

SUPPLEMENT

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Model reactions (values for D1/D2/D3 where applicable)

Name	Reaction	Flux	Parameters	Reference
SERCA2b	$Ca_{cyt}^{2+} \rightarrow Ca_{dts}^{2+}$	$\frac{v[Ca_{cyt}^{2+}]^{1.7}}{K^{1.7} + [Ca_{cyt}^{2+}]^{1.7}}$	$V = k[SERCA2]\mu M \cdot s^{-1}$, $k = 25/35/21$, $K = 0.27\mu M$	[6]
SERCA3	$Ca_{cyt}^{2+} \rightarrow Ca_{dts}^{2+}$	$\frac{v[Ca_{cyt}^{2+}]^{1.8}}{K^{1.8} + [Ca_{cyt}^{2+}]^{1.8}}$	$V = k[SERCA3]\mu M \cdot s^{-1}$, $k = 36/36/39$, $K = 1.1\mu M$	[6]
Leak	$Ca_{dts}^{2+} \leftrightarrow Ca_{cyt}^{2+}$	$\gamma \ln \frac{[Ca_{dts}^{2+}]}{[Ca_{cyt}^{2+}]}$	$\gamma = 21\mu M \cdot s^{-1}$	[6]
IP3R	$Ca_{dts}^{2+} \rightarrow Ca_{cyt}^{2+}$	$\gamma P_0 [IP3R] \ln \frac{[Ca_{dts}^{2+}]}{[Ca_{cyt}^{2+}]}$, $P_0 = \left(0.9 \frac{[IP3Ra]}{[IP3R]} + 0.1 \frac{[IP3Ro]}{[IP3R]} \right)^4$	$\gamma = (13/13/12.5) \cdot 10^4 s^{-1}$	[6]
IP3R	$IP3Ra \rightarrow IP3Ro + Ca_{cyt}^{2+}$	$\frac{k_1 L_1 [IP3Ra]}{L_1 + [Ca_{cyt}^{2+}]}$	$k_1 = 11.94 s^{-1}$	[6]
IP3R	$IP3Ro + Ca_{cyt}^{2+} \rightarrow IP3Ra$	$\frac{(k_5 L_5 + K_5) [Ca_{cyt}^{2+}] [IP3Ro]}{L_5 + [Ca_{cyt}^{2+}]}$	$k_5 = 4(\mu M \cdot s)^{-1}$, $K_5 = 4707 s^{-1}$	[6]
IP3R	$IP3Ro \rightarrow IP3Rn + IP3$	$\frac{(K_3 + k_{m3}) [Ca_{cyt}^{2+}] L_3 [IP3Ro]}{L_3 + [Ca_{cyt}^{2+}]}$	$k_{m3} = 2.5(\mu M \cdot s)^{-1}$, $K_3 = 1.4 s^{-1}$	[6]
IP3R	$IP3Rn + IP3 \rightarrow IP3Ro$	$\frac{(k_3 L_3 + k_{c3}) [Ca_{cyt}^{2+}] [IP3] [IP3Rn]}{L_3 + [Ca_{cyt}^{2+}] \left(1 + \frac{L_3}{L_1} \right)}$	$k_3 = 37.4(\mu M \cdot s)^{-1}$, $k_{c3} = 1.7(\mu M \cdot s)^{-1}$	[6]
IP3R	$IP3Ro \leftrightarrow IP3Rs$	$\frac{k_4 L_5 [IP3Ro]}{L_5 + [Ca_{cyt}^{2+}]} - k_{m4} [IP3Rs]$	$k_4 = 0.11 s^{-1}$, $k_{m4} = 29.8 s^{-1}$	[6]
IP3R	$IP3Rn + Ca_{cyt}^{2+} \leftrightarrow IP3Ri1$	$\frac{k_2 [Ca_{cyt}^{2+}] [IP3Rn]}{L_1 + [Ca_{cyt}^{2+}] \left(1 + \frac{L_1}{L_3} \right)} - k_{m2} [IP3Ri1]$	$k_2 = 1.78 s^{-1}$, $k_{m2} = 0.84 s^{-1}$	[6]
IP3R	$IP3Ra + Ca_{cyt}^{2+} \leftrightarrow IP3Ri2$	$\frac{k_2 [Ca_{cyt}^{2+}] [IP3Ra]}{L_1 + [Ca_{cyt}^{2+}]} - k_{m2} [IP3Ri2]$		[6]
NCLX	$Ca_{mit}^{2+} \rightarrow Ca_{cyt}^{2+}$	$\gamma \left(1 + \frac{K}{[Ca_{mit}^{2+}]} \right)^{-1} e^{-\frac{F(\Delta\psi - \Delta\psi^*)}{2RT}}$	$\gamma = 1.84 \cdot 10^3 \mu M \cdot s^{-1}$, $K = 3 \mu M$, $\Delta\psi^* = 0.091V$	[6]
UNI	$Ca_{cyt}^{2+} \rightarrow Ca_{mit}^{2+}$	$\frac{[Ca_{cyt}^{2+}] (\Delta\psi - \Delta\psi^*)^2}{\gamma K^2 + [Ca_{cyt}^{2+}]^2 (\Delta\psi)^3 + (\Delta\psi - \Delta\psi^*)^3} \frac{2F\Delta\psi}{RT} \left([Ca_{cyt}^{2+}] - [Ca_{mit}^{2+}] e^{-\frac{2F\Delta\psi}{RT}} \right)$	$\gamma = 64.2 \mu M^2 \cdot s^{-1}$, $K = 0.07 \mu M$, $\Delta\psi^* = 0.013V$, $\Delta\psi = 0.124V$	[6]
CaM	$CaM + 4Ca_{cyt}^{2+} \leftrightarrow CaMb$	$k[CaM][Ca_{cyt}^{2+}]^4 - k_m[CaMb]$	$k = 763/657/168(\mu M^4 \cdot s)^{-1}$, $k_m = 7 s^{-1}$	[32]
Calr	$Calr + Ca_{DTs}^{2+} \leftrightarrow CalrB$	$k[Calr][Ca_{DTs}^{2+}] - k_m[CalrB]$	$k = 25(\mu M \cdot s)^{-1}$, $k_m = 100 s^{-1}$	[33]
END	$END + Ca_{DTs}^{2+} \leftrightarrow ENDB$	$k[END][Ca_{DTs}^{2+}] - k_m[ENDB]$	$k = 0.05(\mu M \cdot s)^{-1}$, $k_m = 100 s^{-1}$	[34]
SCaMC	$SC + 2Ca_{Mit}^{2+} \leftrightarrow SCB$	$k[SC][Ca_{cyt}^{2+}]^2 - k_m[SCB]$	$k = 4.5/33/64(\mu M^2 \cdot s)^{-1}$, $k_m = 1 s^{-1}$	[36]
CypD	$CypD + 4Ca_{Mit}^{2+} \leftrightarrow CDB$	$k[CypD][Ca_{cyt}^{2+}]^4 - k_m[CDB]$	$k = 4.5/33/64(\mu M^4 \cdot s)^{-1}$, $k_m = 1 s^{-1}$	[36]

Non-zero initial concentrations (values for D1/D2/D3 where applicable)

Variable	Concentration, μM	Variable	Concentration, μM	Variable	Concentration, μM	Variable	Concentration, μM
CaM	6/14/5	Calr	208/224/70	CypD	32/27/13	UNI	7.3/2.8/7.5
Ca_{DTs}^{2+}	293/242/398	END	116/111/112	SERCA2	10/7.3/11	NCLX	0.2/0.1/0.14
IP3R	2.7/1/1.5	SC	2.1/3.1/1.1	SERCA3	19/9/15		