823defd1f	kPMCA		0.200		☑
mwd21d3f76-_d133-_4053_8e44-_02a538657e0a	PMCA0		0.013		☑

Id	Name	SBO	Value	Unit	Constant
mwf998b218-_be11-_4aa4_81ae-_41141861fb42	kG		1.000		☑
mwfbff577a-_4e9c-_40fe_8777-_eb0ceade28c9	ProtDeg		10^{-6}		☑
mwd8bf5d8f-_ad00-_4119_bde1-_91015ef2cd7c	DirTransf		0.030		☑
mwe3841c25-_6042-_49c2_9feb-_90cbf6751167	kUnip		0.600		☑
mw219cf65d-_18cc-_4f7e_ab5a-_5b87cda6fc43	MitNaCaEx		0.005		☑
mwa3072851-_e3e4-_4767_ac41-_49fa7c0de7a7	Uniport		0.030		☑
mwd3b36919-_202a-_4fed_a3c8-_1a3a60594404	cr		8.000		☑

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.

Table 5: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	kPLC	PLC: Receptor and Ca2+ regulated IP3 production	$\emptyset \xrightarrow{\text{CaI}} \text{IP3}$	
2	JPump	SERCA: Pumps Ca2+ into ER Ca2+ stores	$\text{CaI} \xrightarrow{\text{mw0ebc76ad\_49d7\_4845\_8f88\_04d443fbe7f3}} \text{CaS}$	
3	JChannel	IP3R: IP3 and Ca2+ regulated Ca2+ channel, plus leak	$\text{CaS} \xrightarrow{\text{g, IP3}} \text{CaI}$	
4	kPhosphatase	IP3 phosphatase: Degradation of IP3	$\text{IP3} \longrightarrow \emptyset$	
5	inhibition_parameter1	Inhibition of IP3R (mechanism not well understood)	$\emptyset \xrightarrow{\text{CaI}} \text{g}$	
6	inhibition_parameter2	Recovery of IP3R from Ca2+ iinhibition when Ca2+ drops	$\text{g} \longrightarrow \emptyset$	
7	mwbdcd6a40_1ae7_4c86_a99f_1fba0b8beaf7	Regulation of Orai by STIM, plus leak	$\emptyset \xrightarrow{\text{mw7cb2644a\_384a\_4bbb\_93fd\_fd686e01d7cb, CaS}} \text{CaI}$	
8	mw530793e3_76b2_4483_be11_e94364306712	PMCA: Pumps Ca2+ across PM out of cell	$\text{CaI} \xrightarrow{\text{mwaf195932\_a72c\_4552\_8cf2\_b349b15d39c4}} \emptyset$	

№	Id	Name	Reaction Equation	SBO
9	mw5658298a-_d96a-_4b97_9a4f-_6f06dad35824	PMCA synthesis	$\emptyset \xrightarrow{\text{CaI}}$ mwaf195932_a72c_4552_8cf2_b349b15d39c4	
10	mw700bd02b-_9fc4-_47e7_864a-_967c03874dd6	PMCA degradation	mwaf195932_a72c_4552_8cf2_b349b15d39c4 $\longrightarrow \emptyset$	
11	mw06f8fde4-_d97b-_4d5f_b71e-_d93aa53e9932	SERCA synthesis	$\emptyset \xrightarrow{\text{CaS}}$ mw0ebc76ad_49d7_4845_8f88_04d443fbe7f3	
12	mw8021d532-_dd9b-_4e34_a865-_c2bb1689b0b5	STIM/Orai synthesis	$\emptyset \xrightarrow{\text{CaS, CaI}}$ mw7cb2644a_384a_4bbb_93fd_fd686e01d7cb	
13	mw1f122e51-_99cb-_4a32_a12e-_4c2921920a17	STIM/Orai degradation	mw7cb2644a_384a_4bbb_93fd_fd686e01d7cb $\longrightarrow \emptyset$	
14	mw89d547e1-_8d48-_4cd2_ba3d-_e4390294089d	SERCA degradation	mw0ebc76ad_49d7_4845_8f88_04d443fbe7f3 $\longrightarrow \emptyset$	
15	mwa61047ec-_49c1-_47b2_b78e-_4d84a33d432a	CytToMito	CaI $\longrightarrow$ mw013a7c64_a9ec_483c_b3b8_ed658337ee95	

№	Id	Name	Reaction Equation	SBO
16	ERtoMito	ERtoMito	CaS $\xrightarrow{\text{g, IP3, CaI}}$ mw013a7c64_a9ec_483c_b3b8_ed658337ee95	
17	mw1c50c3d1-_dab9-_423a_8373-_6a4c75479b54	MitoToCytosol	mw013a7c64_a9ec_483c_b3b8_ed658337ee95 $\longrightarrow$ CaI	

6.1 Reaction kPLC

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

Name PLC: Receptor and Ca2+ regulated IP3 production

Reaction equation

$$\emptyset \xrightarrow{\text{CaI}} \text{IP3} \tag{1}$$

Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
CaI	CaI	

Product

Table 7: Properties of each product.

Id	Name	SBO
IP3	IP3	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{R} \cdot [\text{CaI}] \tag{2}$$

6.2 Reaction JPump

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

Name SERCA: Pumps Ca2+ into ER Ca2+ stores

Reaction equation

$$\text{CaI} \xrightarrow{\text{mw0ebc76ad\_49d7\_4845\_8f88\_04d443fbe7f3}} \text{CaS} \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
CaI	CaI	

Modifier

Table 9: Properties of each modifier.

Id	Name	SBO
mw0ebc76ad_49d7_4845_8f88_04d443fbe7f3	SERCA	

Product

Table 10: Properties of each product.

Id	Name	SBO
CaS	CaS	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{[\text{mw0ebc76ad\_49d7\_4845\_8f88\_04d443fbe7f3}] \cdot [\text{CaI}]^2}{[\text{CaI}]^2 + \text{k2}^2} \tag{4}$$

6.3 Reaction JChannel

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

Name IP3R: IP3 and Ca2+ regulated Ca2+ channel, plus leak

Reaction equation

$$\text{CaS} \xrightarrow{\text{g, IP3}} \text{CaI} \tag{5}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
CaS	CaS	

Modifiers

Table 12: Properties of each modifier.

Id	Name	SBO
g	g	
IP3	IP3	

Product

Table 13: Properties of each product.

Id	Name	SBO
CaI	CaI	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = (1 - \text{mwd8bf5d8f\_ad00\_4119\_bde1\_91015ef2cd7c}) \cdot \left(\text{L} + \frac{\frac{(1-[\text{g}])\cdot \text{A}\cdot[\text{IP3}]^2}{[\text{IP3}]^2+\text{mw92b257b7\_00af\_4fd6\_a11b\_8e4655a4ba65}^2} \cdot [\text{CaI}]^2}{[\text{CaI}]^2 + \text{mw78dd80b8\_e003\_4c62\_81d1\_547d001767af}^2} \right) \cdot [\text{CaS}] \quad (6)$$

6.4 Reaction kPhosphatase

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

Name IP3 phosphatase: Degradation of IP3

Reaction equation

$$\text{IP3} \longrightarrow \emptyset \quad (7)$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
IP3	IP3	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{D} \cdot [\mathrm{IP3}] \tag{8}$$

6.5 Reaction inhibition_parameter1

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

Name Inhibition of IP3R (mechanism not well understood)

Reaction equation

$$\emptyset \xrightarrow{\mathrm{CaI}} \mathrm{g} \tag{9}$$

Modifier

Table 15: Properties of each modifier.

Id	Name	SBO
CaI	CaI	

Product

Table 16: Properties of each product.

Id	Name	SBO
g	g	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \frac{\mathrm{E} \cdot [\mathrm{CaI}]^4}{[\mathrm{CaI}]^4 + \mathrm{mwf998b218\_be11\_4aa4\_81ae\_41141861fb42}^4} \cdot (1 - [\mathrm{g}]) \tag{10}$$

6.6 Reaction inhibition_parameter2

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

Name Recovery of IP3R from Ca2+ iinhibition when Ca2+ drops

Reaction equation

$$\mathrm{g} \longrightarrow \emptyset \tag{11}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
g	g	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{F} \cdot [\mathrm{g}] \tag{12}$$

6.7 Reaction mwbdcd6a40_1ae7_4c86_a99f_1fba0b8beaf7

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

Name Regulation of Orai by STIM, plus leak

Reaction equation

$$\emptyset \xrightarrow{\text{mw7cb2644a\_384a\_4bbb\_93fd\_fd686e01d7cb, CaS}} \mathrm{CaI} \tag{13}$$

Modifiers

Table 18: Properties of each modifier.

Id	Name	SBO
mw7cb2644a_384a_4bbb_93fd_fd686e01d7cb	STIM	
CaS	CaS	

Product

Table 19: Properties of each product.

Id	Name	SBO
CaI	CaI	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = [\text{mw7cb2644a\_384a\_4bbb\_93fd\_fd686e01d7cb}] \cdot \left(\text{mw0ad64e84\_bb75\_4be4\_a9c3\_2d4741b0f45f} + \frac{\text{mwfe8e89cf\_3c67\_4dd5\_939e\_b4cfee2e0778}^8}{[\text{CaS}]^8 + \text{mwfe8e89cf\_3c67\_4dd5\_939e\_b4cfee2e0778}^8} \right) \tag{14}$$

6.8 Reaction mw530793e3_76b2_4483_be11_e94364306712

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

Name PMCA: Pumps Ca2+ across PM out of cell

Reaction equation

$$\text{CaI} \xrightarrow{\text{mwaf195932\_a72c\_4552\_8cf2\_b349b15d39c4}} \emptyset \tag{15}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
CaI	CaI	

Modifier

Table 21: Properties of each modifier.

Id	Name	SBO
mwaf195932_a72c_4552_8cf2_b349b15d39c4	PMCA	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \frac{[\text{mwaf195932\_a72c\_4552\_8cf2\_b349b15d39c4}] \cdot [\text{CaI}]^2}{[\text{CaI}]^2 + \text{mw3a93c3a6\_623a\_44fe\_84e9\_a47823defd1f}^2} \tag{16}$$

6.9 Reaction mw5658298a_d96a_4b97_9a4f_6f06dad35824

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

Name PMCA synthesis

Reaction equation

$$\emptyset \xrightarrow{\text{CaI}} \text{mwaf195932\_a72c\_4552\_8cf2\_b349b15d39c4} \tag{17}$$

Modifier

Table 22: Properties of each modifier.

Id	Name	SBO
CaI	CaI	

Product

Table 23: Properties of each product.

Id	Name	SBO
mwaf195932_a72c_4552_8cf2_b349b15d39c4	PMCA	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \frac{\text{mwd3b36919\_202a\_4fed\_a3c8\_1a3a60594404} \cdot \text{mwfbff577a\_4e9c\_40fe\_8777\_eb0ceade28c9} \cdot \text{mwd21d3f76\_d133}}{(\text{mwd3b36919\_202a\_4fed\_a3c8\_1a3a60594404} - 1) \cdot 0.05^4 + [\text{CaI}]^4} \tag{18}$$

6.10 Reaction mw700bd02b_9fc4_47e7_864a_967c03874dd6

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

Name PMCA degradation

Reaction equation

$$\text{mwaf195932\_a72c\_4552\_8cf2\_b349b15d39c4} \longrightarrow \emptyset \tag{19}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
mwaf195932_a72c_4552_8cf2_b349b15d39c4	PMCA	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = [\text{mwaf195932\_a72c\_4552\_8cf2\_b349b15d39c4}] \cdot \text{mwfbff577a\_4e9c\_40fe\_8777\_eb0cead2} \ldots \text{c9} \tag{20}$$

6.11 Reaction mw06f8fde4_d97b_4d5f_b71e_d93aa53e9932

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

Name SERCA synthesis

Reaction equation

$$\emptyset \xrightarrow{\text{CaS}} \text{mw0ebc76ad\_49d7\_4845\_8f88\_04d443fbe7f3} \tag{21}$$

Modifier

Table 25: Properties of each modifier.

Id	Name	SBO
CaS	CaS	

Product

Table 26: Properties of each product.

Id	Name	SBO
mw0ebc76ad_49d7_4845_8f88_04d443fbe7f3	SERCA	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \frac{\frac{1}{\text{mwd3b36919\_202a\_4fed\_a3c8\_1a3a60594404}} \cdot \text{B} \cdot \text{mwfbff577a\_4e9c\_40fe\_8777\_eb0ceade28c9} \cdot \left(\left(\text{mwd3b36919\_202a\_4fed\_}\right.\right.}{[\text{CaS}]^4} \tag{22}$$

6.12 Reaction mw8021d532_dd9b_4e34_a865_c2bb1689b0b5

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

Name STIM/Orai synthesis

Reaction equation

$$\emptyset \xrightarrow{\text{CaS, CaI}} \text{mw7cb2644a\_384a\_4bbb\_93fd\_fd686e01d7cb} \tag{23}$$

Modifiers

Table 27: Properties of each modifier.

Id	Name	SBO
CaS	CaS	
CaI	CaI	

Product

Table 28: Properties of each product.

Id	Name	SBO
mw7cb2644a_384a_4bbb_93fd_fd686e01d7cb	STIM	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \frac{\frac{1}{\text{mwd3b36919\_202a\_4fed\_a3c8\_1a3a60594404}\cdot\text{mwd3b36919\_202a\_4fed\_a3c8\_1a3a60594404}} \cdot \text{mw004dcb62\_da5f\_41c7\_a7bd\_033574894f48} \cdot \text{mwfbff577a\_4e9c\_40fe\_8777\_eb0cea}}{[\text{CaS}]^2} \tag{24}$$

6.13 Reaction mw1f122e51_99cb_4a32_a12e_4c2921920a17

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

Name STIM/Orai degradation

Reaction equation

$$\text{mw7cb2644a\_384a\_4bbb\_93fd\_fd686e01d7cb} \longrightarrow \emptyset \tag{25}$$

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
mw7cb2644a_384a_4bbb_93fd_fd686e01d7cb	STIM	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = [\text{mw7cb2644a\_384a\_4bbb\_93fd\_fd686e01d7cb}] \cdot \text{mwfbff577a\_4e9c\_40fe\_8777\_eb0cead2} \quad (26)$$

6.14 Reaction mw89d547e1_8d48_4cd2_ba3d_e4390294089d

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

Name SERCA degradation

Reaction equation

$$\text{mw0ebc76ad\_49d7\_4845\_8f88\_04d443fbe7f3} \longrightarrow \emptyset \tag{27}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
mw0ebc76ad_49d7_4845_8f88_04d443fbe7f3	SERCA	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = [\text{mw0ebc76ad\_49d7\_4845\_8f88\_04d443fbe7f3}] \cdot \text{mwfbff577a\_4e9c\_40fe\_8777\_eb0cead2} \quad (28)$$

6.15 Reaction mwa61047ec_49c1_47b2_b78e_4d84a33d432a

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

Name CytToMito

Reaction equation

$$\text{CaI} \longrightarrow \text{mw013a7c64\_a9ec\_483c\_b3b8\_ed658337ee95} \tag{29}$$

Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
CaI	CaI	

Product

Table 32: Properties of each product.

Id	Name	SBO
mw013a7c64_a9ec_483c_b3b8_ed658337ee95	CaM	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \frac{\text{mwa3072851\_e3e4\_4767\_ac41\_49fa7c0de7a7} \cdot [\text{CaI}]^4}{[\text{CaI}]^4 + \text{mwe3841c25\_6042\_49c2\_9feb\_90cbf6751167}^4} \tag{30}$$

6.16 Reaction ERtoMito

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

Name ERtoMito

Reaction equation

$$\text{CaS} \xrightarrow{\text{g, IP3, CaI}} \text{mw013a7c64\_a9ec\_483c\_b3b8\_ed658337ee95} \tag{31}$$

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
CaS	CaS	

Modifiers

Table 34: Properties of each modifier.

Id	Name	SBO
g	g	
IP3	IP3	
CaI	CaI	

Product

Table 35: Properties of each product.

Id	Name	SBO
mw013a7c64_a9ec_483c_b3b8_ed658337ee95	CaM	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \text{mwd8bf5d8f\_ad00\_4119\_bde1\_91015ef2cd7c} \cdot \left(\text{L} + \frac{\frac{(1-[\text{g}])\cdot \text{A}\cdot[\text{IP3}]^2}{[\text{IP3}]^2+\text{mw92b257b7\_00af\_4fd6\_a11b\_8e4655a4ba65}^2}\cdot[\text{CaI}]^2}{[\text{CaI}]^2+\text{mw78dd80b8\_e003\_4c62\_81d1\_547d001767af}^2} \right) \cdot [\text{CaS}] \tag{32}$$

6.17 Reaction mw1c50c3d1_dab9_423a_8373_6a4c75479b54

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

Name MitoToCytosol

Reaction equation

$$\text{mw013a7c64\_a9ec\_483c\_b3b8\_ed658337ee95} \longrightarrow \text{CaI} \tag{33}$$

Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
mw013a7c64_a9ec_483c_b3b8_ed658337ee95	CaM	

Product

Table 37: Properties of each product.

Id	Name	SBO
CaI	CaI	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \frac{\text{mw219cf65d\_18cc\_4f7e\_ab5a\_5b87cda6fc43} \cdot [\text{mw013a7c64\_a9ec\_483c\_b3b8\_ed658337ee95}]}{[\text{mw013a7c64\_a9ec\_483c\_b3b8\_ed658337ee95}] + 0.01} \tag{34}$$

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 CaI

Name CaI

SBO:0000247 simple chemical

Initial amount 0.05 mol

This species takes part in eleven reactions (as a reactant in JPump, mw530793e3_76b2_4483-_be11_e94364306712, mwa61047ec_49c1_47b2_b78e_4d84a33d432a and as a product in JChannel, mwbdcd6a40_1ae7_4c86_a99f_1fba0b8beaf7, mw1c50c3d1_dab9_423a_8373_6a4c75479b54

and as a modifier in kPLC, inhibition_parameter1, mw5658298a_d96a_4b97_9a4f_6f06dad35824, mw8021d532_dd9b_4e34_a865_c2bb1689b0b5, ERtoMito).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CaI} = v_3 + v_7 + v_{17} - v_2 - v_8 - v_{15} \tag{35}$$

7.2 Species IP3

Name IP3

SBO:0000247 simple chemical

Initial amount 0 mol

This species takes part in four reactions (as a reactant in kPhosphatase and as a product in kPLC and as a modifier in JChannel, ERtoMito).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IP3} = v_1 - v_4 \tag{36}$$

7.3 Species g

Name g

Initial amount 0.0020 mol

This species takes part in four reactions (as a reactant in inhibition_parameter2 and as a product in inhibition_parameter1 and as a modifier in JChannel, ERtoMito).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{g} = v_5 - v_6 \tag{37}$$

7.4 Species mwaf195932_a72c_4552_8cf2_b349b15d39c4

Name PMCA

SBO:0000242 channel

Initial amount 0.013 mol

This species takes part in three reactions (as a reactant in mw700bd02b_9fc4_47e7_864a-_967c03874dd6 and as a product in mw5658298a_d96a_4b97_9a4f_6f06dad35824 and as a modifier in mw530793e3_76b2_4483_be11_e94364306712).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{mwaf195932\_a72c\_4552\_8cf2\_b349b15d39c4} = v_9 - v_{10} \tag{38}$$

7.5 Species mw0ebc76ad_49d7_4845_8f88_04d443fbe7f3

Name SERCA

SBO:0000242 channel

Initial amount 0.266 mol

This species takes part in three reactions (as a reactant in mw89d547e1_8d48_4cd2_ba3d-_e4390294089d and as a product in mw06f8fde4_d97b_4d5f_b71e_d93aa53e9932 and as a modifier in JPump).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{mw0ebc76ad\_49d7\_4845\_8f88\_04d443fbe7f3} = v_{11} - v_{14} \tag{39}$$

7.6 Species mw7cb2644a_384a_4bbb_93fd_fd686e01d7cb

Name STIM

SBO:0000252 polypeptide chain

Initial amount 0.02 mol

This species takes part in three reactions (as a reactant in mw1f122e51_99cb_4a32_a12e-_4c2921920a17 and as a product in mw8021d532_dd9b_4e34_a865_c2bb1689b0b5 and as a modifier in mwbdcd6a40_1ae7_4c86_a99f_1fba0b8beaf7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{mw7cb2644a\_384a\_4bbb\_93fd\_fd686e01d7cb} = v_{12} - v_{13} \tag{40}$$

7.7 Species mwd6b792d8_c983_42c1_b3bc_2494d6a3363e

Name CaO

SBO:0000247 simple chemical

Initial amount 1000 mol

This species does not take part in any reactions. Its quantity does hence not change over time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{mwd6b792d8\_c983\_42c1\_b3bc\_2494d6a3363e} = 0 \tag{41}$$

7.8 Species mw013a7c64_a9ec_483c_b3b8_ed658337ee95

Name CaM

SBO:0000247 simple chemical

Initial amount 0 mol

This species takes part in three reactions (as a reactant in mw1c50c3d1_dab9_423a_8373-_6a4c75479b54 and as a product in mwa61047ec_49c1_47b2_b78e_4d84a33d432a, ERtoMito).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{mw013a7c64\_a9ec\_483c\_b3b8\_ed658337ee95} = v_{15} + v_{16} - v_{17} \tag{42}$$

7.9 Species CaS

Name CaS

SBO:0000247 simple chemical

Initial amount 2 mol

This species takes part in six reactions (as a reactant in JChannel, ERtoMito and as a product in JPump and as a modifier in mwbdcd6a40_1ae7_4c86_a99f_1fba0b8beaf7, mw06f8fde4-_d97b_4d5f_b71e_d93aa53e9932, mw8021d532_dd9b_4e34_a865_c2bb1689b0b5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CaS} = v_2 - v_3 - v_{16} \tag{43}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000242 channel: A component that allows another component to pass through itself, possibly connecting different compartments

SBO:0000247 simple chemical: Simple, non-repetitive chemical entity

SBO:0000252 polypeptide chain: Naturally occurring macromolecule formed by the repetition of amino-acid residues linked by peptidic bonds. A polypeptide chain is synthesized by the ribosome. CHEBI:1654

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

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