Supporting Information

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SI Text

Parameter Determination

Obtaining *L* and *c* Values. Equations to minimize to obtain estimates for L, c, e_1 (for skMLCK), e_2 (for PhK5), and e_3 (for CaATPase) were obtained by inserting data from Peersen *et al.* (5) into the expression for fractional occupancy in the presence of an allosteric activator from Rubin and Changeux (9). K_R for calcium binding can be obtained from the reported K_d value using the relation $K_R = K_d\,(1 + Lc)/(1 + L)$. The resulting system of equations reads as follows:

No ligand present:

$$\varepsilon_1 = \frac{1}{2} - \frac{\frac{F_{1/2}}{K_R}\left(1+\frac{F_{1/2}}{K_R}\right)^3 + Lc\frac{F_{1/2}}{K_R}\left(1+c\frac{F_{1/2}}{K_R}\right)^3}{\left(1+\frac{F_{1/2}}{K_R}\right)^4 + L\left(1+c\frac{F_{1/2}}{K_R}\right)^4}, \qquad \textbf{[1]}$$

where $F_{1/2} = 7.5 \times 10^{-6}$, and $K_R = 1.4 \times 10^{-5}$.

skMLCK:

$$\varepsilon_2 = \frac{1}{2} - \frac{\frac{F_{1/2}}{K_R}\left(1+\frac{F_{1/2_1}}{K_R}\right)^3 + L\left(\frac{1+\frac{A_1}{K_1^{AR}}e_1}{1+\frac{A_1}{K_1^{AR}}}\right)c\frac{F_{1/2_1}}{K_R}\left(1+c\frac{F_{1/2_1}}{K_R}\right)^3}{\left(1+\frac{F_{1/2_1}}{K_R}\right)^4 + L\left(\frac{1+\frac{A_1}{K_1^{AR}}e_1}{1+\frac{A_1}{K_1^{AR}}}\right)\left(1+c\frac{F_{1/2_1}}{K_R}\right)^4}, \qquad \textbf{[2]}$$

where $F_{1/2_1} = 3.4 \times 10^{-8}$, $A_1 = 1 \times 10^{-5}$, and $K_1^{AR} = 1 \times 10^{-9}$

PhK5:

$$\varepsilon_3 = \frac{1}{2} - \frac{\frac{F_{1/2_2}}{K_R}\left(1+\frac{F_{1/2_2}}{K_R}\right)^3 + L\left(\frac{1+\frac{A_2}{K_2^{AR}}e_2}{1+\frac{A_2}{K_2^{AR}}}\right)c\frac{F_{1/2_2}}{K_R}\left(1+c\frac{F_{1/2_2}}{K_R}\right)^3}{\left(1+\frac{F_{1/2_2}}{K_R}\right)^4 + L\left(\frac{1+\frac{A_2}{K_2^{AR}}e_2}{1+\frac{A_2}{K_2^{AR}}}\right)\left(1+c\frac{F_{1/2_2}}{K_R}\right)^4}, \qquad \textbf{[3]}$$

where $F_{1/2_2} = 6 \times 10^{-7}$, $A_2 = 1 \times 10^{-5}$, and $K_2^{AR} = 2 \times 10^{-8}$

CaATPase:

$$\varepsilon_4 = \frac{1}{2} - \frac{\frac{F_{1/2_3}}{K_R}\left(1+\frac{F_{1/2_3}}{K_R}\right)^3 + L\left(\frac{1+\frac{A_3}{K_3^{AR}}e_3}{1+\frac{A_3}{K_3^{AR}}}\right)c\frac{F_{1/2_3}}{K_R}\left(1+c\frac{F_{1/2_3}}{K_R}\right)^3}{\left(1+\frac{F_{1/2_3}}{K_R}\right)^4 + L\left(\frac{1+\frac{A_3}{K_3^{AR}}e_3}{1+\frac{A_3}{K_3^{AR}}}\right)\left(1+c\frac{F_{1/2_3}}{K_R}\right)^4}, \qquad \textbf{[4]}$$

where $F_{1/2_3} = 1.2 \times 10^{-7}$, $A_3 = 1 \times 10^{-5}$, and $K_3^{AR} = 1 \times 10^{-9}$

We minimized ε_1, ε_2, ε_3, ε_4 by using the leastsquare function provided in Scilab (www.scilab.org). To avoid local minima, we ran 10^5 minimizations, each one with different initial values. Initial values were drawn at random: The grand function provided in Scilab was used to determine the exponent of each parameter, with initial values in the following range: $10^3 \le L < 10^5$, $10^{-4} \le c < 0.1$, and $10^{-15} < e_i < 0.5$. Of 10^5 runs, 13 resulted in the same minimum, which we believe to be global. It is reached at $L = 20{,}670$, $c = 3.96 \times 10^{-3}$, $e_1 = 10^{-15}$, $e_2 = 0.5$, and $e_3 = 1.57 \times 10^{-3}$. e_1 being very small means that skMLCK binds predominantly to the R state. We can therefore assume that, in the presence of sufficient amounts of skMLCK, calmodulin exists predominantly in the R state.

Obtaining K_R Values. The system of equations used to determine K_R values was as follows:

Wild Type. Calcium concentrations at $\bar{Y} = 0.5$ and $\bar{Y} = 0.25$ were taken from ref. 1.

$$\eta_1 = \frac{1}{2} - 0.25$$

$$\frac{\sum_i\left(\frac{F_{1/2}}{K_{Ri}}\prod_j\left(1+\frac{F_{1/2}}{K_{Rj}}\right)\right) + L\sum_i\left(c\frac{F_{1/2}}{K_{Ri}}\prod_j\left(1+c_j\frac{F_{1/2}}{K_{Rj}}\right)\right)}{\prod_i\left(1+\frac{F_{1/2}}{K_{Ri}}\right) + L\prod_i\left(1+c\frac{F_{1/2}}{K_{Ri}}\right)} \qquad \textbf{[5]}$$

$$\eta_2 = \frac{1}{4} - 0.25$$

$$\frac{\sum_i\left(\frac{F_{1/4}}{K_{Ri}}\prod_j\left(1+\frac{F_{1/4}}{K_{Rj}}\right)\right) + L\sum_i\left(c\frac{F_{1/4}}{K_{Ri}}\prod_j\left(1+c_j\frac{F_{1/4}}{K_{Rj}}\right)\right)}{\prod_i\left(1+\frac{F_{1/4}}{K_{Ri}}\right) + L\prod_i\left(1+c\frac{F_{1/4}}{K_{Ri}}\right)} \qquad \textbf{[6]}$$

where $i, j \in \{A, B, C, D\}$, and $j \neq i$, $F_{1/2} = 4.4 \times 10^{-6}$, and $F_{1/4} = 1.4 \times 10^{-6}$.

C-Terminal Mutant. Calcium concentrations at $\bar{Y} = 0.5$ and $\bar{Y} = 0.25$ for mutant calmodulin with intact N-terminal binding sites were taken from ref. 10.

$$\eta_3 = \frac{1}{2} - 0.5 \frac{\sum_i\left(\frac{FN_{1/2}}{K_{Ri}}\prod_j\left(1+\frac{FN_{1/2}}{K_{Rj}}\right)\right) + L\sum_i\left(c\frac{FN_{1/2}}{K_{Ri}}\prod_j\left(1+c_j\frac{FN_{1/2}}{K_{Rj}}\right)\right)}{\prod_i\left(1+\frac{FN_{1/2}}{K_{Ri}}\right) + L\prod_i\left(1+c\frac{FN_{1/2}}{K_{Ri}}\right)} \quad [7]$$

$$\eta_4 = \frac{1}{4} - 0.5 \frac{\sum_i\left(\frac{FN_{1/4}}{K_{Ri}}\prod_j\left(1+\frac{FN_{1/4}}{K_{Rj}}\right)\right) + L\sum_i\left(c\frac{FN_{1/4}}{K_{Ri}}\prod_j\left(1+c_j\frac{FN_{1/4}}{K_{Rj}}\right)\right)}{\prod_i\left(1+\frac{FN_{1/4}}{K_{Ri}}\right) + L\prod_i\left(1+c\frac{FN_{1/4}}{K_{Ri}}\right)} \quad [8]$$

where $i, j \in \{A, B\}$, and $j \neq i$, $FN_{1/2} = 3.3 \times 10^{-5}$, and $FN_{1/4} = 1.3 \times 10^{-5}$.

N-Terminal Mutant. Calcium concentrations at $\bar{Y} = 0.5$ and $\bar{Y} = 0.25$ for mutant calmodulin with intact C-terminal binding sites were taken from ref. 10.

$$\eta_5 = \frac{1}{2} - 0.5 \frac{\sum_i\left(\frac{FC_{1/2}}{K_{Ri}}\prod_j\left(1+\frac{FC_{1/2}}{K_{Rj}}\right)\right) + L\sum_i\left(c\frac{FC_{1/2}}{K_{Ri}}\prod_j\left(1+c_j\frac{FC_{1/2}}{K_{Rj}}\right)\right)}{\prod_i\left(1+\frac{FC_{1/2}}{K_{Ri}}\right) + L\prod_i\left(1+c\frac{FC_{1/2}}{K_{Ri}}\right)} \quad [9]$$

$$\eta_6 = \frac{1}{4} - 0.5 \frac{\sum_i\left(\frac{FC_{1/4}}{K_{Ri}}\prod_j\left(1+\frac{FC_{1/4}}{K_{Rj}}\right)\right) + L\sum_i\left(c\frac{FC_{1/4}}{K_{Ri}}\prod_j\left(1+c_j\frac{FC_{1/4}}{K_{Rj}}\right)\right)}{\prod_i\left(1+\frac{FC_{1/4}}{K_{Ri}}\right) + L\prod_i\left(1+c\frac{FC_{1/4}}{K_{Ri}}\right)} \quad [10]$$

where $i, j \in \{C, D\}$, and $j \neq i$, $FC_{1/2} = 3.5 \times 10^{-5}$, and $FC_{1/4} = 1.4 \times 10^{-5}$.

***R* State Only.** Calcium concentrations at $\bar{Y} = 0.5$ and $\bar{Y} = 0.25$ in the presence of skMLCK were taken from ref. 5.

$$\eta_7 = \frac{1}{2} - 0.25 \frac{\sum_i\left(\frac{FR_{1/2}}{K_{Ri}}\prod_j\left(1+\frac{FR_{1/2}}{K_{Rj}}\right)\right)}{\prod_i\left(1+\frac{FR_{1/2}}{K_{Ri}}\right)} \quad [11]$$

$$\eta_8 = \frac{1}{4} - 0.25 \frac{\sum_i\left(\frac{FR_{1/4}}{K_{Ri}}\prod_j\left(1+\frac{FR_{1/4}}{K_{Rj}}\right)\right)}{\prod_i\left(1+\frac{FR_{1/4}}{K_{Ri}}\right)}, \quad [12]$$

where $i, j \in \{A, B, C, D\}$ and $j \neq i$, $FR_{1/2} = 3.4 \times 10^{-8}$, and $FR_{1/4} = 1.5 \times 10^{-8}$.

We first sampled all possible combinations of $K^R{}_i$ values in a broad range ($10^{-9} \leq K_{Ri} < 10^{-4}$, using a logarithmic scan with 50 sample points per dimension). Of these, we selected the parameter configuration that minimizes $\Sigma_{i=1}^{8} \eta_i{}^2$. The result was then used as an initial vector for a refined search using a smaller intervals (of 2 orders of magnitude) around the initial results and 66 sample points per dimension.

Robustness of k_{RT}. To determine whether the choice of the R to T transition rate, k_{RT}, affects the outcome of the simulation, we performed a robustness analysis on this parameter. We looked at calcium binding to calmodulin as a function of calcium concentration for k_{RT} values between 10^3 and 10^9 and found no difference in output (see Fig. S1).

Comparison of Calcium-Binding Curve to Experimental Results

In addition to comparing our simulation results to experimental data reported by Crouch and Klee (3), we also compared them to experimental data reported by Peersen *et al.* (5) (see Fig. 2) and Porumb (7) (see Fig. 3).

List of Reactions Included in the Simulation

Reactions included in the simulation are listed in Table S1.

List of Parameters for Simulation

Parameters used in the simulation are listed in Table S2.

1. Bayley PM, Findlay WA, Martin SR (1996) Target recognition by calmodulin: dissecting the kinetics and affinity of interaction using short peptide sequences. *Protein Sci* 5:1215–1228.
2. Carlisle HJ, Kennedy MB (2005) Spine architecture and synaptic plasticity. *Trends Neurosci* 28:182–187.
3. Crouch TH, Klee CB (1980) Positive cooperative binding of calcium to bovine brain calmodulin. *Biochemistry* 19:3692–3698.
4. Goto S, Matsukado Y, Mihara Y, Inoue N, Miyamoto E (1986) The distribution of calcineurin in rat brain by light and electron microscopic immunohistochemistry and enzyme-immunoassay. *Brain Res* 397:161–172.
5. Peersen OB, Madsen TS, Falke JJ (1997) Intermolecular tuning of calmodulin by target peptides and proteins: differential effects on Ca2+ binding and implications for kinase activation. *Protein Sci* 6:794–807.
6. Petersen JD, *et al.* (2003) Distribution of postsynaptic density (PSD)-95 and Ca2+/calmodulin-dependent protein kinase II at the PSD. *J Neurosci* 23:11270–11278.
7. Porumb T (1994) Determination of calcium-binding constants by flow dialysis. *Anal Biochem* 220:227–237.
8. Quintana AR, Wang D, Forbes JE, Waxham MN (2005) Kinetics of calmodulin binding to calcineurin. *Biochem Biophys Res Commun* 334:674–680.
9. Rubin MM, Changeux JP (1966) On the nature of allosteric transitions: implications of non-exclusive ligand binding. *J Mol Biol* 21:265–274.
10. Shifman JM, Choi MH, Mihalas S, Mayo SL, Kennedy MB (2006) Ca2+/calmodulin-dependent protein kinase II (CaMKII) is activated by calmodulin with two bound calciums. *Proc Natl Acad Sci USA* 103:13968–13973.
11. Tzortzopoulos A, Török K (2004) Mechanism of the T286A-mutant alphaCaMKII interactions with Ca2+/calmodulin and ATP. *Biochemistry* 43:6404–6414.

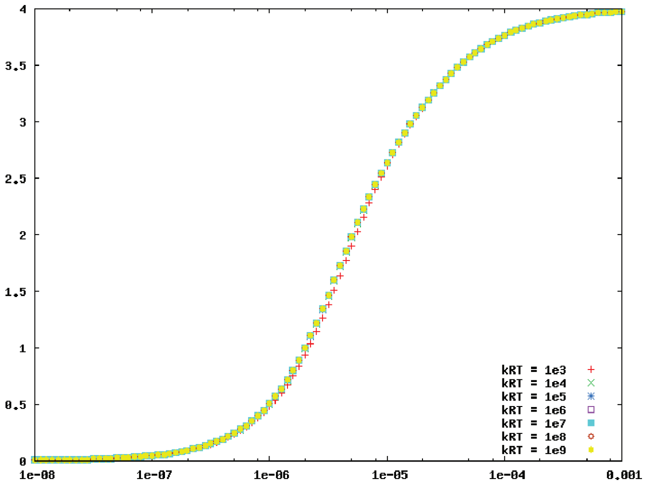

Fig. S1. Robustness of the parameter k_{RT}: Moles of calcium bound per mole of calmodulin are shown as a function of calcium concentration. Each curve represents a different value of k_{RT}. Calmodulin concentration used was 2×10^{-7} M.

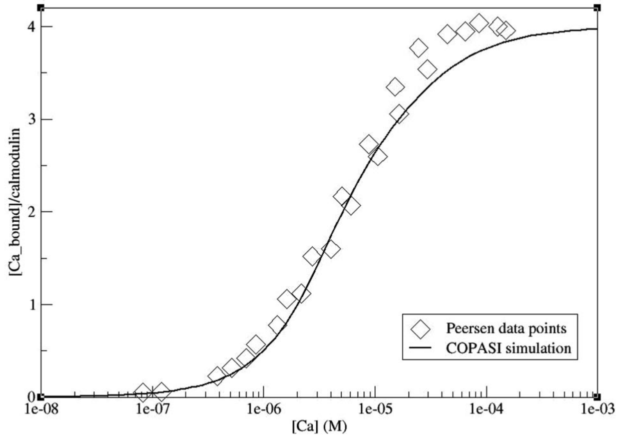

Fig. S2. Comparison between simulation results and experimental results reported by Peersen *et al.* (5). Moles of calcium bound per mole of calmodulin are shown as a function of calcium concentration. Diamonds: data points measured by Peersen *et al.*; solid line: steady-state results of simulations at different initial calcium concentrations. Calmodulin concentration used was 2×10^{-7} M.

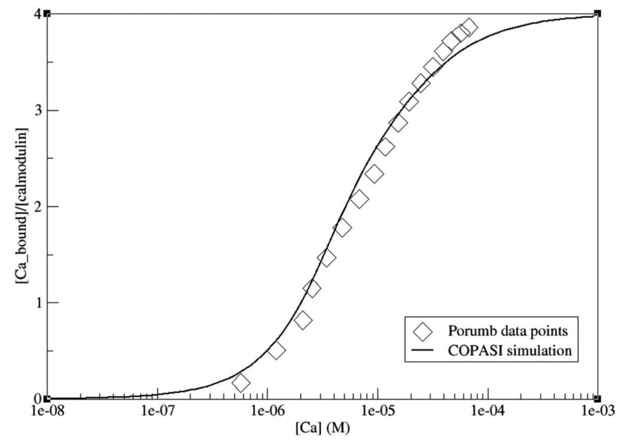

Fig. S3. Comparison between simulation results and experimental results reported by Porumb (7). Moles of calcium bound per mole of calmodulin are shown as a function of calcium concentration. Diamonds: data points measured by Porumb; solid line: steady state results of simulations at different initial calcium concentrations. Calmodulin concentration used was 2×10^{-7} M.

Table S1. List of reactions included in our simulation with their respective reaction rates

camT + ca -> camT_ca1_A	k_{on}
camT + ca -> camT_ca1_B	k_{on}
camT + ca -> camT_ca1_C	k_{on}
camT + ca -> camT_ca1_D	k_{on}
camT_ca1_A + ca -> camT_ca2_AB	k_{on}
camT_ca1_A + ca -> camT_ca2_AC	k_{on}
camT_ca1_A + ca -> camT_ca2_AD	k_{on}
camT_ca1_B + ca -> camT_ca2_AB	k_{on}
camT_ca1_B + ca -> camT_ca2_BC	k_{on}
camT_ca1_B + ca -> camT_ca2_BD	k_{on}
camT_ca1_C + ca -> camT_ca2_AC	k_{on}
camT_ca1_C + ca -> camT_ca2_BC	k_{on}
camT_ca1_C + ca -> camT_ca2_CD	k_{on}
camT_ca1_D + ca -> camT_ca2_AD	k_{on}
camT_ca1_D + ca -> camT_ca2_BD	k_{on}
camT_ca1_D + ca -> camT_ca2_CD	k_{on}
camT_ca2_AB + ca -> camT_ca3_ABC	k_{on}
camT_ca2_AB + ca -> camT_ca3_ABD	k_{on}
camT_ca2_AC + ca -> camT_ca3_ABC	k_{on}
camT_ca2_AC + ca -> camT_ca3_ACD	k_{on}
camT_ca2_AD + ca -> camT_ca3_ABD	k_{on}
camT_ca2_AD + ca -> camT_ca3_ACD	k_{on}
camT_ca2_BC + ca -> camT_ca3_ABC	k_{on}
camT_ca2_BC + ca -> camT_ca3_BCD	k_{on}
camT_ca2_BD + ca -> camT_ca3_ABD	k_{on}
camT_ca2_BD + ca -> camT_ca3_BCD	k_{on}
camT_ca2_CD + ca -> camT_ca3_ACD	k_{on}
camT_ca2_CD + ca -> camT_ca3_BCD	k_{on}
camT_ca3_ABC + ca -> camT_ca4_ABCD	k_{on}
camT_ca3_ABD + ca -> camT_ca4_ABCD	k_{on}
camT_ca3_ACD + ca -> camT_ca4_ABCD	k_{on}
camT_ca3_BCD + ca -> camT_ca4_ABCD	k_{on}
camT_ca1_A -> camT + ca	k^T_{offA}
camT_ca1_B -> camT + ca	k^T_{offB}
camT_ca1_C -> camT + ca	k^T_{offC}
camT_ca1_D -> camT + ca	k^T_{offD}
camT_ca2_AB -> camT_ca1_A + ca	k^T_{offB}
camT_ca2_AB -> camT_ca1_B + ca	k^T_{offA}
camT_ca2_AC -> camT_ca1_A + ca	k^T_{offC}
camT_ca2_AC -> camT_ca1_C + ca	k^T_{offA}
camT_ca2_AD -> camT_ca1_A + ca	k^T_{offD}
camT_ca2_AD -> camT_ca1_D + ca	k^T_{offA}
camT_ca2_BC -> camT_ca1_B + ca	k^T_{offC}
camT_ca2_BC -> camT_ca1_C + ca	k^T_{offB}
camT_ca2_BD -> camT_ca1_B + ca	k^T_{offD}
camT_ca2_BD -> camT_ca1_D + ca	k^T_{offB}
camT_ca2_CD -> camT_ca1_C + ca	k^T_{offD}
camT_ca2_CD -> camT_ca1_D + ca	k^T_{offC}
camT_ca3_ABC -> camT_ca2_AB + ca	k^T_{offC}
camT_ca3_ABC -> camT_ca2_AC + ca	k^T_{offB}
camT_ca3_ABC -> camT_ca2_BC + ca	k^T_{offA}

Table S1. Continued

camT_ca3_ABD -> camT_ca2_AB + ca	k^T_{offD}
camT_ca3_ABD -> camT_ca2_AD + ca	k^T_{offB}
camT_ca3_ABD -> camT_ca2_BD + ca	k^T_{offA}
camT_ca3_ACD -> camT_ca2_AC + ca	k^T_{offD}
camT_ca3_ACD -> camT_ca2_AD + ca	k^T_{offC}
camT_ca3_ACD -> camT_ca2_CD + ca	k^T_{offA}
camT_ca3_BCD -> camT_ca2_BC + ca	k^T_{offD}
camT_ca3_BCD -> camT_ca2_BD + ca	k^T_{offC}
camT_ca3_BCD -> camT_ca2_CD + ca	k^T_{offB}
camT_ca4_ABCD -> camT_ca3_ABC + ca	k^T_{offD}
camT_ca4_ABCD -> camT_ca3_ABD + ca	k^T_{offC}
camT_ca4_ABCD -> camT_ca3_ACD + ca	k^T_{offB}
camT_ca4_ABCD -> camT_ca3_BCD + ca	k^T_{offA}
camR + ca -> camR_ca1_A	k_{on}
camR + ca -> camR_ca1_B	k_{on}
camR + ca -> camR_ca1_C	k_{on}
camR + ca -> camR_ca1_D	k_{on}
camR_ca1_A + ca -> camR_ca2_AB	k_{on}
camR_ca1_A + ca -> camR_ca2_AC	k_{on}
camR_ca1_A + ca -> camR_ca2_AD	k_{on}
camR_ca1_B + ca -> camR_ca2_AB	k_{on}
camR_ca1_B + ca -> camR_ca2_BC	k_{on}
camR_ca1_B + ca -> camR_ca2_BD	k_{on}
camR_ca1_C + ca -> camR_ca2_AC	k_{on}
camR_ca1_C + ca -> camR_ca2_BC	k_{on}
camR_ca1_C + ca -> camR_ca2_CD	k_{on}
camR_ca1_D + ca -> camR_ca2_AD	k_{on}
camR_ca1_D + ca -> camR_ca2_BD	k_{on}
camR_ca1_D + ca -> camR_ca2_CD	k_{on}
camR_ca2_AB + ca -> camR_ca3_ABC	k_{on}
camR_ca2_AB + ca -> camR_ca3_ABD	k_{on}
camR_ca2_AC + ca -> camR_ca3_ABC	k_{on}
camR_ca2_AC + ca -> camR_ca3_ACD	k_{on}
camR_ca2_AD + ca -> camR_ca3_ABD	k_{on}
camR_ca2_AD + ca -> camR_ca3_ACD	k_{on}
camR_ca2_BC + ca -> camR_ca3_ABC	k_{on}
camR_ca2_BC + ca -> camR_ca3_BCD	k_{on}
camR_ca2_BD + ca -> camR_ca3_ABD	k_{on}
camR_ca2_BD + ca -> camR_ca3_BCD	k_{on}
camR_ca2_CD + ca -> camR_ca3_ACD	k_{on}
camR_ca2_CD + ca -> camR_ca3_BCD	k_{on}
camR_ca3_ABC + ca -> camR_ca4_ABCD	k_{on}
camR_ca3_ABD + ca -> camR_ca4_ABCD	k_{on}
camR_ca3_ACD + ca -> camR_ca4_ABCD	k_{on}
camR_ca3_BCD + ca -> camR_ca4_ABCD	k_{on}
camR_ca1_A -> camR + ca	k^R_{offA}
camR_ca1_B -> camR + ca	k^R_{offB}
camR_ca1_C -> camR + ca	k^R_{offC}
camR_ca1_D -> camR + ca	k^R_{offD}
camR_ca2_AB -> camR_ca1_A + ca	k^R_{offB}
camR_ca2_AB -> camR_ca1_B + ca	k^R_{offA}
camR_ca2_AC -> camR_ca1_A + ca	k^R_{offC}
camR_ca2_AC -> camR_ca1_C + ca	k^R_{offA}

Table S1. Continued

camR_ca2_AC -> camR_ca1_C + ca	k^R_{offA}
camR_ca2_AD -> camR_ca1_A + ca	k^R_{offD}
camR_ca2_AD -> camR_ca1_D + ca	k^R_{offA}
camR_ca2_BC -> camR_ca1_B + ca	k^R_{offC}
camR_ca2_BC -> camR_ca1_C + ca	k^R_{offB}
camR_ca2_BD -> camR_ca1_B + ca	k^R_{offD}
camR_ca2_BD -> camR_ca1_D + ca	k^R_{offB}
camR_ca2_CD -> camR_ca1_C + ca	k^R_{offD}
camR_ca2_CD -> camR_ca1_D + ca	k^R_{offC}
camR_ca3_ABC -> camR_ca2_AB + ca	k^R_{offC}
camR_ca3_ABC -> camR_ca2_AC + ca	k^R_{offB}
camR_ca3_ABC -> camR_ca2_BC + ca	k^R_{offA}
camR_ca3_ABD -> camR_ca2_AB + ca	k^R_{offD}
camR_ca3_ABD -> camR_ca2_AD + ca	k^R_{offB}
camR_ca3_ABD -> camR_ca2_BD + ca	k^R_{offA}
camR_ca3_ACD -> camR_ca2_AC + ca	k^R_{offD}
camR_ca3_ACD -> camR_ca2_AD + ca	k^R_{offC}
camR_ca3_ACD -> camR_ca2_CD + ca	k^R_{offA}
camR_ca3_BCD -> camR_ca2_BC + ca	k^R_{offD}
camR_ca3_BCD -> camR_ca2_BD + ca	k^R_{offC}
camR_ca3_BCD -> camR_ca2_CD + ca	k^R_{offB}
camR_ca4_ABCD -> camR_ca3_ABC + ca	k^R_{offD}
camR_ca4_ABCD -> camR_ca3_ABD + ca	k^R_{offC}
camR_ca4_ABCD -> camR_ca3_ACD + ca	k^R_{offB}
camR_ca4_ABCD -> camR_ca3_BCD + ca	k^R_{offA}
camR -> camT	k^R_{RT}
camR_ca1_A -> camT_ca1_A	$k^R_{\text{RT}} * \sqrt{c}$
camR_ca1_B -> camT_ca1_B	$k^R_{\text{RT}} * \sqrt{c}$
camR_ca1_C -> camT_ca1_C	$k^R_{\text{RT}} * \sqrt{c}$
camR_ca1_D -> camT_ca1_D	$k^R_{\text{RT}} * \sqrt{c}$
camR_ca2_AB -> camT_ca2_AB	$k^R_{\text{RT}} * \sqrt{c} * \sqrt{c}$
camR_ca2_AC -> camT_ca2_AC	$k^R_{\text{RT}} * \sqrt{c} * \sqrt{c}$
camR_ca2_AD -> camT_ca2_AD	$k^R_{\text{RT}} * \sqrt{c} * \sqrt{c}$
camR_ca2_BC -> camT_ca2_BC	$k^R_{\text{RT}} * \sqrt{c} * \sqrt{c}$
camR_ca2_BD -> camT_ca2_BD	$k^R_{\text{RT}} * \sqrt{c} * \sqrt{c}$
camR_ca2_CD -> camT_ca2_CD	$k^R_{\text{RT}} * \sqrt{c} * \sqrt{c}$
camR_ca3_ABC -> camT_ca3_ABC	$k^R_{\text{RT}} * \sqrt{c} * \sqrt{c} * \sqrt{c}$
camR_ca3_ABD -> camT_ca3_ABD	$k^R_{\text{RT}} * \sqrt{c} * \sqrt{c} * \sqrt{c}$
camR_ca3_ACD -> camT_ca3_ACD	$k^R_{\text{RT}} * \sqrt{c} * \sqrt{c} * \sqrt{c}$
camR_ca3_BCD -> camT_ca3_BCD	$k^R_{\text{RT}} * \sqrt{c} * \sqrt{c} * \sqrt{c}$
camR_ca4_ABCD -> camT_ca4_ABD	$k^R_{\text{RT}} * \sqrt{c} * \sqrt{c} * \sqrt{c} * \sqrt{c}$
camT -> camR	k^R_{TR}
camT_ca1_A -> camR_ca1_A	$k^R_{\text{TR}}/\sqrt{c}$
camT_ca1_B -> camR_ca1_B	$k^R_{\text{TR}}/\sqrt{c}$
camT_ca1_C -> camR_ca1_C	$k^R_{\text{TR}}/\sqrt{c}$
camT_ca1_D -> camR_ca1_D	$k^R_{\text{TR}}/\sqrt{c}$
camT_ca2_AB -> camR_ca2_AB	$k^R_{\text{TR}}/(\sqrt{c} * \sqrt{c})$
camT_ca2_AC -> camR_ca2_AC	$k^R_{\text{TR}}/(\sqrt{c} * \sqrt{c})$
camT_ca2_AD -> camR_ca2_AD	$k^R_{\text{TR}}/(\sqrt{c} * \sqrt{c})$
camT_ca2_BC -> camR_ca2_BC	$k^R_{\text{TR}}/(\sqrt{c} * \sqrt{c})$
camT_ca2_BD -> camR_ca2_BD	$k^R_{\text{TR}}/(\sqrt{c} * \sqrt{c})$
camT_ca2_CD -> camR_ca2_CD	$k^R_{\text{TR}}/(\sqrt{c} * \sqrt{c})$
camT_ca3_ABC -> camR_ca3_ABC	$k^R_{\text{TR}}/(\sqrt{c} * \sqrt{c} * \sqrt{c})$

Table S1. Continued

camT_ca3_ABD -> camR_ca3_ABD	$k^R_{\mathrm{TR}}/(\sqrt{c}*\sqrt{c}*\sqrt{c})$
camT_ca3_ACD -> camR_ca3_ACD	$k^R_{\mathrm{TR}}/(\sqrt{c}*\sqrt{c}*\sqrt{c})$
camT_ca3_BCD -> camR_ca3_BCD	$k^R_{\mathrm{TR}}/(\sqrt{c}*\sqrt{c}*\sqrt{c})$
camT_ca4_ABCD -> camR_ca4_ABD	$k^R_{\mathrm{TR}}/(\sqrt{c}*\sqrt{c}*\sqrt{c}*\sqrt{c})$
camR + CaMKII -> camR_CaMKII	k^R_{onCaMKII}
camR_ca1_A + CaMKII -> camR_ca1_A_CaMKII	k^R_{onCaMKII}
camR_ca1_B + CaMKII -> camR_ca1_B_CaMKII	k^R_{onCaMKII}
camR_ca1_C + CaMKII -> camR_ca1_C_CaMKII	k^R_{onCaMKII}
camR_ca1_D + CaMKII -> camR_ca1_D_CaMKII	k^R_{onCaMKII}
camR_ca2_AB + CaMKII -> camR_ca2_AB_CaMKII	k^R_{onCaMKII}
camR_ca2_AC + CaMKII -> camR_ca2_AC_CaMKII	k^R_{onCaMKII}
camR_ca2_AD + CaMKII -> camR_ca2_AD_CaMKII	k^R_{onCaMKII}
camR_ca2_BC + CaMKII -> camR_ca2_BC_CaMKII	k^R_{onCaMKII}
camR_ca2_BD + CaMKII -> camR_ca2_BD_CaMKII	k^R_{onCaMKII}
camR_ca2_CD + CaMKII -> camR_ca2_CD_CaMKII	k^R_{onCaMKII}
camR_ca3_ABC + CaMKII -> camR_ca3_ABC_CaMKII	k^R_{onCaMKII}
camR_ca3_ABD + CaMKII -> camR_ca3_ABD_CaMKII	k^R_{onCaMKII}
camR_ca3_ACD + CaMKII -> camR_ca3_ACD_CaMKII	k^R_{onCaMKII}
camR_ca3_BCD + CaMKII -> camR_ca3_BCD_CaMKII	k^R_{onCaMKII}
camR_ca4_ABCD + CaMKII -> camR_ca4_ABCD_CaMKII	k^R_{onCaMKII}
camR_CaMKII -> camR + CaMKII	$k^R_{\mathrm{offCaMKII}}$
camR_ca1_A_CaMKII -> camR_ca1_A + CaMKII	$k^R_{\mathrm{offCaMKII}}$
camR_ca1_B_CaMKII -> camR_ca1_B + CaMKII	$k^R_{\mathrm{offCaMKII}}$
camR_ca1_C_CaMKII -> camR_ca1_C + CaMKII	$k^R_{\mathrm{offCaMKII}}$
camR_ca1_D_CaMKII -> camR_ca1_D + CaMKII	$k^R_{\mathrm{offCaMKII}}$
camR_ca2_AB_CaMKII -> camR_ca2_AB + CaMKII	$k^R_{\mathrm{offCaMKII}}$
camR_ca2_AC_CaMKII -> camR_ca2_AC + CaMKII	$k^R_{\mathrm{offCaMKII}}$
camR_ca2_AD_CaMKII -> camR_ca2_AD + CaMKII	$k^R_{\mathrm{offCaMKII}}$
camR_ca2_BC_CaMKII -> camR_ca2_BC + CaMKII	$k^R_{\mathrm{offCaMKII}}$
camR_ca2_BD_CaMKII -> camR_ca2_BD + CaMKII	$k^R_{\mathrm{offCaMKII}}$
camR_ca2_CD_CaMKII -> camR_ca2_CD + CaMKII	$k^R_{\mathrm{offCaMKII}}$
camR_ca3_ABC_CaMKII -> camR_ca3_ABC + CaMKII	$k^R_{\mathrm{offCaMKII}}$
camR_ca3_ABD_CaMKII -> camR_ca3_ABD + CaMKII	$k^R_{\mathrm{offCaMKII}}$
camR_ca3_ACD_CaMKII -> camR_ca3_ACD + CaMKII	$k^R_{\mathrm{offCaMKII}}$
camR_ca3_BCD_CaMKII -> camR_ca3_BCD + CaMKII	$k^R_{\mathrm{offCaMKII}}$
camR_ca4_ABCD_CaMKII -> camR_ca4_ABCD + CaMKII	$k^R_{\mathrm{offCaMKII}}$
camR + PP2B -> camR_PP2B	k^R_{onPP2B}
camR_ca1_A + PP2B -> camR_ca1_A_PP2B	k^R_{onPP2B}
camR_ca1_B + PP2B -> camR_ca1_B_PP2B	k^R_{onPP2B}
camR_ca1_C + PP2B -> camR_ca1_C_PP2B	k^R_{onPP2B}
camR_ca1_D + PP2B -> camR_ca1_D_PP2B	k^R_{onPP2B}
camR_ca2_AB + PP2B -> camR_ca2_AB_PP2B	k^R_{onPP2B}
camR_ca2_AC + PP2B -> camR_ca2_AC_PP2B	k^R_{onPP2B}
camR_ca2_AD + PP2B -> camR_ca2_AD_PP2B	k^R_{onPP2B}
camR_ca2_BC + PP2B -> camR_ca2_BC_PP2B	k^R_{onPP2B}
camR_ca2_BD + PP2B -> camR_ca2_BD_PP2B	k^R_{onPP2B}
camR_ca2_CD + PP2B -> camR_ca2_CD_PP2B	k^R_{onPP2B}
camR_ca3_ABC + PP2B -> camR_ca3_ABC_PP2B	k^R_{onPP2B}
camR_ca3_ABD + PP2B -> camR_ca3_ABD_PP2B	k^R_{onPP2B}
camR_ca3_ACD + PP2B -> camR_ca3_ACD_PP2B	k^R_{onPP2B}
camR_ca3_BCD + PP2B -> camR_ca3_BCD_PP2B	k^R_{onPP2B}
camR_ca4_ABCD + PP2B -> camR_ca4_ABCD_PP2B	k^R_{onPP2B}
camR_PP2B -> camR + PP2B	k^R_{offPP2B}

Table S1. Continued

camR_ca1_B_PP2B -> camR_ca1_B + PP2B	k^R_{offPP2B}
camR_ca1_C_PP2B -> camR_ca1_C + PP2B	k^R_{offPP2B}
camR_ca1_D_PP2B -> camR_ca1_D + PP2B	k^R_{offPP2B}
camR_ca2_AB_PP2B -> camR_ca2_AB + PP2B	k^R_{offPP2B}
camR_ca2_AC_PP2B -> camR_ca2_AC + PP2B	k^R_{offPP2B}
camR_ca2_AD_PP2B -> camR_ca2_AD + PP2B	k^R_{offPP2B}
camR_ca2_BC_PP2B -> camR_ca2_BC + PP2B	k^R_{offPP2B}
camR_ca2_BD_PP2B -> camR_ca2_BD + PP2B	k^R_{offPP2B}
camR_ca2_CD_PP2B -> camR_ca2_CD + PP2B	k^R_{offPP2B}
camR_ca3_ABC_PP2B -> camR_ca3_ABC + PP2B	k^R_{offPP2B}
camR_ca3_ABD_PP2B -> camR_ca3_ABD + PP2B	k^R_{offPP2B}
camR_ca3_ACD_PP2B -> camR_ca3_ACD + PP2B	k^R_{offPP2B}
camR_ca3_BCD_PP2B -> camR_ca3_BCD + PP2B	k^R_{offPP2B}
camR_ca4_ABCD_PP2B -> camR_ca4_ABCD + PP2B	k^R_{offPP2B}
camR_CaMKII + ca -> camR_ca1_A_CaMKII	k^R_{on}
camR_CaMKII + ca -> camR_ca1_B_CaMKII	k^R_{on}
camR_CaMKII + ca -> camR_ca1_C_CaMKII	k^R_{on}
camR_CaMKII + ca -> camR_ca1_D_CaMKII	k^R_{on}
camR_ca1_A_CaMKII + ca -> camR_ca2_AB_CaMKII	k^R_{on}
camR_ca1_A_CaMKII + ca -> camR_ca2_AC_CaMKII	k^R_{on}
camR_ca1_A_CaMKII + ca -> camR_ca2_AD_CaMKII	k^R_{on}
camR_ca1_B_CaMKII + ca -> camR_ca2_AB_CaMKII	k^R_{on}
camR_ca1_B_CaMKII + ca -> camR_ca2_BC_CaMKII	k^R_{on}
camR_ca1_B_CaMKII + ca -> camR_ca2_BD_CaMKII	k^R_{on}
camR_ca1_C_CaMKII + ca -> camR_ca2_AC_CaMKII	k^R_{on}
camR_ca1_C_CaMKII + ca -> camR_ca2_BC_CaMKII	k^R_{on}
camR_ca1_C_CaMKII + ca -> camR_ca2_CD_CaMKII	k^R_{on}
camR_ca1_D_CaMKII + ca -> camR_ca2_AD_CaMKII	k^R_{on}
camR_ca1_D_CaMKII + ca -> camR_ca2_BD_CaMKII	k^R_{on}
camR_ca1_D_CaMKII + ca -> camR_ca2_CD_CaMKII	k^R_{on}
camR_ca2_AB_CaMKII + ca -> camR_ca3_ABC_CaMKII	k^R_{on}
camR_ca2_AB_CaMKII + ca -> camR_ca3_ABD_CaMKII	k^R_{on}
camR_ca2_AC_CaMKII + ca -> camR_ca3_ABC_CaMKII	k^R_{on}
camR_ca2_AC_CaMKII + ca -> camR_ca3_ACD_CaMKII	k^R_{on}
camR_ca2_AD_CaMKII + ca -> camR_ca3_ABD_CaMKII	k^R_{on}
camR_ca2_AD_CaMKII + ca -> camR_ca3_ACD_CaMKII	k^R_{on}
camR_ca2_BC_CaMKII + ca -> camR_ca3_ABC_CaMKII	k^R_{on}
camR_ca2_BC_CaMKII + ca -> camR_ca3_BCD_CaMKII	k^R_{on}
camR_ca2_BD_CaMKII + ca -> camR_ca3_ABD_CaMKII	k^R_{on}
camR_ca2_BD_CaMKII + ca -> camR_ca3_BCD_CaMKII	k^R_{on}
camR_ca2_CD_CaMKII + ca -> camR_ca3_ACD_CaMKII	k^R_{on}
camR_ca2_CD_CaMKII + ca -> camR_ca3_BCD_CaMKII	k^R_{on}
camR_ca3_ABC_CaMKII + ca -> camR_ca4_ABCD_CaMKII	k^R_{on}
camR_ca3_ABD_CaMKII + ca -> camR_ca4_ABCD_CaMKII	k^R_{on}
camR_ca3_ACD_CaMKII + ca -> camR_ca4_ABCD_CaMKII	k^R_{on}
camR_ca3_BCD_CaMKII + ca -> camR_ca4_ABCD_CaMKII	k^R_{on}
camR_ca1_A_CaMKII -> camR_CaMKII + ca	k^R_{offA}
camR_ca1_B_CaMKII -> camR_CaMKII + ca	k^R_{offB}
camR_ca1_C_CaMKII -> camR_CaMKII + ca	k^R_{offC}
camR_ca1_D_CaMKII -> camR_CaMKII + ca	k^R_{offD}
camR_ca2_AB_CaMKII -> camR_ca1_A_CaMKII + ca	k^R_{offB}
camR_ca2_AB_CaMKII -> camR_ca1_B_CaMKII + ca	k^R_{offA}
camR_ca2_AC_CaMKII -> camR_ca1_A_CaMKII + ca	k^R_{offC}

Table S1. Continued

camR_ca2_AC_CaMKII -> camR_ca1_C_CaMKII + ca	k^R_{offA}
camR_ca2_AD_CaMKII -> camR_ca1_A_CaMKII + ca	k^R_{offD}
camR_ca2_AD_CaMKII -> camR_ca1_D_CaMKII + ca	k^R_{offA}
camR_ca2_BC_CaMKII -> camR_ca1_B_CaMKII + ca	k^R_{offC}
camR_ca2_BC_CaMKII -> camR_ca1_C_CaMKII + ca	k^R_{offB}
camR_ca2_BD_CaMKII -> camR_ca1_B_CaMKII + ca	k^R_{offD}
camR_ca2_BD_CaMKII -> camR_ca1_D_CaMKII + ca	k^R_{offB}
camR_ca2_CD_CaMKII -> camR_ca1_C_CaMKII + ca	k^R_{offD}
camR_ca2_CD_CaMKII -> camR_ca1_D_CaMKII + ca	k^R_{offC}
camR_ca3_ABC_CaMKII -> camR_ca2_AB_CaMKII + ca	k^R_{offC}
camR_ca3_ABC_CaMKII -> camR_ca2_AC_CaMKII + ca	k^R_{offB}
camR_ca3_ABC_CaMKII -> camR_ca2_BC_CaMKII + ca	k^R_{offA}
camR_ca3_ABD_CaMKII -> camR_ca2_AB_CaMKII + ca	k^R_{offD}
camR_ca3_ABD_CaMKII -> camR_ca2_AD_CaMKII + ca	k^R_{offB}
camR_ca3_ABD_CaMKII -> camR_ca2_BD_CaMKII + ca	k^R_{offA}
camR_ca3_ACD_CaMKII -> camR_ca2_AC_CaMKII + ca	k^R_{offD}
camR_ca3_ACD_CaMKII -> camR_ca2_AD_CaMKII + ca	k^R_{offC}
camR_ca3_ACD_CaMKII -> camR_ca2_CD_CaMKII + ca	k^R_{offA}
camR_ca3_BCD_CaMKII -> camR_ca2_BC_CaMKII + ca	k^R_{offD}
camR_ca3_BCD_CaMKII -> camR_ca2_BD_CaMKII + ca	k^R_{offC}
camR_ca3_BCD_CaMKII -> camR_ca2_CD_CaMKII + ca	k^R_{offB}
camR_ca4_ABCD_CaMKII -> camR_ca3_ABC_CaMKII + ca	k^R_{offD}
camR_ca4_ABCD_CaMKII -> camR_ca3_ABD_CaMKII + ca	k^R_{offC}
camR_ca4_ABCD_CaMKII -> camR_ca3_ACD_CaMKII + ca	k^R_{offB}
camR_ca4_ABCD_CaMKII -> camR_ca3_BCD_CaMKII + ca	k^R_{offA}
camR_PP2B + ca -> camR_ca1_A_PP2B	k^R_{on}
camR_PP2B + ca -> camR_ca1_B_PP2B	k^R_{on}
camR_PP2B + ca -> camR_ca1_C_PP2B	k^R_{on}
camR_PP2B + ca -> camR_ca1_D_PP2B	k^R_{on}
camR_ca1_A_PP2B + ca -> camR_ca2_AB_PP2B	k^R_{on}
camR_ca1_A_PP2B + ca -> camR_ca2_AC_PP2B	k^R_{on}
camR_ca1_A_PP2B + ca -> camR_ca2_AD_PP2B	k^R_{on}
camR_ca1_B_PP2B + ca -> camR_ca2_AB_PP2B	k^R_{on}
camR_ca1_B_PP2B + ca -> camR_ca2_BC_PP2B	k^R_{on}
camR_ca1_B_PP2B + ca -> camR_ca2_BD_PP2B	k^R_{on}
camR_ca1_C_PP2B + ca -> camR_ca2_AC_PP2B	k^R_{on}
camR_ca1_C_PP2B + ca -> camR_ca2_BC_PP2B	k^R_{on}
camR_ca1_C_PP2B + ca -> camR_ca2_CD_PP2B	k^R_{on}
camR_ca1_D_PP2B + ca -> camR_ca2_AD_PP2B	k^R_{on}
camR_ca1_D_PP2B + ca -> camR_ca2_BD_PP2B	k^R_{on}
camR_ca1_D_PP2B + ca -> camR_ca2_CD_PP2B	k^R_{on}
camR_ca2_AB_PP2B + ca -> camR_ca3_ABC_PP2B	k^R_{on}
camR_ca2_AB_PP2B + ca -> camR_ca3_ABD_PP2B	k^R_{on}
camR_ca2_AC_PP2B + ca -> camR_ca3_ABC_PP2B	k^R_{on}
camR_ca2_AC_PP2B + ca -> camR_ca3_ACD_PP2B	k^R_{on}
camR_ca2_AD_PP2B + ca -> camR_ca3_ABD_PP2B	k^R_{on}
camR_ca2_AD_PP2B + ca -> camR_ca3_ACD_PP2B	k^R_{on}
camR_ca2_BC_PP2B + ca -> camR_ca3_ABC_PP2B	k^R_{on}
camR_ca2_BC_PP2B + ca -> camR_ca3_BCD_PP2B	k^R_{on}
camR_ca2_BD_PP2B + ca -> camR_ca3_ABD_PP2B	k^R_{on}
camR_ca2_BD_PP2B + ca -> camR_ca3_BCD_PP2B	k^R_{on}
camR_ca2_CD_PP2B + ca -> camR_ca3_ACD_PP2B	k^R_{on}
camR_ca2_CD_PP2B + ca -> camR_ca3_BCD_PP2B	k^R_{on}

Table S1. Continued

camR_ca3_ABC_PP2B + ca -> camR_ca4_ABCD_PP2B	k^R_{on}
camR_ca3_ABD_PP2B + ca -> camR_ca4_ABCD_PP2B	k^R_{on}
camR_ca3_ACD_PP2B + ca -> camR_ca4_ABCD_PP2B	k^R_{on}
camR_ca3_BCD_PP2B + ca -> camR_ca4_ABCD_PP2B	k^R_{on}
camR_ca1_A_PP2B -> camR_PP2B + ca	k^R_{offA}
camR_ca1_B_PP2B -> camR_PP2B + ca	k^R_{offB}
camR_ca1_C_PP2B -> camR_PP2B + ca	k^R_{offC}
camR_ca1_D_PP2B -> camR_PP2B + ca	k^R_{offD}
camR_ca2_AB_PP2B -> camR_ca1_A_PP2B + ca	k^R_{offB}
camR_ca2_AB_PP2B -> camR_ca1_B_PP2B + ca	k^R_{offA}
camR_ca2_AC_PP2B -> camR_ca1_A_PP2B + ca	k^R_{offC}
camR_ca2_AC_PP2B -> camR_ca1_C_PP2B + ca	k^R_{offA}
camR_ca2_AD_PP2B -> camR_ca1_A_PP2B + ca	k^R_{offD}
camR_ca2_AD_PP2B -> camR_ca1_D_PP2B + ca	k^R_{offA}
camR_ca2_BC_PP2B -> camR_ca1_B_PP2B + ca	k^R_{offC}
camR_ca2_BC_PP2B -> camR_ca1_C_PP2B + ca	k^R_{offB}
camR_ca2_BD_PP2B -> camR_ca1_B_PP2B + ca	k^R_{offD}
camR_ca2_BD_PP2B -> camR_ca1_D_PP2B + ca	k^R_{offB}
camR_ca2_CD_PP2B -> camR_ca1_C_PP2B + ca	k^R_{offD}
camR_ca2_CD_PP2B -> camR_ca1_D_PP2B + ca	k^R_{offC}
camR_ca3_ABC_PP2B -> camR_ca2_AB_PP2B + ca	k^R_{offC}
camR_ca3_ABC_PP2B -> camR_ca2_AC_PP2B + ca	k^R_{offB}
camR_ca3_ABC_PP2B -> camR_ca2_BC_PP2B + ca	k^R_{offA}
camR_ca3_ABD_PP2B -> camR_ca2_AB_PP2B + ca	k^R_{offD}
camR_ca3_ABD_PP2B -> camR_ca2_AD_PP2B + ca	k^R_{offB}
camR_ca3_ABD_PP2B -> camR_ca2_BD_PP2B + ca	k^R_{offA}
camR_ca3_ACD_PP2B -> camR_ca2_AC_PP2B + ca	k^R_{offD}
camR_ca3_ACD_PP2B -> camR_ca2_AD_PP2B + ca	k^R_{offC}
camR_ca3_ACD_PP2B -> camR_ca2_CD_PP2B + ca	k^R_{offA}
camR_ca3_BCD_PP2B -> camR_ca2_BC_PP2B + ca	k^R_{offD}
camR_ca3_BCD_PP2B -> camR_ca2_BD_PP2B + ca	k^R_{offC}
camR_ca3_BCD_PP2B -> camR_ca2_CD_PP2B + ca	k^R_{offB}
camR_ca4_ABCD_PP2B -> camR_ca3_ABC_PP2B + ca	k^R_{offD}
camR_ca4_ABCD_PP2B -> camR_ca3_ABD_PP2B + ca	k^R_{offC}
camR_ca4_ABCD_PP2B -> camR_ca3_ACD_PP2B + ca	k^R_{offB}
camR_ca4_ABCD_PP2B -> camR_ca3_BCD_PP2B + ca	k^R_{offA}

Table S2. List of parameters used for simulation

K_A^R	8.32×10^{-6} M	this article
K_B^R	1.66×10^{-8} M	this article
K_C^R	1.74×10^{-5} M	this article
K_D^R	1.45×10^{-8} M	this article
K_A^T	2.10×10^{-3} M	K_A^R/c
K_B^T	4.19×10^{-6} M	K_B^R/c
K_C^T	4.39×10^{-3} M	K_C^R/c
K_D^T	3.66×10^{-6} M	K_D^R/c
k_{on}	10^6 $M^{-1}s^{-1}$	assumption
k^R_{offA}	$8.32\ s^{-1}$	$K_A^R * k_{on}$
k^R_{offB}	$1.66 \times 10^{-2}\ s^{-1}$	$K_B^R * k_{on}$
k^R_{offC}	$17.4\ s^{-1}$	$K_C^R * k_{on}$
k^R_{offD}	$1.45 \times 10^{-2}\ s^{-1}$	$K_D^R * k_{on}$
k^T_{offA}	$2.10 \times 10^3\ s^{-1}$	$K_A^T * k_{on}$
k^T_{offB}	$4.19\ s^{-1}$	$K_B^T * k_{on}$
k^T_{offC}	$4.39 \times 10^3\ s^{-1}$	$K_C^T * k_{on}$
k^T_{offD}	$3.66\ s^{-1}$	$K_D^T * k_{on}$
L	20670	this article
k_{RT}	1×10^6	assumption
k_{TR}	48.38	k_{RT}/L
c	0.00396	this article
$k_{onCaMKII}$	3.2×10^6 $M^{-1}s^{-1}$	[11]
$k_{offCaMKII}$	$0.343\ s^{-1}$	[11]
k_{onPP2B}	4.6×10^7 $M^{-1}s^{-1}$	[8]
$k_{offPP2B}$	$0.0013\ s^{-1}$	[8]
$[T_0]$	2×10^{-7} M – 3×10^{-5} M	depending on simulation run
[calcium]	10^{-8} M – 10^{-1} M	multiple simulations with various concentrations
[PP2B]	1.6×10^{-6} M	cf [4]
[CaMKII]	7×10^{-5} M	cf [6]
spine volume	10^{-15} L	cf [2]