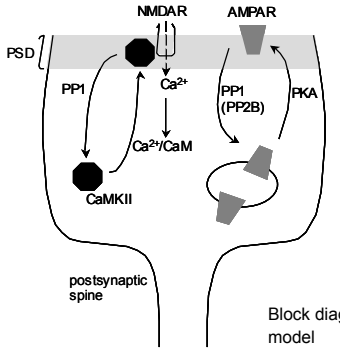
A. Model Parameters for basic synaptic traffic model.
Components: AMPA receptor (AMPAR), Calcium Calmodulin type II Kinase (CaMKII), Calmodulin (CaM), Inhibitor 1 (I1), Protein phosphatase 2 B (PP2B), Adenylyl Cyclase (AC), Protein Kinase A (PKA).

Concentration units: uM (micromolar) for rate constants presented as Kf, Kb, Km
#/cell for rate constants presented as kf, kb, k1, k2, k3. This formulation of rates may depend on cellular volume.
Time units: Seconds in all cases.
Total Volume of Synapse = 0.1 femtoliters (fl)
Volume of cytosolic portion = 0.09 fl
Volume of Postsynaptic Density (PSD) = 0.01 fl

The enzyme rates are related as follows:
Km = (k2 + k3)/k1 (after conversion of units)
Kcat = k3.
Ratio = k2/k3

Initial concentrations (CoInit) are mostly zero, except for a few key molecules.
There is a flag for 'buffered' in the molecule concentration table. When this flag is zero the molecule concentrations are computed according to the reaction equations. If the flag is one the molecule concentration is held fixed to its initial concentration.

For clarity, the model is organized into 'groups' which roughly correspond to individual pathways. The '/kinetics' group is a set of shared molecules interacting with more than one pathway. The entire model scheme is then repeated as composite tables for molecules, reactions and enzymes.



Block diagram of model

Concentration units: uM
Time units: sec
Default Volume (m^3) : 9e-20

Equations for group /kinetics
Reactions for group /kinetics

Reaction	kf	kb	Kf	Kb
PKC-control <===> PKC-active	2.5	2.5	2.5	2.5
Ca_control_cyt <===> Ca	100	100	100	100
Ca_control_PSD <===> Ca-PSD	100	100	100	100

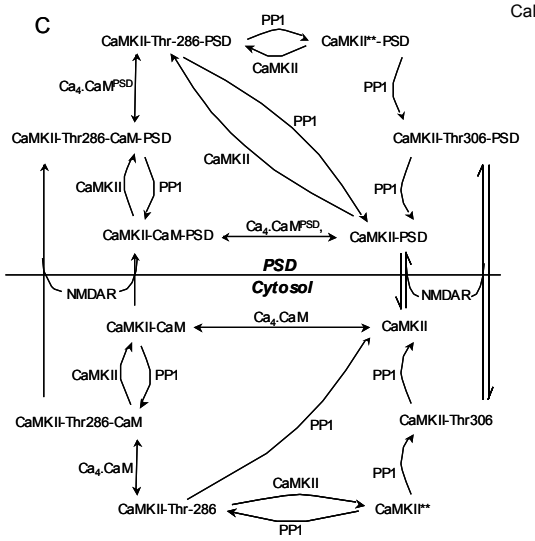
Enzymes for group /kinetics

Enzyme-reaction	k1	k2	k3	Km	Vmax	ratio
neurogranin ---PKC-active--> neurogranin*	0.001889	2.34	0.58	28.627	0.58	4.0345
neurogranin-CaM ---PKC-active--> CaM + neurogranin*	0.001133	1.4	0.35	28.596	0.35	4
AC2 ---PKC-active--> AC2*	0.011111	16	4	33.334	4	4
neurogranin-CaM[1] ---PKC-active--> CaM-PSD + neurogranin*[1]	0.001133	1.4	0.35	28.596	0.35	4
neurogranin[1] ---PKC-active--> neurogranin*[1]	0.001889	2.34	0.58	28.627	0.58	4.0345

Pools for group /kinetics

name	CoInit	buffered
Ca	0.08	0
Ca-PSD	0.08	0
PKC-active	0.1	0
PKC-control	0.1	1
Ca_control_cyt	0.08	1
Ca_control_PSD	0.08	1

CaMKII reactions



Equations for group /kinetics/CaMKII

Reactions for group /kinetics/CaMKII

Reaction	kf	kb	Kf	Kb
CaM-Ca4 + CaMKII <===> CaMKII-CaM	0.92592	5	50	5
CaMKII-thr286 + CaM-Ca4 <===> CaMKII-thr286*-CaM	18.522	0.1	1000.2	0.1
CaMKII-thr306-PSD <===> CaMK-thr306 + NMDAR	0.3	1.00E-05	0.3	6.00E-05
CaMKII-PSD <===> CaMKII + NMDAR	0.3	1.00E-05	0.3	6.00E-05
CaMKII-CaM + NMDAR <===> CaMKII-CaM-PSD	2.00E-05	0	0.00108	0
CaMKII-thr286*-CaM + NMDAR <===> CaMKII-thr286-CaM-PSD	2.00E-05	0	0.00108	0
CaMKII-CaM-PSD <===> CaM-Ca4-PSD + CaMKII-PSD	5	0	5	0
CaMKII-PSD + CaM-Ca4-PSD <===> CaMKII-CaM-PSD	8.3333	0	50	0
CaMKII-thr286-PSD + CaM-Ca4-PSD <===> CaMKII-thr286-CaM-PSD	166.67	0.1	1000	0.1
basal_CaMKII_PSD_control <===> basal_CaMKII_PSD	1	1	1	1

Enzymes for group /kinetics/CaMKII

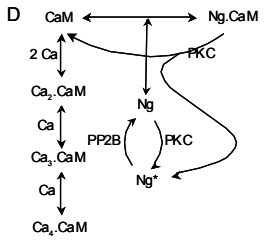
Enzyme-reaction	k1	k2	k3	Km	Vmax	ratio
CaMKII-thr286 ---tot_CaM_CaMKII--> CaMKII***	0.00489	24	6	113.6	6	4
CaMKII-CaM ---tot_CaM_CaMKII--> CaMKII-thr286*-CaM	0.000408	2	0.5	113.6	0.5	4
CaMKII-thr286 ---tot_autonomous_CaMKII--> CaMKII***	0.003175	24	6	175	6	4
CaMKII-CaM ---tot_autonomous_CaMKII--> CaMKII-thr286*-CaM	0.000265	2	0.5	174.99	0.5	4
CaMKII-thr286-PSD ---tot-auto-PSD--> CaMKII***-PSD	0.04	24	6	125	6	4
CaMKII-CaM-PSD ---tot-auto-PSD--> CaMKII-thr286-CaM-PSD	0.003333	2	0.5	125	0.5	4
CaMKII-thr286-PSD ---tot-CaM-CaMKII-PSD--> CaMKII***-PSD	0.061599	24	6	81.17	6	4
CaMKII-CaM-PSD ---tot-CaM-CaMKII-PSD--> CaMKII-thr286-CaM-PSD	0.005133	2	0.5	81.169	0.5	4
A12_B12 ---actCaMKII-PSD--> A1'2_B12[1]	0.00463	2	0.5	90.001	0.5	4
A12_B12'[1] ---actCaMKII-PSD--> A1'2_B12'	0.00463	2	0.5	90.001	0.5	4
A12'_B12[2] ---actCaMKII-PSD--> A1'2'_B12	0.00463	2	0.5	90.001	0.5	4
A12_B12[3] ---actCaMKII-PSD--> A1'2_B12[5]	0.00463	2	0.5	90.001	0.5	4
A12_B12 ---actCaMKII-PSD--> A12_B12[2]	0.00463	2	0.5	90.001	0.5	4
A12_B12'[1] ---actCaMKII-PSD--> A12_B12'[2]	0.00463	2	0.5	90.001	0.5	4
A12'_B12[2] ---actCaMKII-PSD--> A12'_B12[1]	0.00463	2	0.5	90.001	0.5	4
A12_B12[3] ---actCaMKII-PSD--> A12_B12[6]	0.00463	2	0.5	90.001	0.5	4
A12_B12[2] ---actCaMKII-PSD--> A12_B12[4]	0.00463	2	0.5	90.001	0.5	4
A12_B12'[2] ---actCaMKII-PSD--> A12_B12'[3]	0.00463	2	0.5	90.001	0.5	4
A12'_B12[1] ---actCaMKII-PSD--> A12'_B12[3]	0.00463	2	0.5	90.001	0.5	4
A12_B12[6] ---actCaMKII-PSD--> A12_B12[7]	0.00463	2	0.5	90.001	0.5	4
A1'2_B12[1] ---actCaMKII-PSD--> A12_B12[4]	0.00463	2	0.5	90.001	0.5	4
A1'2_B12' ---actCaMKII-PSD--> A12_B12'[3]	0.00463	2	0.5	90.001	0.5	4
A1'2'_B12 ---actCaMKII-PSD--> A12'_B12[3]	0.00463	2	0.5	90.001	0.5	4
A1'2_B12[5] ---actCaMKII-PSD--> A12_B12[7]	0.00463	2	0.5	90.001	0.5	4

Pools for group /kinetics/CaMKII

name	CoInit	buffered
CaMKII	20	0
CaMKII-CaM	0	0
CaMKII-thr286*-CaM	0	0
CaMKII***	0	0
CaMKII-thr286	0	0
CaMK-thr306	0	0

tot_CaM_CaMKII	0	0
tot_autonomous_CaMKII	2	0
tot_CaMKII_cyt	22	0
act_CaMKII_cyt	2	0
basal_CaMKII_cyt	2	1
NMDAR	120	0
CaMKII-thr306-PSD	0	0
CaMKII***-PSD	0	0
CaMKII-PSD	0	0
CaMKII-thr286-PSD	0	0
CaMKII-CaM-PSD	0	0
CaMKII-thr286-CaM-PSD	0	0
tot-auto-PSD	2	0
tot-CaM-CaMKII-PSD	0	0
basal_CaMKII_PSD_control	2	1
basal_CaMKII_PSD	2	0
tot_CaMKII_PSD	2	0
actCaMKII-PSD	2	0
286P-PSD	0	0

CaM reactions



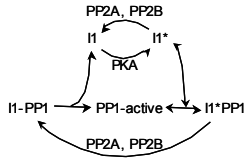
Equations for group /kinetics/CaM
Reactions for group /kinetics/CaM

Reaction	kf	kb	Kf	Kb
CaM + 2 Ca <===> CaM-TR2-Ca2	0.024691	72	71.999	72
CaM-TR2-Ca2 + Ca <===> CaM-Ca3	0.066667	10	3.6	10
neurogranin + CaM <===> neurogranin-CaM	0.005556	1	0.3	1
neurogranin* <===> neurogranin	0.005	0	0.005	0
CaM-PSD + 2 Ca-PSD <===> CaM-TR2-Ca2-PSD	2	72	72	72
CaM-TR2-Ca2-PSD + Ca-PSD <===> CaM-Ca3-PSD	0.6	10	3.6	10
neurogranin[1] + CaM-PSD <===> neurogranin-CaM[1]	0.05	1	0.3	1
neurogranin*[1] <===> neurogranin[1]	0.005	0	0.005	0
CaM-Ca3 + Ca <===> CaM-Ca4	0.008611	10	0.465	10
CaM-Ca3-PSD + Ca-PSD <===> CaM-Ca4-PSD	0.077502	10	0.46501	10
CaM-Ca4-PSD <===> CaM-Ca4	540	60	540	60

Pools for group /kinetics/CaM

name	CoInit	buffered
CaM	26.333	0
neurogranin-CaM	0	0
neurogranin*	0	0
neurogranin	10	0
CaM-PSD	26.333	0
neurogranin-CaM[1]	0	0
neurogranin[1]	10	0
neurogranin*[1]	0	0
CaM-TR2-Ca2	0	0
CaM-Ca3	0	0
CaM-Ca4	0	0
CaM-TR2-Ca2-PSD	0	0
CaM-Ca3-PSD	0	0
CaM-Ca4-PSD	0	0

PP1 reactions



Equations for group /kinetics/PP1
Reactions for group /kinetics/PP1

Reaction	kf	kb	Kf	Kb
I1* + PP1-active <===> PP1-I1*	9.2589	0.1	499.98	0.1
PP1-I1 <===> PP1-active + I1	1	0	1	0

Enzymes for group /kinetics/PP1

Enzyme-reaction	k1	k2	k3	Km	Vmax	ratio
CaMKII-thr286*-CaM ---PP1-active--> CaMKII-CaM	0.045397	10	2.5	5.099	2.5	4
CaMKII-thr286 ---PP1-active--> CaMKII	0.045397	10	2.5	5.099	2.5	4
CaMKII*** ---PP1-active--> CaMKII-thr286	0.045397	10	2.5	5.099	2.5	4
CaMK-thr306 ---PP1-active--> CaMKII	0.045397	10	2.5	5.099	2.5	4
CaMKII*** ---PP1-active--> CaMK-thr306	0.045397	10	2.5	5.099	2.5	4
I1* ---PP2A--> I1	0.01196	8.3334	2	16	2	4.1667
PP1-I1* ---PP2A--> PP1-I1	0.01196	8.3334	2	16	2	4.1667
I1*_PSD ---PP2A--> I1_PSD	0.01196	8.3334	2	16	2	4.1667
PP1-I1*_PSD ---PP2A--> PP1-I1_PSD	0.01196	8.3334	2	16	2	4.1667

Pools for group /kinetics/PP1

name	CoInit	buffered
I1	1.8	0
I1*	0	0
PP1-I1*	0	0
PP1-I1	0	0
PP1-active	1.8	0
PP2A	0.11111	0

Equations for group /kinetics/PP1_PSD
Reactions for group /kinetics/PP1_PSD

Reaction	kf	kb	Kf	Kb
PP1-I1_PSD <===> I1_PSD + PP1-active_PSD	1	0	1	0
I1*_PSD + PP1-active_PSD <===> PP1-I1*_PSD	83.33	0.1	499.98	0.1

Enzymes for group /kinetics/PP1_PSD

Enzyme-reaction	k1	k2	k3	Km	Vmax	ratio
CaMKII-thr286-CaM-PSD ---PP1-active_PSD--> CaMKII-CaM-PSD	1.0417	10	2.5	1.9999	2.5	4
CaMKII-thr286-PSD ---PP1-active_PSD--> CaMKII-PSD	1.0417	10	2.5	1.9999	2.5	4
CaMKII***-PSD ---PP1-active_PSD--> CaMKII-thr286-PSD	0.40857	10	2.5	5.0991	2.5	4
CaMKII-thr306-PSD ---PP1-active_PSD--> CaMKII-PSD	0.40857	10	2.5	5.0991	2.5	4
CaMKII***-PSD ---PP1-active_PSD--> CaMKII-thr306-PSD	1.0417	10	2.5	1.9999	2.5	4
A12_B12 ---PP1-active_PSD--> A12_B12'[1]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12 ---PP1-active_PSD--> A12'_B12[2]	0.14583	0.68	0.17	0.97145	0.17	4
A12'_B12[2] ---PP1-active_PSD--> A12_B12[3]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12'[1] ---PP1-active_PSD--> A12_B12[3]	0.14583	0.68	0.17	0.97145	0.17	4
A1'2_B12[1] ---PP1-active_PSD--> A1'2_B12'	0.14583	0.68	0.17	0.97145	0.17	4
A1'2_B12[1] ---PP1-active_PSD--> A1'2'_B12	0.14583	0.68	0.17	0.97145	0.17	4
A1'2_B12' ---PP1-active_PSD--> A1'2_B12[5]	0.14583	0.68	0.17	0.97145	0.17	4
A1'2'_B12 ---PP1-active_PSD--> A1'2_B12[5]	0.14583	0.68	0.17	0.97145	0.17	4
A1'2_B12[1] ---PP1-active_PSD--> A12_B12	0.14583	1.4	0.35	2	0.35	4
A1'2_B12' ---PP1-active_PSD--> A12_B12'[1]	0.14583	1.4	0.35	2	0.35	4
A1'2'_B12 ---PP1-active_PSD--> A12'_B12[2]	0.14583	1.4	0.35	2	0.35	4
A1'2_B12[5] ---PP1-active_PSD--> A12_B12[3]	0.14583	1.4	0.35	2	0.35	4
A12_B12[2] ---PP1-active_PSD--> A12_B12'[2]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12[2] ---PP1-active_PSD--> A12'_B12[1]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12'[2] ---PP1-active_PSD--> A12_B12[6]	0.14583	0.68	0.17	0.97145	0.17	4
A12'_B12[1] ---PP1-active_PSD--> A12_B12[6]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12[4] ---PP1-active_PSD--> A12_B12'[3]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12[4] ---PP1-active_PSD--> A12'_B12[3]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12'[3] ---PP1-active_PSD--> A12_B12[7]	0.14583	0.68	0.17	0.97145	0.17	4
A12'_B12[3] ---PP1-active_PSD--> A12_B12[7]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12'[2] ---PP1-active_PSD--> A12_B12'[1]	0.14583	1.4	0.35	2	0.35	4
A12_B12[2] ---PP1-active_PSD--> A12_B12	0.14583	1.4	0.35	2	0.35	4

A12'_B12[1] ---PP1-active_PSD--> A12'_B12[2]	0.14583	1.4	0.35	2	0.35	4
A12_B12[6] ---PP1-active_PSD--> A12_B12[3]	0.14583	1.4	0.35	2	0.35	4
A12_B12[4] ---PP1-active_PSD--> A12_B12[2]	0.14583	1.4	0.35	2	0.35	4
A12_B12'[3] ---PP1-active_PSD--> A12_B12'[2]	0.14583	1.4	0.35	2	0.35	4
A12'_B12[3] ---PP1-active_PSD--> A12'_B12[1]	0.14583	1.4	0.35	2	0.35	4
A12_B12[7] ---PP1-active_PSD--> A12_B12[6]	0.14583	1.4	0.35	2	0.35	4
A12_B12[4] ---PP1-active_PSD--> A1'2_B12[1]	0.14583	1.4	0.35	2	0.35	4
A12_B12'[3] ---PP1-active_PSD--> A1'2_B12'	0.14583	1.4	0.35	2	0.35	4
A12'_B12[3] ---PP1-active_PSD--> A1'2'_B12	0.14583	1.4	0.35	2	0.35	4
A12_B12[7] ---PP1-active_PSD--> A1'2_B12[5]	0.14583	1.4	0.35	2	0.35	4

Pools for group /kinetics/PP1_PSD

name	CoInit	buffered
PP1-active_PSD	4	0
I1_PSD	4	0
I1*_PSD	0	0
PP1-I1_PSD	0	0
PP1-I1*_PSD	0	0

PP2B/Calcineurin
reactions

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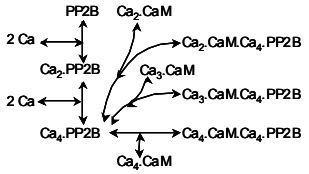


Equations for group /kinetics/PP2B
Reactions for group /kinetics/PP2B

Reaction	kf	kb	Kf	Kb
2 Ca + CaNAB-Ca2 <===> CaNAB-Ca4	0.001235	1	3.6001	1
CaNAB + 2 Ca <===> CaNAB-Ca2	3.4321	1	10008	1
CaM-Ca4 + CaNAB-Ca4 <===> CaM_Ca_n-CaNAB	11.111	1	599.99	1

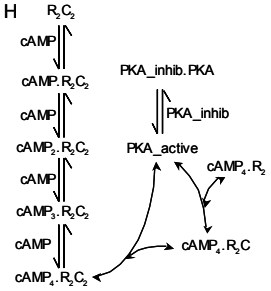
Enzymes for group /kinetics/PP2B

Enzyme-reaction	k1	k2	k3	Km	Vmax	ratio
I1* ---CaNAB-Ca4--> I1	0.000633	0.136	0.034	4.9708	0.034	4
I1*_PSD ---CaNAB-Ca4--> I1_PSD	0.000633	0.136	0.034	4.9707	0.034	4
neurogranin* ---CaM_Ca_n-CaNAB--> neurogranin	0.006178	2.67	0.67	10.012	0.67	3.9851
I1* ---CaM_Ca_n-CaNAB--> I1	0.006333	1.36	0.34	4.9708	0.34	4
PP1-I1* ---CaM_Ca_n-CaNAB--> PP1-I1	0.006333	1.36	0.34	4.9708	0.34	4
I1*_PSD ---CaM_Ca_n-CaNAB--> I1_PSD	0.006333	1.36	0.34	4.9707	0.34	4
PP1-I1*_PSD ---CaM_Ca_n-CaNAB--> PP1-I1_PSD	0.006333	1.36	0.34	4.9707	0.34	4
A12_B12' ---CaM_Ca_n-CaNAB--> A12_B12	0.037256	8	2	4.9706	2	4
A1'2_B12' ---CaM_Ca_n-CaNAB--> A1'2_B12	0.037256	8	2	4.9706	2	4
A12_B1'2' ---CaM_Ca_n-CaNAB--> A12_B1'2	0.037256	8	2	4.9706	2	4
A1'2_B1'2' ---CaM_Ca_n-CaNAB--> A1'2_B1'2	0.037256	8	2	4.9706	2	4
A12'_B12 ---CaM_Ca_n-CaNAB--> A12_B12	0.037256	8	2	4.9706	2	4
A1'2'_B12 ---CaM_Ca_n-CaNAB--> A1'2_B12	0.037256	8	2	4.9706	2	4
A12'_B1'2 ---CaM_Ca_n-CaNAB--> A12_B1'2	0.037256	8	2	4.9706	2	4
A1'2'_B1'2 ---CaM_Ca_n-CaNAB--> A1'2_B1'2	0.037256	8	2	4.9706	2	4
A12'_B12'[1] ---CaM_Ca_n-CaNAB--> A12'_B12	0.037256	8	2	4.9706	2	4
A1'2'_B12'[1] ---CaM_Ca_n-CaNAB--> A1'2'_B12	0.037256	8	2	4.9706	2	4
A12'_B1'2'[1] ---CaM_Ca_n-CaNAB--> A12'_B1'2	0.037256	8	2	4.9706	2	4
A1'2'_B1'2'[1] ---CaM_Ca_n-CaNAB--> A1'2'_B1'2	0.037256	8	2	4.9706	2	4
A12'_B12'[1] ---CaM_Ca_n-CaNAB--> A12_B12'	0.037256	8	2	4.9706	2	4
A1'2'_B12'[1] ---CaM_Ca_n-CaNAB--> A1'2_B12'	0.037256	8	2	4.9706	2	4
A12'_B1'2'[1] ---CaM_Ca_n-CaNAB--> A12_B1'2'	0.037256	8	2	4.9706	2	4
A1'2'_B1'2'[1] ---CaM_Ca_n-CaNAB--> A1'2_B1'2'	0.037256	8	2	4.9706	2	4
A12_B12 ---CaM_Ca_n-CaNAB--> A12_B12'[1]	0.037256	8	2	4.9706	2	4
A12_B12 ---CaM_Ca_n-CaNAB--> A12'_B12[2]	0.037256	8	2	4.9706	2	4
A12_B12'[1] ---CaM_Ca_n-CaNAB--> A12_B12[3]	0.037256	8	2	4.9706	2	4
A12'_B12[2] ---CaM_Ca_n-CaNAB--> A12_B12[3]	0.037256	8	2	4.9706	2	4
A1'2_B12[1] ---CaM_Ca_n-CaNAB--> A1'2_B12'	0.037256	8	2	4.9706	2	4
A1'2_B12[1] ---CaM_Ca_n-CaNAB--> A1'2'_B12	0.037256	8	2	4.9706	2	4
A1'2_B12' ---CaM_Ca_n-CaNAB--> A1'2_B12[5]	0.037256	8	2	4.9706	2	4
A1'2'_B12 ---CaM_Ca_n-CaNAB--> A1'2_B12[5]	0.037256	8	2	4.9706	2	4
A12_B12[2] ---CaM_Ca_n-CaNAB--> A12_B12'[2]	0.037256	8	2	4.9706	2	4
A12_B12[2] ---CaM_Ca_n-CaNAB--> A12'_B12[1]	0.037256	8	2	4.9706	2	4
A12_B12'[2] ---CaM_Ca_n-CaNAB--> A12_B12[6]	0.037256	8	2	4.9706	2	4
A12'_B12[1] ---CaM_Ca_n-CaNAB--> A12_B12[6]	0.037256	8	2	4.9706	2	4
A12_B12[4] ---CaM_Ca_n-CaNAB--> A12_B12'[3]	0.037256	8	2	4.9706	2	4
A12_B12[4] ---CaM_Ca_n-CaNAB--> A12'_B12[3]	0.037256	8	2	4.9706	2	4
A12'_B12[3] ---CaM_Ca_n-CaNAB--> A12_B12[7]	0.037256	8	2	4.9706	2	4
A12_B12'[3] ---CaM_Ca_n-CaNAB--> A12_B12[7]	0.037256	8	2	4.9706	2	4
neurogranin*[1] ---CaM_Ca_n-CaNAB--> neurogranin[1]	0.006178	2.67	0.67	10.012	0.67	3.9851

Pools for group /kinetics/PP2B

name	CoInit	buffered
CaNAB	1	0
CaNAB-Ca2	0	0
CaNAB-Ca4	0	0
CaM_Ca_n-CaNAB	0	0

PKA reactions



Equations for group /kinetics/PKA

Reactions for group /kinetics/PKA

Reaction	kf	kb	Kf	Kb
R2C2 + cAMP <===> R2C2-cAMP	1	33	54	33
R2C2-cAMP + cAMP <===> R2C2-cAMP2	1	33	54	33
R2C2-cAMP2 + cAMP <===> R2C2-cAMP3	1.3889	110	75.001	110
cAMP + R2C2-cAMP3 <===> R2C2-cAMP4	1.3889	32.5	75.001	32.5
R2C2-cAMP4 <===> PKA-active + R2C-cAMP4	60	0.33333	60	18
R2C-cAMP4 <===> PKA-active + R2-cAMP4	60	0.33333	60	18
PKA-active + PKA-inhibitor <===> inhibited-PKA	1.1111	1	59.999	1

Enzymes for group /kinetics/PKA

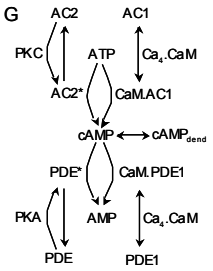
Enzyme-reaction	k1	k2	k3	Km	Vmax	ratio	
cAMP-PDE ---PKA-active--> cAMP-PDE*	0.11111	36	9	7.5001	9	4	
I1 ---PKA-active--> I1*	0.11111	36	9	7.5001	9	4	
I1_PSD ---PKA-active--> I1*_PSD	0.11111	36	9	7.5001	9	4	
A12_B12 ---PKA-active--> A12_B12'	0.074072	24	6	7.5002	6	4	
A1'2_B12 ---PKA-active--> A1'2_B12'	0.074072	24	6	7.5002	6	4	
A12_B1'2 ---PKA-active--> A12_B1'2'	0.074072	24	6	7.5002	6	4	
A1'2_B1'2 ---PKA-active--> A1'2_B1'2'	0.074072	24	6	7.5002	6	4	
A12_B12 ---PKA-active--> A12'_B12	0.074072	24	6	7.5002	6	4	
A1'2_B12 ---PKA-active--> A1'2'_B12	0.074072	24	6	7.5002	6	4	
A12_B1'2 ---PKA-active--> A12'_B1'2	0.074072	24	6	7.5002	6	4	
A1'2_B1'2 ---PKA-active--> A1'2'_B1'2	0.074072	24	6	7.5002	6	4	
A12'_B12 ---PKA-active--> A12'_B12'[1]	0.074072	24	6	7.5002	6	4	
A1'2'_B12 ---PKA-active--> A1'2'_B12'[1]	0.074072	24	6	7.5002	6	4	
A12'_B1'2 ---PKA-active--> A12'_B1'2'[1]	0.074072	24	6	7.5002	6	4	
A1'2'_B1'2 ---PKA-active--> A1'2'_B1'2'[1]	0.074072	24	6	7.5002	6	4	
A12_B12' ---PKA-active--> A12'_B12'[1]	0.074072	24	6	7.5002	6	4	
A1'2_B12' ---PKA-active--> A1'2'_B12'[1]	0.074072	24	6	7.5002	6	4	
A12_B1'2' ---PKA-active--> A12'_B1'2'[1]	0.074072	24	6	7.5002	6	4	
A1'2_B1'2' ---PKA-active--> A1'2'_B1'2'[1]	0.074072	24	6	7.5002	6	4	
A12_B12'[1] ---PKA-active--> A12_B12	0.074072	24	6	7.5002	6	4	
A12'_B12[2] ---PKA-active--> A12_B12	0.074072	24	6	7.5002	6	4	
A12_B12[3] ---PKA-active--> A12'_B12[2]	0.074072	24	6	7.5002	6	4	
A12_B12[3] ---PKA-active--> A12_B12'[1]	0.074072	24	6	7.5002	6	4	
A1'2_B12' ---PKA-active--> A1'2_B12[1]	0.074072	24	6	7.5002	6	4	
A1'2'_B12 ---PKA-active--> A1'2_B12[1]	0.074072	24	6	7.5002	6	4	
A1'2_B12[5] ---PKA-active--> A1'2_B12'	0.074072	24	6	7.5002	6	4	
A1'2_B12[5] ---PKA-active--> A1'2'_B12	0.074072	24	6	7.5002	6	4	
A12_B12'[2] ---PKA-active--> A12_B12[2]	0.074072	24	6	7.5002	6	4	
A12'_B12[1] ---PKA-active--> A12_B12[2]	0.074072	24	6	7.5002	6	4	
A12_B12[6] ---PKA-active--> A12_B12'[2]	0.074072	24	6	7.5002	6	4	
A12_B12[6] ---PKA-active--> A12'_B12[1]	0.074072	24	6	7.5002	6	4	
A12_B12'[3] ---PKA-active--> A12_B12[4]	0.074072	24	6	7.5002	6	4	
A12'_B12[3] ---PKA-active--> A12_B12[4]	0.074072	24	6	7.5002	6	4	
A12_B12[7] ---PKA-active--> A12_B12'[3]	0.074072	24	6	7.5002	6	4	
A12_B12[7] ---PKA-active--> A12'_B12[3]	0.074072	24	6	7.5002	6	4	

Pools for group /kinetics/PKA

name	CoInit	buffered
R2C2	0.5	0
R2C2-cAMP	0	0
R2C2-cAMP2	0	0
R2C2-cAMP3	0	0
R2C2-cAMP4	0	0
R2C-cAMP4	0	0

R2-cAMP4	0	0
PKA-inhibitor	0.25926	0
inhibited-PKA	0	0
PKA-active	0	0

AC/cAMP reactions



Equations for group /kinetics/AC

Reactions for group /kinetics/AC

Reaction	kf	kb	Kf	Kb
CaM-Ca4 + AC1 <===> AC1-CaM	0.92592	1	50	1
AC2* <===> AC2	0.1	0	0.1	0
cAMP-PDE* <===> cAMP-PDE	0.01	0	0.01	0
PDE1 + CaM-Ca4 <===> CaM.PDE1	13.333	5	719.98	5
cAMP <===> cAMP_in_dend	300	5.4	300	5.4

Enzymes for group /kinetics/AC

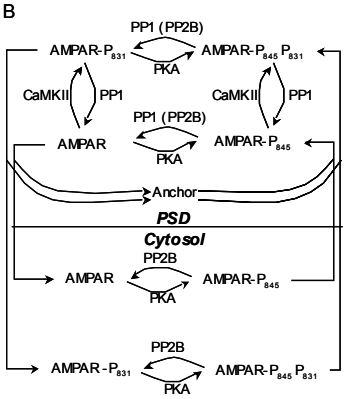
Enzyme-reaction	k1	k2	k3	Km	Vmax	ratio
ATP ---AC1-CaM--> cAMP	0.001389	18	4.5	300	4.5	4
ATP ---AC2*--> cAMP	0.000617	8	2	300	2	4
cAMP ---cAMP-PDE--> AMP	0.046667	40	10	19.841	10	4
cAMP ---cAMP-PDE*--> AMP	0.093333	80	20	19.841	20	4
cAMP ---PDE1--> AMP	0.003889	6.67	1.667	39.7	1.667	4.0012
cAMP ---CaM.PDE1--> AMP	0.023333	40	10	39.683	10	4

Pools for group /kinetics/AC

name	CoInit	buffered
ATP	2000	1
AC1-CaM	0	0
AC1	0.074074	0
AC2*	0	0
AC2	0.074074	0
AMP	0	0
cAMP-PDE	0.55556	0
cAMP-PDE*	0	0
PDE1	2.5926	0
CaM.PDE1	0	0
cAMP_in_dend	0	0
cAMP	0	0

AMPAR trafficking reactions

B



Equations for group /kinetics/AMPAR
Reactions for group /kinetics/AMPAR

Reaction	kf	kb	Kf	Kb
A1'2_B12[5] <===> A1'2_B12 + Anchor	0.0008	0	0.0008	0
A12_B12[6] <===> A12_B1'2 + Anchor	0.0008	0	0.0008	0
A12_B12[7] <===> A1'2_B1'2 + Anchor	0.0008	0	0.0008	0
A1'2'_B12'[1] + Anchor <===> A1'2_B12[1]	0.0002	0.008	0.0108	0.008
A12'_B12'[1] + Anchor <===> A12_B12	0.0002	0.008	0.0108	0.008
A1'2'_B1'2'[1] + Anchor <===> A12_B12[4]	0.0002	0.008	0.0108	0.008
A12_B12[3] <===> A12_B12 + Anchor	0.0008	0	0.0008	0
A12'_B1'2'[1] + Anchor <===> A12_B12[2]	0.0002	0.008	0.0108	0.008
A1'2'_B1'2'[1] <===> AMPAR_deg	3.60E-05	0	3.60E-05	0
A12'_B1'2'[1] <===> AMPAR_deg	3.60E-05	0	3.60E-05	0
A1'2'_B12'[1] <===> AMPAR_deg	3.60E-05	0	3.60E-05	0
A12'_B12'[1] <===> AMPAR_deg	3.60E-05	0	3.60E-05	0
GluR23_M <===> GluR23_I	0.00035	0.0014	0.00035	0.0014
AMPA_bulk <===> A12_B12	1	1	1	1

Pools for group /kinetics/AMPAR

name	CoInit	buffered
GluR23_I	0.092593	0
A12_B12'	0	0
A1'2_B12'	0	0
A12_B1'2'	0	0
A1'2_B1'2'	0	0
A12'_B12	0	0
A1'2'_B12	0	0
A12'_B1'2	0	0
A1'2'_B1'2	0	0
A12_B12	0	0
A1'2_B12	0	0
A12_B1'2	0	0
A1'2_B1'2	0	0
A12'_B12'[1]	0	0
A1'2'_B12'[1]	0	0
A12'_B1'2'[1]	0	0
A1'2'_B1'2'[1]	0	0
AMPAR_deg	0	1
AMPA_bulk	0.009259	1
I_845	0	0
I_845-P	0	0
I_845_PP	0	0
tot_I_GluR12	0	0
total_Int	0.096296	0

Equations for group /kinetics/AMPAR_memb
Pools for group /kinetics/AMPAR_memb

name	CoInit	buffered
Ser831-PP	0	0

Ser831-P	0	0
Ser831	0	0
A12_B12	0	0
A1'2_B12[1]	0	0
A12_B12[2]	0	0
A12_B12[4]	0	0
A12_B12'[3]	0	0
A12_B12'[2]	0	0
A1'2_B12'	0	0
A12_B12'[1]	0	0
Ser845-PP	0	0
Ser845-P	0	0
A12'_B12[2]	0	0
A1'2'_B12	0	0
A12'_B12[1]	0	0
A12'_B12[3]	0	0
A12_B12[7]	0	0
A12_B12[6]	0	0
A1'2_B12[5]	0	0
A12_B12[3]	0	0
tot_mem_GluR12	0	0
total_mem	3.4667	0
GluR23_M	3.5	0
Anchor	27.333	0
Ser845	0	0

Same data, sorting by data type:

Equations for group /##[]
Reactions for group /##[]

Reaction	kf	kb	Kf	Kb
PKC-control <===> PKC-active	2.5	2.5	2.5	2.5
Ca_control_cyt <===> Ca	100	100	100	100
Ca_control_PSD <===> Ca-PSD	100	100	100	100
CaM-Ca4 + CaMKII <===> CaMKII-CaM	0.92592	5	50	5
CaMKII-thr286 + CaM-Ca4 <===> CaMKII-thr286*-CaM	18.522	0.1	1000.2	0.1
CaMKII-thr306-PSD <===> CaMK-thr306 + NMDAR	0.3	1.00E-05	0.3	6.00E-05
CaMKII-PSD <===> CaMKII + NMDAR	0.3	1.00E-05	0.3	6.00E-05
CaMKII-CaM + NMDAR <===> CaMKII-CaM-PSD	2.00E-05	0	0.00108	0
CaMKII-thr286*-CaM + NMDAR <===> CaMKII-thr286-CaM-PSD	2.00E-05	0	0.00108	0
CaMKII-CaM-PSD <===> CaM-Ca4-PSD + CaMKII-PSD	5	0	5	0
CaMKII-PSD + CaM-Ca4-PSD <===> CaMKII-CaM-PSD	8.3333	0	50	0
CaMKII-thr286-PSD + CaM-Ca4-PSD <===> CaMKII-thr286-CaM-PSD	166.67	0.1	1000	0.1
basal_CaMKII_PSD_control <===> basal_CaMKII_PSD	1	1	1	1
CaM + 2 Ca <===> CaM-TR2-Ca2	0.024691	72	71.999	72
CaM-TR2-Ca2 + Ca <===> CaM-Ca3	0.066667	10	3.6	10
neurogranin + CaM <===> neurogranin-CaM	0.005556	1	0.3	1
neurogranin* <===> neurogranin	0.005	0	0.005	0
CaM-PSD + 2 Ca-PSD <===> CaM-TR2-Ca2-PSD	2	72	72	72
CaM-TR2-Ca2-PSD + Ca-PSD <===> CaM-Ca3-PSD	0.6	10	3.6	10
neurogranin[1] + CaM-PSD <===> neurogranin-CaM[1]	0.05	1	0.3	1
neurogranin*[1] <===> neurogranin[1]	0.005	0	0.005	0
CaM-Ca3 + Ca <===> CaM-Ca4	0.008611	10	0.465	10
CaM-Ca3-PSD + Ca-PSD <===> CaM-Ca4-PSD	0.077502	10	0.46501	10
CaM-Ca4-PSD <===> CaM-Ca4	540	60	540	60
I1* + PP1-active <===> PP1-I1*	9.2589	0.1	499.98	0.1
PP1-I1 <===> PP1-active + I1	1	0	1	0
2 Ca + CaNAB-Ca2 <===> CaNAB-Ca4	0.001235	1	3.6001	1
CaNAB + 2 Ca <===> CaNAB-Ca2	3.4321	1	10008	1
CaM-Ca4 + CaNAB-Ca4 <===> CaM_Ca_n-CaNAB	11.111	1	599.99	1
R2C2 + cAMP <===> R2C2-cAMP	1	33	54	33
R2C2-cAMP + cAMP <===> R2C2-cAMP2	1	33	54	33
R2C2-cAMP2 + cAMP <===> R2C2-cAMP3	1.3889	110	75.001	110
cAMP + R2C2-cAMP3 <===> R2C2-cAMP4	1.3889	32.5	75.001	32.5
R2C2-cAMP4 <===> PKA-active + R2C-cAMP4	60	0.33333	60	18
R2C-cAMP4 <===> PKA-active + R2-cAMP4	60	0.33333	60	18
PKA-active + PKA-inhibitor <===> inhibited-PKA	1.1111	1	59.999	1
CaM-Ca4 + AC1 <===> AC1-CaM	0.92592	1	50	1
AC2* <===> AC2	0.1	0	0.1	0
cAMP-PDE* <===> cAMP-PDE	0.01	0	0.01	0
PDE1 + CaM-Ca4 <===> CaM.PDE1	13.333	5	719.98	5
cAMP <===> cAMP_in_dend	300	5.4	300	5.4
PP1-I1_PSD <===> I1_PSD + PP1-active_PSD	1	0	1	0
I1*_PSD + PP1-active_PSD <===> PP1-I1*_PSD	83.33	0.1	499.98	0.1
A1'2_B12[5] <===> A1'2_B12 + Anchor	0.0008	0	0.0008	0
A12_B12[6] <===> A12_B1'2 + Anchor	0.0008	0	0.0008	0
A12_B12[7] <===> A1'2_B1'2 + Anchor	0.0008	0	0.0008	0
A1'2'_B12'[1] + Anchor <===> A1'2_B12[1]	0.0002	0.008	0.0108	0.008
A12'_B12'[1] + Anchor <===> A12_B12	0.0002	0.008	0.0108	0.008
A1'2'_B1'2'[1] + Anchor <===> A12_B12[4]	0.0002	0.008	0.0108	0.008
A12_B12[3] <===> A12_B12 + Anchor	0.0008	0	0.0008	0
A12'_B1'2'[1] + Anchor <===> A12_B12[2]	0.0002	0.008	0.0108	0.008
A1'2'_B1'2'[1] <===> AMPAR_deg	3.60E-05	0	3.60E-05	0
A12'_B1'2'[1] <===> AMPAR_deg	3.60E-05	0	3.60E-05	0
A1'2'_B12'[1] <===> AMPAR_deg	3.60E-05	0	3.60E-05	0
A12'_B12'[1] <===> AMPAR_deg	3.60E-05	0	3.60E-05	0
GluR23_M <===> GluR23_I	0.00035	0.0014	0.00035	0.0014
AMPA_bulk <===> A12_B12	1	1	1	1

Enzymes for group /##[]

Enzyme-reaction	k1	k2	k3	Km	Vmax	ratio
neurogranin ---PKC-active--> neurogranin*	0.001889	2.34	0.58	28.627	0.58	4.0345
neurogranin-CaM ---PKC-active--> CaM + neurogranin*	0.001133	1.4	0.35	28.596	0.35	4
AC2 ---PKC-active--> AC2*	0.011111	16	4	33.334	4	4
neurogranin-CaM[1] ---PKC-active--> CaM-PSD + neurogranin*[1]	0.001133	1.4	0.35	28.596	0.35	4
neurogranin[1] ---PKC-active--> neurogranin*[1]	0.001889	2.34	0.58	28.627	0.58	4.0345
CaMKII-thr286 ---tot_CaM_CaMKII--> CaMKII***	0.00489	24	6	113.6	6	4

CaMKII-CaM ---tot_CaM_CaMKII--> CaMKII-thr286*-CaM	0.000408	2	0.5	113.6	0.5	4
CaMKII-thr286 ---tot_autonomous_CaMKII--> CaMKII***	0.003175	24	6	175	6	4
CaMKII-CaM ---tot_autonomous_CaMKII--> CaMKII-thr286*-CaM	0.000265	2	0.5	174.99	0.5	4
CaMKII-thr286-PSD ---tot-auto-PSD--> CaMKII***-PSD	0.04	24	6	125	6	4
CaMKII-CaM-PSD ---tot-auto-PSD--> CaMKII-thr286-CaM-PSD	0.003333	2	0.5	125	0.5	4
CaMKII-thr286-PSD ---tot-CaM-CaMKII-PSD--> CaMKII***-PSD	0.061599	24	6	81.17	6	4
CaMKII-CaM-PSD ---tot-CaM-CaMKII-PSD--> CaMKII-thr286-CaM-PSD	0.005133	2	0.5	81.169	0.5	4
A12_B12 ---actCaMKII-PSD--> A1'2_B12[1]	0.00463	2	0.5	90.001	0.5	4
A12_B12'[1] ---actCaMKII-PSD--> A1'2_B12'	0.00463	2	0.5	90.001	0.5	4
A12'_B12[2] ---actCaMKII-PSD--> A1'2'_B12	0.00463	2	0.5	90.001	0.5	4
A12_B12[3] ---actCaMKII-PSD--> A1'2_B12[5]	0.00463	2	0.5	90.001	0.5	4
A12_B12 ---actCaMKII-PSD--> A12_B12[2]	0.00463	2	0.5	90.001	0.5	4
A12_B12'[1] ---actCaMKII-PSD--> A12_B12'[2]	0.00463	2	0.5	90.001	0.5	4
A12'_B12[2] ---actCaMKII-PSD--> A12'_B12[1]	0.00463	2	0.5	90.001	0.5	4
A12_B12[3] ---actCaMKII-PSD--> A12_B12[6]	0.00463	2	0.5	90.001	0.5	4
A12_B12[2] ---actCaMKII-PSD--> A12_B12[4]	0.00463	2	0.5	90.001	0.5	4
A12_B12'[2] ---actCaMKII-PSD--> A12_B12'[3]	0.00463	2	0.5	90.001	0.5	4
A12'_B12[1] ---actCaMKII-PSD--> A12'_B12[3]	0.00463	2	0.5	90.001	0.5	4
A12_B12[6] ---actCaMKII-PSD--> A12_B12[7]	0.00463	2	0.5	90.001	0.5	4
A1'2_B12[1] ---actCaMKII-PSD--> A12_B12[4]	0.00463	2	0.5	90.001	0.5	4
A1'2_B12' ---actCaMKII-PSD--> A12_B12'[3]	0.00463	2	0.5	90.001	0.5	4
A1'2'_B12 ---actCaMKII-PSD--> A12'_B12[3]	0.00463	2	0.5	90.001	0.5	4
A1'2_B12[5] ---actCaMKII-PSD--> A12_B12[7]	0.00463	2	0.5	90.001	0.5	4
CaMKII-thr286*-CaM ---PP1-active--> CaMKII-CaM	0.045397	10	2.5	5.099	2.5	4
CaMKII-thr286 ---PP1-active--> CaMKII	0.045397	10	2.5	5.099	2.5	4
CaMKII*** ---PP1-active--> CaMKII-thr286	0.045397	10	2.5	5.099	2.5	4
CaMK-thr306 ---PP1-active--> CaMKII	0.045397	10	2.5	5.099	2.5	4
CaMKII*** ---PP1-active--> CaMK-thr306	0.045397	10	2.5	5.099	2.5	4
I1* ---PP2A--> I1	0.01196	8.3334	2	16	2	4.1667
PP1-I1* ---PP2A--> PP1-I1	0.01196	8.3334	2	16	2	4.1667
I1*_PSD ---PP2A--> I1_PSD	0.01196	8.3334	2	16	2	4.1667
PP1-I1*_PSD ---PP2A--> PP1-I1_PSD	0.01196	8.3334	2	16	2	4.1667
I1* ---CaNAB-Ca4--> I1	0.000633	0.136	0.034	4.9708	0.034	4
I1*_PSD ---CaNAB-Ca4--> I1_PSD	0.000633	0.136	0.034	4.9707	0.034	4
neurogranin* ---CaM_Ca_n-CaNAB--> neurogranin	0.006178	2.67	0.67	10.012	0.67	3.9851
I1* ---CaM_Ca_n-CaNAB--> I1	0.006333	1.36	0.34	4.9708	0.34	4
PP1-I1* ---CaM_Ca_n-CaNAB--> PP1-I1	0.006333	1.36	0.34	4.9708	0.34	4
I1*_PSD ---CaM_Ca_n-CaNAB--> I1_PSD	0.006333	1.36	0.34	4.9707	0.34	4
PP1-I1*_PSD ---CaM_Ca_n-CaNAB--> PP1-I1_PSD	0.006333	1.36	0.34	4.9707	0.34	4
A12_B12' ---CaM_Ca_n-CaNAB--> A12_B12	0.037256	8	2	4.9706	2	4
A1'2_B12' ---CaM_Ca_n-CaNAB--> A1'2_B12	0.037256	8	2	4.9706	2	4
A12_B1'2' ---CaM_Ca_n-CaNAB--> A12_B1'2	0.037256	8	2	4.9706	2	4
A1'2_B1'2' ---CaM_Ca_n-CaNAB--> A1'2_B1'2	0.037256	8	2	4.9706	2	4
A12'_B12 ---CaM_Ca_n-CaNAB--> A12_B12	0.037256	8	2	4.9706	2	4
A1'2'_B12 ---CaM_Ca_n-CaNAB--> A1'2_B12	0.037256	8	2	4.9706	2	4
A12'_B1'2 ---CaM_Ca_n-CaNAB--> A12_B1'2	0.037256	8	2	4.9706	2	4
A1'2'_B1'2 ---CaM_Ca_n-CaNAB--> A1'2_B1'2	0.037256	8	2	4.9706	2	4
A12'_B12'[1] ---CaM_Ca_n-CaNAB--> A12'_B12	0.037256	8	2	4.9706	2	4
A1'2'_B12'[1] ---CaM_Ca_n-CaNAB--> A1'2'_B12	0.037256	8	2	4.9706	2	4
A12'_B1'2'[1] ---CaM_Ca_n-CaNAB--> A12'_B1'2	0.037256	8	2	4.9706	2	4
A1'2'_B1'2'[1] ---CaM_Ca_n-CaNAB--> A1'2'_B1'2	0.037256	8	2	4.9706	2	4
A12'_B12'[1] ---CaM_Ca_n-CaNAB--> A12_B12'	0.037256	8	2	4.9706	2	4
A1'2'_B12'[1] ---CaM_Ca_n-CaNAB--> A1'2_B12'	0.037256	8	2	4.9706	2	4
A12'_B1'2'[1] ---CaM_Ca_n-CaNAB--> A12_B1'2'	0.037256	8	2	4.9706	2	4
A1'2'_B1'2'[1] ---CaM_Ca_n-CaNAB--> A1'2_B1'2'	0.037256	8	2	4.9706	2	4
A12_B12 ---CaM_Ca_n-CaNAB--> A12_B12'[1]	0.037256	8	2	4.9706	2	4
A12_B12 ---CaM_Ca_n-CaNAB--> A12'_B12[2]	0.037256	8	2	4.9706	2	4
A12_B12'[1] ---CaM_Ca_n-CaNAB--> A12_B12[3]	0.037256	8	2	4.9706	2	4
A12'_B12[2] ---CaM_Ca_n-CaNAB--> A12_B12[3]	0.037256	8	2	4.9706	2	4
A1'2_B12[1] ---CaM_Ca_n-CaNAB--> A1'2_B12'	0.037256	8	2	4.9706	2	4
A1'2_B12[1] ---CaM_Ca_n-CaNAB--> A1'2'_B12	0.037256	8	2	4.9706	2	4
A1'2_B12' ---CaM_Ca_n-CaNAB--> A1'2_B12[5]	0.037256	8	2	4.9706	2	4
A1'2'_B12 ---CaM_Ca_n-CaNAB--> A1'2_B12[5]	0.037256	8	2	4.9706	2	4
A12_B12[2] ---CaM_Ca_n-CaNAB--> A12_B12'[2]	0.037256	8	2	4.9706	2	4
A12_B12[2] ---CaM_Ca_n-CaNAB--> A12'_B12[1]	0.037256	8	2	4.9706	2	4
A12_B12'[2] ---CaM_Ca_n-CaNAB--> A12_B12[6]	0.037256	8	2	4.9706	2	4
A12'_B12[1] ---CaM_Ca_n-CaNAB--> A12_B12[6]	0.037256	8	2	4.9706	2	4
A12_B12[4] ---CaM_Ca_n-CaNAB--> A12_B12'[3]	0.037256	8	2	4.9706	2	4
A12_B12[4] ---CaM_Ca_n-CaNAB--> A12'_B12[3]	0.037256	8	2	4.9706	2	4
A12'_B12[3] ---CaM_Ca_n-CaNAB--> A12_B12[7]	0.037256	8	2	4.9706	2	4
A12_B12'[3] ---CaM_Ca_n-CaNAB--> A12_B12[7]	0.037256	8	2	4.9706	2	4
neurogranin*[1] ---CaM_Ca_n-CaNAB--> neurogranin[1]	0.006178	2.67	0.67	10.012	0.67	3.9851
cAMP-PDE ---PKA-active--> cAMP-PDE*	0.11111	36	9	7.5001	9	4
I1 ---PKA-active--> I1*	0.11111	36	9	7.5001	9	4
I1_PSD ---PKA-active--> I1*_PSD	0.11111	36	9	7.5001	9	4
A12_B12 ---PKA-active--> A12_B12'	0.074072	24	6	7.5002	6	4

A1'2_B12 ---PKA-active--> A1'2_B12'	0.074072	24	6	7.5002	6	4
A12_B1'2 ---PKA-active--> A12_B1'2'	0.074072	24	6	7.5002	6	4
A1'2_B1'2 ---PKA-active--> A1'2_B1'2'	0.074072	24	6	7.5002	6	4
A12_B12 ---PKA-active--> A12'_B12	0.074072	24	6	7.5002	6	4
A1'2_B12 ---PKA-active--> A1'2'_B12	0.074072	24	6	7.5002	6	4
A12_B1'2 ---PKA-active--> A12'_B1'2	0.074072	24	6	7.5002	6	4
A1'2_B1'2 ---PKA-active--> A1'2'_B1'2	0.074072	24	6	7.5002	6	4
A12'_B12 ---PKA-active--> A12'_B12'[1]	0.074072	24	6	7.5002	6	4
A1'2'_B12 ---PKA-active--> A1'2'_B12'[1]	0.074072	24	6	7.5002	6	4
A12'_B1'2 ---PKA-active--> A12'_B1'2'[1]	0.074072	24	6	7.5002	6	4
A1'2'_B1'2 ---PKA-active--> A1'2'_B1'2'[1]	0.074072	24	6	7.5002	6	4
A12_B12' ---PKA-active--> A12'_B12'[1]	0.074072	24	6	7.5002	6	4
A1'2_B12' ---PKA-active--> A1'2'_B12'[1]	0.074072	24	6	7.5002	6	4
A12_B1'2' ---PKA-active--> A12'_B1'2'[1]	0.074072	24	6	7.5002	6	4
A1'2_B1'2' ---PKA-active--> A1'2'_B1'2'[1]	0.074072	24	6	7.5002	6	4
A12_B12'[1] ---PKA-active--> A12_B12	0.074072	24	6	7.5002	6	4
A12'_B12[2] ---PKA-active--> A12_B12	0.074072	24	6	7.5002	6	4
A12_B12[3] ---PKA-active--> A12'_B12[2]	0.074072	24	6	7.5002	6	4
A12_B12[3] ---PKA-active--> A12_B12'[1]	0.074072	24	6	7.5002	6	4
A1'2_B12' ---PKA-active--> A1'2_B12[1]	0.074072	24	6	7.5002	6	4
A1'2'_B12 ---PKA-active--> A1'2_B12[1]	0.074072	24	6	7.5002	6	4
A1'2_B12[5] ---PKA-active--> A1'2_B12'	0.074072	24	6	7.5002	6	4
A1'2_B12[5] ---PKA-active--> A1'2'_B12	0.074072	24	6	7.5002	6	4
A12_B12'[2] ---PKA-active--> A12_B12[2]	0.074072	24	6	7.5002	6	4
A12'_B12[1] ---PKA-active--> A12_B12[2]	0.074072	24	6	7.5002	6	4
A12_B12[6] ---PKA-active--> A12_B12'[2]	0.074072	24	6	7.5002	6	4
A12_B12[6] ---PKA-active--> A12'_B12[1]	0.074072	24	6	7.5002	6	4
A12_B12'[3] ---PKA-active--> A12_B12[4]	0.074072	24	6	7.5002	6	4
A12'_B12[3] ---PKA-active--> A12_B12[4]	0.074072	24	6	7.5002	6	4
A12_B12[7] ---PKA-active--> A12_B12'[3]	0.074072	24	6	7.5002	6	4
A12_B12[7] ---PKA-active--> A12'_B12[3]	0.074072	24	6	7.5002	6	4
ATP ---AC1-CaM--> cAMP	0.001389	18	4.5	300	4.5	4
ATP ---AC2*--> cAMP	0.000617	8	2	300	2	4
cAMP ---cAMP-PDE--> AMP	0.046667	40	10	19.841	10	4
cAMP ---cAMP-PDE*--> AMP	0.093333	80	20	19.841	20	4
cAMP ---PDE1--> AMP	0.003889	6.67	1.667	39.7	1.667	4.0012
cAMP ---CaM.PDE1--> AMP	0.023333	40	10	39.683	10	4
CaMKII-thr286-CaM-PSD ---PP1-active_PSD--> CaMKII-CaM-PSD	1.0417	10	2.5	1.9999	2.5	4
CaMKII-thr286-PSD ---PP1-active_PSD--> CaMKII-PSD	1.0417	10	2.5	1.9999	2.5	4
CaMKII***-PSD ---PP1-active_PSD--> CaMKII-thr286-PSD	0.40857	10	2.5	5.0991	2.5	4
CaMKII-thr306-PSD ---PP1-active_PSD--> CaMKII-PSD	0.40857	10	2.5	5.0991	2.5	4
CaMKII***-PSD ---PP1-active_PSD--> CaMKII-thr306-PSD	1.0417	10	2.5	1.9999	2.5	4
A12_B12 ---PP1-active_PSD--> A12_B12'[1]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12 ---PP1-active_PSD--> A12'_B12[2]	0.14583	0.68	0.17	0.97145	0.17	4
A12'_B12[2] ---PP1-active_PSD--> A12_B12[3]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12'[1] ---PP1-active_PSD--> A12_B12[3]	0.14583	0.68	0.17	0.97145	0.17	4
A1'2_B12[1] ---PP1-active_PSD--> A1'2_B12'	0.14583	0.68	0.17	0.97145	0.17	4
A1'2_B12[1] ---PP1-active_PSD--> A1'2'_B12	0.14583	0.68	0.17	0.97145	0.17	4
A1'2_B12' ---PP1-active_PSD--> A1'2_B12[5]	0.14583	0.68	0.17	0.97145	0.17	4
A1'2'_B12 ---PP1-active_PSD--> A1'2_B12[5]	0.14583	0.68	0.17	0.97145	0.17	4
A1'2_B12[1] ---PP1-active_PSD--> A12_B12	0.14583	1.4	0.35	2	0.35	4
A1'2_B12' ---PP1-active_PSD--> A12_B12'[1]	0.14583	1.4	0.35	2	0.35	4
A1'2'_B12 ---PP1-active_PSD--> A12'_B12[2]	0.14583	1.4	0.35	2	0.35	4
A1'2_B12[5] ---PP1-active_PSD--> A12_B12[3]	0.14583	1.4	0.35	2	0.35	4
A12_B12[2] ---PP1-active_PSD--> A12_B12'[2]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12[2] ---PP1-active_PSD--> A12'_B12[1]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12'[2] ---PP1-active_PSD--> A12_B12[6]	0.14583	0.68	0.17	0.97145	0.17	4
A12'_B12[1] ---PP1-active_PSD--> A12_B12[6]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12[4] ---PP1-active_PSD--> A12_B12'[3]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12[4] ---PP1-active_PSD--> A12'_B12[3]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12'[3] ---PP1-active_PSD--> A12_B12[7]	0.14583	0.68	0.17	0.97145	0.17	4
A12'_B12[3] ---PP1-active_PSD--> A12_B12[7]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12'[2] ---PP1-active_PSD--> A12_B12'[1]	0.14583	1.4	0.35	2	0.35	4
A12_B12[2] ---PP1-active_PSD--> A12_B12	0.14583	1.4	0.35	2	0.35	4
A12'_B12[1] ---PP1-active_PSD--> A12'_B12[2]	0.14583	1.4	0.35	2	0.35	4
A12_B12[6] ---PP1-active_PSD--> A12_B12[3]	0.14583	1.4	0.35	2	0.35	4
A12_B12[4] ---PP1-active_PSD--> A12_B12[2]	0.14583	1.4	0.35	2	0.35	4
A12_B12'[3] ---PP1-active_PSD--> A12_B12'[2]	0.14583	1.4	0.35	2	0.35	4
A12'_B12[3] ---PP1-active_PSD--> A12'_B12[1]	0.14583	1.4	0.35	2	0.35	4
A12_B12[7] ---PP1-active_PSD--> A12_B12[6]	0.14583	1.4	0.35	2	0.35	4
A12_B12[4] ---PP1-active_PSD--> A1'2_B12[1]	0.14583	1.4	0.35	2	0.35	4
A12_B12'[3] ---PP1-active_PSD--> A1'2_B12'	0.14583	1.4	0.35	2	0.35	4
A12'_B12[3] ---PP1-active_PSD--> A1'2'_B12	0.14583	1.4	0.35	2	0.35	4
A12_B12[7] ---PP1-active_PSD--> A1'2_B12[5]	0.14583	1.4	0.35	2	0.35	4

Pools for group /##[]

name	CoInit	buffered
Ca	0.08	0
Ca-PSD	0.08	0
PKC-active	0.1	0
PKC-control	0.1	1
Ca_control_cyt	0.08	1
Ca_control_PSD	0.08	1
CaMKII	20	0
CaMKII-CaM	0	0
CaMKII-thr286*-CaM	0	0
CaMKII***	0	0
CaMKII-thr286	0	0
CaMK-thr306	0	0
tot_CaM_CaMKII	0	0
tot_autonomous_CaMKII	2	0
tot_CaMKII_cyt	22	0
act_CaMKII_cyt	2	0
basal_CaMKII_cyt	2	1
NMDAR	120	0
CaMKII-thr306-PSD	0	0
CaMKII***-PSD	0	0
CaMKII-PSD	0	0
CaMKII-thr286-PSD	0	0
CaMKII-CaM-PSD	0	0
CaMKII-thr286-CaM-PSD	0	0
tot-auto-PSD	2	0
tot-CaM-CaMKII-PSD	0	0
basal_CaMKII_PSD_control	2	1
basal_CaMKII_PSD	2	0
tot_CaMKII_PSD	2	0
actCaMKII-PSD	2	0
286P-PSD	0	0
CaM	26.333	0
neurogranin-CaM	0	0
neurogranin*	0	0
neurogranin	10	0
CaM-PSD	26.333	0
neurogranin-CaM[1]	0	0
neurogranin[1]	10	0
neurogranin*[1]	0	0
CaM-TR2-Ca2	0	0
CaM-Ca3	0	0
CaM-Ca4	0	0
CaM-TR2-Ca2-PSD	0	0
CaM-Ca3-PSD	0	0
CaM-Ca4-PSD	0	0
I1	1.8	0
I1*	0	0
PP1-I1*	0	0
PP1-I1	0	0
PP1-active	1.8	0
PP2A	0.11111	0
CaNAB	1	0
CaNAB-Ca2	0	0
CaNAB-Ca4	0	0
CaM_Ca_n-CaNAB	0	0
R2C2	0.5	0
R2C2-cAMP	0	0
R2C2-cAMP2	0	0
R2C2-cAMP3	0	0
R2C2-cAMP4	0	0
R2C-cAMP4	0	0
R2-cAMP4	0	0
PKA-inhibitor	0.25926	0
inhibited-PKA	0	0
PKA-active	0	0
ATP	2000	1
AC1-CaM	0	0
AC1	0.074074	0
AC2*	0	0
AC2	0.074074	0
AMP	0	0
cAMP-PDE	0.55556	0
cAMP-PDE*	0	0
PDE1	2.5926	0
CaM.PDE1	0	0

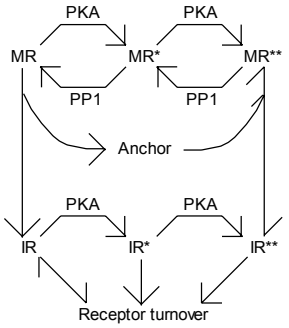
cAMP_in_dend	0	0
cAMP	0	0
PP1-active_PSD	4	0
I1_PSD	4	0
I1*_PSD	0	0
PP1-I1_PSD	0	0
PP1-I1*_PSD	0	0
GluR23_I	0.092593	0
A12_B12'	0	0
A1'2_B12'	0	0
A12_B1'2'	0	0
A1'2_B1'2'	0	0
A12'_B12	0	0
A1'2'_B12	0	0
A12'_B1'2	0	0
A1'2'_B1'2	0	0
A12_B12	0	0
A1'2_B12	0	0
A12_B1'2	0	0
A1'2_B1'2	0	0
A12'_B12'[1]	0	0
A1'2'_B12'[1]	0	0
A12'_B1'2'[1]	0	0
A1'2'_B1'2'[1]	0	0
AMPAR_deg	0	1
AMPA_bulk	0.009259	1
I_845	0	0
I_845-P	0	0
I_845_PP	0	0
tot_I_GluR12	0	0
total_Int	0.096296	0
Ser831-PP	0	0
Ser831-P	0	0
Ser831	0	0
A12_B12	0	0
A1'2_B12[1]	0	0
A12_B12[2]	0	0
A12_B12[4]	0	0
A12_B12'[3]	0	0
A12_B12'[2]	0	0
A1'2_B12'	0	0
A12_B12'[1]	0	0
Ser845-PP	0	0
Ser845-P	0	0
A12'_B12[2]	0	0
A1'2'_B12	0	0
A12'_B12[1]	0	0
A12'_B12[3]	0	0
A12_B12[7]	0	0
A12_B12[6]	0	0
A1'2_B12[5]	0	0
A12_B12[3]	0	0
tot_mem_GluR12	0	0
total_mem	3.4667	0
GluR23_M	3.5	0
Anchor	27.333	0
Ser845	0	0

Model Parameters for simplified AMPAR bistability model.

Concentration units: uM (micromolar) for rate constants presented as Kf, Kb, Km
#/cell for rate constants presented as kf, kb, k1, k2, k3. This formulation of rates may depend on cellular volume.
Time units: Seconds in all cases.
Total Volume of Synapse = 0.1 femtoliters (fl)
Volume of cytosolic portion = 0.09 fl
Volume of Postsynaptic Density (PSD) = 0.01 fl

The enzyme rates are related as follows:
Km = (k2 + k3)/k1 (after conversion of units)
Kcat = k3.
Ratio = k2/k3

Initial concentrations (CoInit) are mostly zero, except for a few key molecules.
There is a flag for 'buffered' in the molecule concentration table. When this flag is zero the molecule concentrations are computed according to the reaction equations. If the flag is one the molecule concentration is held fixed to its initial concentration.



Equations for group /##[]
Reactions for group /##[]

Reaction	kf	kb	Kf	Kb
Anchor + IR** <===> MR**	0.0002	0.008	0.0108	0.008
MR <===> Anchor + IR	0.0008	0	0.0008	0
Bulk_AMPAR <===> IR	1	1	1	1
IR** <===> Bulk_AMPAR	2.00E-05	0	2.00E-05	0
IR* <===> Bulk_AMPAR	2.00E-05	0	2.00E-05	0

Enzymes for group /##[]

Enzyme-reaction	k1	k2	k3	Km	Vmax	ratio
MR ---PKA-active--> MR*	0.074074	24	6	7.5	6	4
IR ---PKA-active--> IR*	0.074074	24	6	7.5	6	4
MR* ---PKA-active--> MR**	0.074074	24	6	7.5	6	4
IR* ---PKA-active--> IR**	0.074074	24	6	7.5	6	4
MR* ---PP1-active--> MR	0.14583	1.4	0.35	2	0.35	4
MR** ---PP1-active--> MR*	0.14583	1.4	0.35	2	0.35	4

Pools for group /##[]

name	CoInit	buffered
PKA-active	0.018519	1
Anchor	3.037	0
Bulk_AMPAR	0.014815	1
PP1-active	0.33333	0
MR*	0	0
MR	0	0
MR**	0	0
IR**	0	0
IR	0	0
IR*	0	0

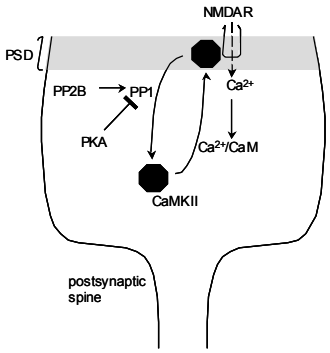
Model Parameters for CaMKII bistability model.

Concentration units: uM (micromolar) for rate constants presented as Kf, Kb, Km
#/cell for rate constants presented as kf, kb, k1, k2, k3. This formulation of rates may depend on cellular volume.
Time units: Seconds in all cases.
Total Volume of Synapse = 0.1 femtoliters (fl)
Volume of cytosolic portion = 0.09 fl
Volume of Postsynaptic Density (PSD) = 0.01 fl

The enzyme rates are related as follows:
Km = (k2 + k3)/k1 (after conversion of units)
Kcat = k3.
Ratio = k2/k3

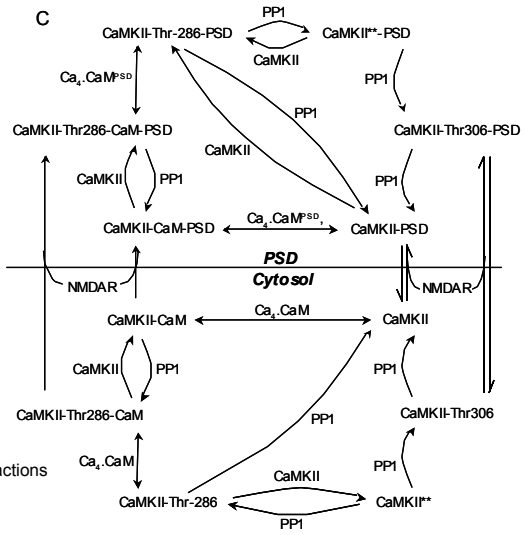
Initial concentrations (CoInit) are mostly zero, except for a few key molecules.
There is a flag for 'buffered' in the molecule concentration table. When this flag is zero the molecule concentrations are computed according to the reaction equations. If the flag is one the molecule concentration is held fixed to its initial concentration.

The entire model scheme is presented as composite tables for molecules, reactions and enzymes.



Block Diagram. Only the CaMKII traffic and regulatory molecules are implemented in this model.

CaMKII reactions



Equations for all groups

Reactions

Reaction	kf	kb	Kf	Kb
CaMKII-PSD + CaM-Ca4-PSD <===> CaMKII-CaM-PSD	8.3333	0	50	0
CaMKII-CaM + NMDAR <===> CaMKII-CaM-PSD	2.00E-05	0	0.00108	0
CaMKII-thr286*-CaM + NMDAR <===> CaMKII-thr286-CaM-PSD	2.00E-05	0	0.00108	0
CaMKII-PSD <===> CaMKII + NMDAR	0.3	1.00E-05	0.3	6.00E-05
CaMKII-thr306-PSD <===> CaMK-thr306 + NMDAR	0.3	1.00E-05	0.3	6.00E-05
CaMKII-thr286-PSD + CaM-Ca4-PSD <===> CaMKII-thr286-CaM-PSD	166.67	0.1	1000	0.1
CaM-Ca4-PSD <===> CaM-Ca4	540	60	540	60
I1* + PP1-active_PSD <===> PP1-I1*	83.33	0.1	499.98	0.1
CaM-Ca3 + Ca <===> CaM-Ca4	0.0086111	10	0.465	10
CaMKII-CaM-PSD <===> CaM-Ca4-PSD + CaMKII-PSD	5	0	5	0
Ca_control_cyt <===> Ca	100	100	100	100
Ca_control_PSD <===> Ca-PSD	100	100	100	100
basal_CaMKII_PSD_control <===> basal_CaMKII_PSD	1	1	1	1
CaM-Ca4 + CaMKII <===> CaMKII-CaM	0.92592	5	50	5
CaMKII-thr286 + CaM-Ca4 <===> CaMKII-thr286*-CaM	18.522	0.1	1000.2	0.1
CaM + 2 Ca <===> CaM-TR2-Ca2	0.024691	72	71.999	72
CaM-TR2-Ca2 + Ca <===> CaM-Ca3	0.066667	10	3.6	10
CaM-PSD + 2 Ca-PSD <===> CaM-TR2-Ca2-PSD	2	72	72	72
CaM-TR2-Ca2-PSD + Ca-PSD <===> CaM-Ca3-PSD	0.6	10	3.6	10
CaM-Ca3-PSD + Ca-PSD <===> CaM-Ca4-PSD	0.077502	10	0.46501	10
I1* + PP1-active <===> PP1-I1*	9.2589	0.1	499.98	0.1
PP1-I1 <===> PP1-active + I1	1	0	1	0
2 Ca + CaNAB-Ca2 <===> CaNAB-Ca4	0.0012346	1	3.6001	1
CaNAB + 2 Ca <===> CaNAB-Ca2	3.4321	1	10008	1
CaM-Ca4 + CaNAB-Ca4 <===> CaM_Ca_n-CaNAB	11.111	1	599.99	1
PP1-I1 <===> I1 + PP1-active_PSD	1	0	1	0

Enzymes

Enzyme-reaction	k1	k2	k3	Km	Vmax	ratio
CaMKII-thr286*-CaM ---PP1-active--> CaMKII-CaM	0.045397	10	2.5	5.099	2.5	4
CaMKII-thr286 ---PP1-active--> CaMKII	0.045397	10	2.5	5.099	2.5	4
CaMKII*** ---PP1-active--> CaMKII-thr286	0.045397	10	2.5	5.099	2.5	4
CaMK-thr306 ---PP1-active--> CaMKII	0.045397	10	2.5	5.099	2.5	4
CaMKII*** ---PP1-active--> CaMK-thr306	0.045397	10	2.5	5.099	2.5	4
I1 ---PKA-active--> I1*	0.11111	36	9	7.5001	9	4
I1 ---PKA-active--> I1*	0.11111	36	9	7.5001	9	4
I1* ---PP2A--> I1	0.01196	8.3334	2	16	2	4.1667
PP1-I1* ---PP2A--> PP1-I1	0.01196	8.3334	2	16	2	4.1667
I1* ---PP2A--> I1	0.01196	8.3334	2	16	2	4.1667
PP1-I1* ---PP2A--> PP1-I1	0.01196	8.3334	2	16	2	4.1667
I1* ---CaNAB-Ca4--> I1	0.0006333	0.136	0.034	4.9708	0.034	4
I1* ---CaNAB-Ca4--> I1	0.0006333	0.136	0.034	4.9707	0.034	4
CaMKII-thr286-PSD ---tot-auto-PSD--> CaMKII***-PSD	0.01	24	6	500	6	4
CaMKII-CaM-PSD ---tot-auto-PSD--> CaMKII-thr286-CaM-PSD	0.0008333	2	0.5	500	0.5	4
CaMKII-PSD ---tot-auto-PSD--> CaMKII-thr286-PSD	0.0033333	8	2	500.01	2	4
CaMKII-thr286-CaM-PSD ---PP1-active_PSD--> CaMKII-CaM-PSD	0.083333	0.8	0.2	2	0.2	4
CaMKII-thr286-PSD ---PP1-active_PSD--> CaMKII-PSD	0.083333	0.8	0.2	2	0.2	4
CaMKII***-PSD ---PP1-active_PSD--> CaMKII-thr286-PSD	0.083333	0.8	0.2	2	0.2	4
CaMKII-thr306-PSD ---PP1-active_PSD--> CaMKII-PSD	0.083333	0.8	0.2	2	0.2	4
CaMKII***-PSD ---PP1-active_PSD--> CaMKII-thr306-PSD	0.083333	0.8	0.2	2	0.2	4
I1* ---CaM_Ca_n-CaNAB--> I1	0.0063333	1.36	0.34	4.9708	0.34	4
PP1-I1* ---CaM_Ca_n-CaNAB--> PP1-I1	0.0063333	1.36	0.34	4.9708	0.34	4
I1* ---CaM_Ca_n-CaNAB--> I1	0.0063334	1.36	0.34	4.9707	0.34	4
PP1-I1* ---CaM_Ca_n-CaNAB--> PP1-I1	0.0063334	1.36	0.34	4.9707	0.34	4
CaMKII-thr286-PSD ---tot-CaM-CaMKII-PSD--> CaMKII***-PSD	0.015625	24	6	320	6	4
CaMKII-CaM-PSD ---tot-CaM-CaMKII-PSD--> CaMKII-thr286-CaM-PSD	0.0013021	2	0.5	320	0.5	4
CaMKII-PSD ---tot-CaM-CaMKII-PSD--> CaMKII-thr286-PSD	0.0052083	8	2	320	2	4
CaMKII-thr286 ---tot_CaM_CaMKII--> CaMKII***	0.0024474	24	6	227	6	4
CaMKII-CaM ---tot_CaM_CaMKII--> CaMKII-thr286*-CaM	0.000204	2	0.5	227	0.5	4
CaMKII-thr286 ---tot_autonomous_CaMKII--> CaMKII***	0.0015873	24	6	350	6	4
CaMKII-CaM ---tot_autonomous_CaMKII--> CaMKII-thr286*-CaM	0.0001323	2	0.5	349.99	0.5	4

Pools

name	CoInit	buffered
CaM-Ca4	0	0
PP1-active	1.8	0
Ca	0.08	0
PKA-active	0.018519	0
CaM-Ca3	0	0
CaM-TR2-Ca2	0	0
PP2A	0.11111	0
CaNAB-Ca4	0	0
CaMKII-thr286-CaM-PSD	0	0
CaMKII-CaM-PSD	0	0
CaMKII-thr286-PSD	0	0
CaMKII-PSD	0	0
CaMKII***-PSD	0	0
CaMKII-thr306-PSD	0	0
tot-auto-PSD	2	0
CaM-TR2-Ca2-PSD	0	0
CaM-Ca3-PSD	0.0025458	0
CaM-Ca4-PSD	0	0
Ca-PSD	0.08	0
286P-PSD	0	0
actCaMKII-PSD	2	0
tot_CaMKII_PSD	2	0
tot_CaMKII_cyt	22	0
PP1-active_PSD	4	0
act_CaMKII_cyt	2	0
NMDAR	120	0
CaM_Ca_n-CaNAB	0	0
basal_CaMKII_cyt	2	1
basal_CaMKII_PSD	2	0
Ca_control_cyt	0.08	1
Ca_control_PSD	0.08	1
basal_CaMKII_PSD_control	2	1
tot-CaM-CaMKII-PSD	0	0
CaMKII	20	0
CaMKII-CaM	0	0
CaMKII-thr286*-CaM	0	0
CaMKII***	0	0
CaMKII-thr286	0	0
CaMK-thr306	0	0
tot_CaM_CaMKII	0	0
tot_autonomous_CaMKII	2	0
CaM	26.333	0
CaM-PSD	26.333	0
I1	1.8	0
I1*	0	0
PP1-I1*	0	0
PP1-I1	0	0
CaNAB	1	0
	0	0
I1	4	0
I1*	0	0
PP1-I1*	0	0
PP1-I1	0	0

Model Parameters for lockstep model.

Concentration units: uM (micromolar) for rate constants presented as Kf, Kb, Km
#/cell for rate constants presented as kf, kb, k1, k2, k3. This formulation of rates may depend on cellular volume.
Time units: Seconds in all cases.
Total Volume of Synapse = 0.1 femtoliters (fl)
Volume of cytosolic portion = 0.09 fl
Volume of Postsynaptic Density (PSD) = 0.01 fl

The enzyme rates are related as follows:
Km = (k2 + k3)/k1 (after conversion of units)
Kcat = k3.
Ratio = k2/k3

Initial concentrations (CoInit) are mostly zero, except for a few key molecules.
There is a flag for 'buffered' in the molecule concentration table. When this flag is zero the molecule concentrations are computed according to the reaction equations. If the flag is one the molecule concentration is held fixed to its initial concentration.

The entire model scheme is presented as composite tables for molecules, reactions and enzymes.

All equations.
Reactions.

Reaction	kf	kb	Kf	Kb
CaMKII-PSD + CaM-Ca4-PSD <===> CaMKII-CaM-PSD	8.3333	0	50	0
CaMKII-CaM + NMDAR <===> CaMKII-CaM-PSD	2.00E-05	0	0.00108	0
CaMKII-thr286*-CaM + NMDAR <===> CaMKII-thr286-CaM-PSD	2.00E-05	0	0.00108	0
CaMKII-PSD <===> CaMKII + NMDAR	0.3	1.00E-05	0.3	6.00E-05
CaMKII-thr306-PSD <===> CaMK-thr306 + NMDAR	0.3	1.00E-05	0.3	6.00E-05
CaMKII-thr286-PSD + CaM-Ca4-PSD <===> CaMKII-thr286-CaM-PSD	166.67	0.1	1000	0.1
CaM-Ca4-PSD <===> CaM-Ca4	540	60	540	60
I1* + PP1-active_PSD <===> PP1-I1*	83.33	0.1	499.98	0.1
CaM-Ca3 + Ca <===> CaM-Ca4	0.0086111	10	0.465	10
GluR23_M <===> GluR23_I	0.00035	0.0014	0.00035	0.0014
CaMKII-CaM-PSD <===> CaM-Ca4-PSD + CaMKII-PSD	5	0	5	0
PKC-control <===> PKC-active	2.5	2.5	2.5	2.5
Ca_control_cyt <===> Ca	100	100	100	100
Ca_control_PSD <===> Ca-PSD	100	100	100	100
basal_CaMKII_PSD_control <===> basal_CaMKII_PSD	1	1	1	1
AMPA_bulk <===> A12_B12	1	1	1	1
CaM-Ca4 + CaMKII <===> CaMKII-CaM	0.92592	5	50	5
CaMKII-thr286 + CaM-Ca4 <===> CaMKII-thr286*-CaM	18.522	0.1	1000.2	0.1
CaM + 2 Ca <===> CaM-TR2-Ca2	0.024691	72	71.999	72
CaM-TR2-Ca2 + Ca <===> CaM-Ca3	0.066667	10	3.6	10
neurogranin + CaM <===> neurogranin-CaM	0.0055556	1	0.3	1
neurogranin* <===> neurogranin	0.005	0	0.005	0
CaM-PSD + 2 Ca-PSD <===> CaM-TR2-Ca2-PSD	2	72	72	72
CaM-TR2-Ca2-PSD + Ca-PSD <===> CaM-Ca3-PSD	0.6	10	3.6	10
CaM-Ca3-PSD + Ca-PSD <===> CaM-Ca4-PSD	0.077502	10	0.46501	10
neurogranin[1] + CaM-PSD <===> neurogranin-CaM[1]	0.05	1	0.3	1
neurogranin*[1] <===> neurogranin[1]	0.005	0	0.005	0
I1* + PP1-active <===> PP1-I1*	9.2589	0.1	499.98	0.1
PP1-I1 <===> PP1-active + I1	1	0	1	0
2 Ca + CaNAB-Ca2 <===> CaNAB-Ca4	0.0012346	1	3.6001	1
CaNAB + 2 Ca <===> CaNAB-Ca2	3.4321	1	10008	1
CaM-Ca4 + CaNAB-Ca4 <===> CaM_Ca_n-CaNAB	11.111	1	599.99	1
R2C2 + cAMP <===> R2C2-cAMP	1	33	54	33
R2C2-cAMP + cAMP <===> R2C2-cAMP2	1	33	54	33
R2C2-cAMP2 + cAMP <===> R2C2-cAMP3	1.3889	110	75.001	110
cAMP + R2C2-cAMP3 <===> R2C2-cAMP4	1.3889	32.5	75.001	32.5
R2C2-cAMP4 <===> PKA-active + R2C-cAMP4	60	0.33333	60	18
R2C-cAMP4 <===> PKA-active + R2-cAMP4	60	0.33333	60	18
PKA-active + PKA-inhibitor <===> inhibited-PKA	1.1111	1	59.999	1
CaM-Ca4 + AC1 <===> AC1-CaM	0.92592	1	50	1
AC2* <===> AC2	0.1	0	0.1	0
cAMP-PDE* <===> cAMP-PDE	0.01	0	0.01	0
PDE1 + CaM-Ca4 <===> CaM.PDE1	13.333	5	719.98	5
cAMP <===> cAMP_in_dend	300	5.4	300	5.4
PP1-I1 <===> I1 + PP1-active_PSD	1	0	1	0
A1'2_B12[5] <===> A1'2_B12 + Anchor	0.0008	0	0.0008	0
A12_B12[6] <===> A12_B1'2 + Anchor	0.0008	0	0.0008	0

A12_B12[7] <===> A1'2_B1'2 + Anchor	0.0008	0	0.0008	0
A1'2'_B12'[1] + Anchor <===> A1'2_B12[1]	0.0002	0.008	0.0108	0.008
A12'_B12'[1] + Anchor <===> A12_B12	0.0002	0.008	0.0108	0.008
A1'2'_B1'2'[1] + Anchor <===> A12_B12[4]	0.0002	0.008	0.0108	0.008
A12_B12[3] <===> A12_B12 + Anchor	0.0008	0	0.0008	0
A12'_B1'2'[1] + Anchor <===> A12_B12[2]	0.0002	0.008	0.0108	0.008
A1'2'_B1'2'[1] <===> AMPAR_deg	3.60E-05	0	3.60E-05	0
A12'_B1'2'[1] <===> AMPAR_deg	3.60E-05	0	3.60E-05	0
A1'2'_B12'[1] <===> AMPAR_deg	3.60E-05	0	3.60E-05	0
A12'_B12'[1] <===> AMPAR_deg	3.60E-05	0	3.60E-05	0

Enzymes

Enzyme-reaction	k1	k2	k3	Km	Vmax	ratio
CaMKII-thr286*-CaM ---PP1-active--> CaMKII-CaM	0.045397	10	2.5	5.099	2.5	4
CaMKII-thr286 ---PP1-active--> CaMKII	0.045397	10	2.5	5.099	2.5	4
CaMKII*** ---PP1-active--> CaMKII-thr286	0.045397	10	2.5	5.099	2.5	4
CaMK-thr306 ---PP1-active--> CaMKII	0.045397	10	2.5	5.099	2.5	4
CaMKII*** ---PP1-active--> CaMK-thr306	0.045397	10	2.5	5.099	2.5	4
cAMP-PDE ---PKA-active--> cAMP-PDE*	0.11111	36	9	7.5001	9	4
I1 ---PKA-active--> I1*	0.11111	36	9	7.5001	9	4
I1 ---PKA-active--> I1*	0.11111	36	9	7.5001	9	4
A12_B12 ---PKA-active--> A12_B12'	0.074072	24	6	7.5002	6	4
A1'2_B12 ---PKA-active--> A1'2_B12'	0.074072	24	6	7.5002	6	4
A12_B1'2 ---PKA-active--> A12_B1'2'	0.074072	24	6	7.5002	6	4
A1'2_B1'2 ---PKA-active--> A1'2_B1'2'	0.074072	24	6	7.5002	6	4
A12_B12 ---PKA-active--> A12'_B12	0.074072	24	6	7.5002	6	4
A1'2_B12 ---PKA-active--> A1'2'_B12	0.074072	24	6	7.5002	6	4
A12_B1'2 ---PKA-active--> A12'_B1'2	0.074072	24	6	7.5002	6	4
A1'2_B1'2 ---PKA-active--> A1'2'_B1'2	0.074072	24	6	7.5002	6	4
A12'_B12 ---PKA-active--> A12'_B12'[1]	0.074072	24	6	7.5002	6	4
A1'2'_B12 ---PKA-active--> A1'2'_B12'[1]	0.074072	24	6	7.5002	6	4
A12'_B1'2 ---PKA-active--> A12'_B1'2'[1]	0.074072	24	6	7.5002	6	4
A1'2'_B1'2 ---PKA-active--> A1'2'_B1'2'[1]	0.074072	24	6	7.5002	6	4
A12_B12' ---PKA-active--> A12'_B12'[1]	0.074072	24	6	7.5002	6	4
A1'2_B12' ---PKA-active--> A1'2'_B12'[1]	0.074072	24	6	7.5002	6	4
A12_B1'2' ---PKA-active--> A12'_B1'2'[1]	0.074072	24	6	7.5002	6	4
A1'2_B1'2' ---PKA-active--> A1'2'_B1'2'[1]	0.074072	24	6	7.5002	6	4
A12_B12'[1] ---PKA-active--> A12_B12	0.074072	24	6	7.5002	6	4
A12'_B12[2] ---PKA-active--> A12_B12	0.074072	24	6	7.5002	6	4
A12_B12[3] ---PKA-active--> A12'_B12[2]	0.074072	24	6	7.5002	6	4
A12_B12[3] ---PKA-active--> A12_B12'[1]	0.074072	24	6	7.5002	6	4
A1'2_B12' ---PKA-active--> A1'2_B12[1]	0.074072	24	6	7.5002	6	4
A1'2'_B12 ---PKA-active--> A1'2_B12[1]	0.074072	24	6	7.5002	6	4
A1'2_B12[5] ---PKA-active--> A1'2_B12'	0.074072	24	6	7.5002	6	4
A1'2_B12[5] ---PKA-active--> A1'2'_B12	0.074072	24	6	7.5002	6	4
A12_B12'[2] ---PKA-active--> A12_B12[2]	0.074072	24	6	7.5002	6	4
A12'_B12[1] ---PKA-active--> A12_B12[2]	0.074072	24	6	7.5002	6	4
A12_B12[6] ---PKA-active--> A12_B12'[2]	0.074072	24	6	7.5002	6	4
A12_B12[6] ---PKA-active--> A12'_B12[1]	0.074072	24	6	7.5002	6	4
A12_B12'[3] ---PKA-active--> A12_B12[4]	0.074072	24	6	7.5002	6	4
A12'_B12[3] ---PKA-active--> A12_B12[4]	0.074072	24	6	7.5002	6	4
A12_B12[7] ---PKA-active--> A12_B12'[3]	0.074072	24	6	7.5002	6	4
A12_B12[7] ---PKA-active--> A12'_B12[3]	0.074072	24	6	7.5002	6	4
I1* ---PP2A--> I1	0.01196	8.3334	2	16	2	4.1667
PP1-I1* ---PP2A--> PP1-I1	0.01196	8.3334	2	16	2	4.1667
I1* ---PP2A--> I1	0.01196	8.3334	2	16	2	4.1667
PP1-I1* ---PP2A--> PP1-I1	0.01196	8.3334	2	16	2	4.1667
I1* ---CaNAB-Ca4--> I1	0.0006333	0.136	0.034	4.9708	0.034	4
I1* ---CaNAB-Ca4--> I1	0.0006333	0.136	0.034	4.9707	0.034	4
CaMKII-thr286-PSD ---tot-auto-PSD--> CaMKII***-PSD	0.01	24	6	500	6	4
CaMKII-CaM-PSD ---tot-auto-PSD--> CaMKII-thr286-CaM-PSD	0.0008333	2	0.5	500	0.5	4
CaMKII-PSD ---tot-auto-PSD--> CaMKII-thr286-PSD	0.0033333	8	2	500.01	2	4
A12_B12 ---actCaMKII-PSD--> A1'2_B12[1]	0.0046296	2	0.5	90.001	0.5	4
A12_B12'[1] ---actCaMKII-PSD--> A1'2_B12'	0.0046296	2	0.5	90.001	0.5	4
A12'_B12[2] ---actCaMKII-PSD--> A1'2'_B12	0.0046296	2	0.5	90.001	0.5	4
A12_B12[3] ---actCaMKII-PSD--> A1'2_B12[5]	0.0046296	2	0.5	90.001	0.5	4
A12_B12 ---actCaMKII-PSD--> A12_B12[2]	0.0046296	2	0.5	90.001	0.5	4
A12_B12'[1] ---actCaMKII-PSD--> A12_B12'[2]	0.0046296	2	0.5	90.001	0.5	4
A12'_B12[2] ---actCaMKII-PSD--> A12'_B12[1]	0.0046296	2	0.5	90.001	0.5	4
A12_B12[3] ---actCaMKII-PSD--> A12_B12[6]	0.0046296	2	0.5	90.001	0.5	4
A12_B12[2] ---actCaMKII-PSD--> A12_B12[4]	0.0046296	2	0.5	90.001	0.5	4
A12_B12'[2] ---actCaMKII-PSD--> A12_B12'[3]	0.0046296	2	0.5	90.001	0.5	4
A12'_B12[1] ---actCaMKII-PSD--> A12'_B12[3]	0.0046296	2	0.5	90.001	0.5	4
A12_B12[6] ---actCaMKII-PSD--> A12_B12[7]	0.0046296	2	0.5	90.001	0.5	4
A1'2_B12[1] ---actCaMKII-PSD--> A12_B12[4]	0.0046296	2	0.5	90.001	0.5	4
A1'2_B12' ---actCaMKII-PSD--> A12_B12'[3]	0.0046296	2	0.5	90.001	0.5	4
A1'2'_B12 ---actCaMKII-PSD--> A12'_B12[3]	0.0046296	2	0.5	90.001	0.5	4
A1'2_B12[5] ---actCaMKII-PSD--> A12_B12[7]	0.0046296	2	0.5	90.001	0.5	4
CaMKII-thr286-CaM-PSD ---PP1-active_PSD--> CaMKII-CaM-PSD	0.083333	0.8	0.2	2	0.2	4
CaMKII-thr286-PSD ---PP1-active_PSD--> CaMKII-PSD	0.083333	0.8	0.2	2	0.2	4
CaMKII***-PSD ---PP1-active_PSD--> CaMKII-thr286-PSD	0.083333	0.8	0.2	2	0.2	4
CaMKII-thr306-PSD ---PP1-active_PSD--> CaMKII-PSD	0.083333	0.8	0.2	2	0.2	4
CaMKII***-PSD ---PP1-active_PSD--> CaMKII-thr306-PSD	0.083333	0.8	0.2	2	0.2	4
A12_B12 ---PP1-active_PSD--> A12_B12'[1]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12 ---PP1-active_PSD--> A12'_B12[2]	0.14583	0.68	0.17	0.97145	0.17	4
A12'_B12[2] ---PP1-active_PSD--> A12_B12[3]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12'[1] ---PP1-active_PSD--> A12_B12[3]	0.14583	0.68	0.17	0.97145	0.17	4

A1'2_B12[1] ---PP1-active_PSD--> A1'2_B12'	0.14583	0.68	0.17	0.97145	0.17	4
A1'2_B12[1] ---PP1-active_PSD--> A1'2'_B12	0.14583	0.68	0.17	0.97145	0.17	4
A1'2_B12' ---PP1-active_PSD--> A1'2_B12[5]	0.14583	0.68	0.17	0.97145	0.17	4
A1'2'_B12 ---PP1-active_PSD--> A1'2_B12[5]	0.14583	0.68	0.17	0.97145	0.17	4
A1'2_B12[1] ---PP1-active_PSD--> A12_B12	0.14583	1.4	0.35	2	0.35	4
A1'2_B12' ---PP1-active_PSD--> A12_B12'[1]	0.14583	1.4	0.35	2	0.35	4
A1'2'_B12 ---PP1-active_PSD--> A12'_B12[2]	0.14583	1.4	0.35	2	0.35	4
A1'2_B12[5] ---PP1-active_PSD--> A12_B12[3]	0.14583	1.4	0.35	2	0.35	4
A12_B12[2] ---PP1-active_PSD--> A12_B12'[2]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12[2] ---PP1-active_PSD--> A12'_B12[1]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12'[2] ---PP1-active_PSD--> A12_B12[6]	0.14583	0.68	0.17	0.97145	0.17	4
A12'_B12[1] ---PP1-active_PSD--> A12_B12[6]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12[4] ---PP1-active_PSD--> A12_B12'[3]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12[4] ---PP1-active_PSD--> A12'_B12[3]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12'[3] ---PP1-active_PSD--> A12_B12[7]	0.14583	0.68	0.17	0.97145	0.17	4
A12'_B12[3] ---PP1-active_PSD--> A12_B12[7]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12'[2] ---PP1-active_PSD--> A12_B12'[1]	0.14583	1.4	0.35	2	0.35	4
A12_B12[2] ---PP1-active_PSD--> A12_B12	0.14583	1.4	0.35	2	0.35	4
A12'_B12[1] ---PP1-active_PSD--> A12'_B12[2]	0.14583	1.4	0.35	2	0.35	4
A12_B12[6] ---PP1-active_PSD--> A12_B12[3]	0.14583	1.4	0.35	2	0.35	4
A12_B12[4] ---PP1-active_PSD--> A12_B12[2]	0.14583	1.4	0.35	2	0.35	4
A12_B12'[3] ---PP1-active_PSD--> A12_B12'[2]	0.14583	1.4	0.35	2	0.35	4
A12'_B12[3] ---PP1-active_PSD--> A12'_B12[1]	0.14583	1.4	0.35	2	0.35	4
A12_B12[7] ---PP1-active_PSD--> A12_B12[6]	0.14583	1.4	0.35	2	0.35	4
A12_B12[4] ---PP1-active_PSD--> A1'2_B12[1]	0.14583	1.4	0.35	2	0.35	4
A12_B12'[3] ---PP1-active_PSD--> A1'2_B12'	0.14583	1.4	0.35	2	0.35	4
A12'_B12[3] ---PP1-active_PSD--> A1'2'_B12	0.14583	1.4	0.35	2	0.35	4
A12_B12[7] ---PP1-active_PSD--> A1'2_B12[5]	0.14583	1.4	0.35	2	0.35	4
neurogranin ---PKC-active--> neurogranin*	0.0018889	2.34	0.58	28.627	0.58	4.0345
neurogranin-CaM ---PKC-active--> CaM + neurogranin*	0.0011333	1.4	0.35	28.596	0.35	4
AC2 ---PKC-active--> AC2*	0.011111	16	4	33.334	4	4
neurogranin-CaM[1] ---PKC-active--> CaM-PSD + neurogranin*[1]	0.0011333	1.4	0.35	28.596	0.35	4
neurogranin[1] ---PKC-active--> neurogranin*[1]	0.0018889	2.34	0.58	28.627	0.58	4.0345
neurogranin* ---CaM_Ca_n-CaNAB--> neurogranin	0.0061778	2.67	0.67	10.012	0.67	3.9851
I1* ---CaM_Ca_n-CaNAB--> I1	0.0063333	1.36	0.34	4.9708	0.34	4
PP1-I1* ---CaM_Ca_n-CaNAB--> PP1-I1	0.0063333	1.36	0.34	4.9708	0.34	4
I1* ---CaM_Ca_n-CaNAB--> I1	0.0063334	1.36	0.34	4.9707	0.34	4
PP1-I1* ---CaM_Ca_n-CaNAB--> PP1-I1	0.0063334	1.36	0.34	4.9707	0.34	4
A12_B12' ---CaM_Ca_n-CaNAB--> A12_B12	0.037256	8	2	4.9706	2	4
A1'2_B12' ---CaM_Ca_n-CaNAB--> A1'2_B12	0.037256	8	2	4.9706	2	4
A12_B1'2' ---CaM_Ca_n-CaNAB--> A12_B1'2	0.037256	8	2	4.9706	2	4
A1'2_B1'2' ---CaM_Ca_n-CaNAB--> A1'2_B1'2	0.037256	8	2	4.9706	2	4
A12'_B12 ---CaM_Ca_n-CaNAB--> A12_B12	0.037256	8	2	4.9706	2	4
A1'2'_B12 ---CaM_Ca_n-CaNAB--> A1'2_B12	0.037256	8	2	4.9706	2	4
A12'_B1'2 ---CaM_Ca_n-CaNAB--> A12_B1'2	0.037256	8	2	4.9706	2	4
A1'2'_B1'2 ---CaM_Ca_n-CaNAB--> A1'2_B1'2	0.037256	8	2	4.9706	2	4
A12'_B12'[1] ---CaM_Ca_n-CaNAB--> A12'_B12	0.037256	8	2	4.9706	2	4
A1'2'_B12'[1] ---CaM_Ca_n-CaNAB--> A1'2'_B12	0.037256	8	2	4.9706	2	4
A12'_B1'2'[1] ---CaM_Ca_n-CaNAB--> A12'_B1'2	0.037256	8	2	4.9706	2	4
A1'2'_B1'2'[1] ---CaM_Ca_n-CaNAB--> A1'2'_B1'2	0.037256	8	2	4.9706	2	4
A12'_B12'[1] ---CaM_Ca_n-CaNAB--> A12_B12'	0.037256	8	2	4.9706	2	4
A1'2'_B12'[1] ---CaM_Ca_n-CaNAB--> A1'2_B12'	0.037256	8	2	4.9706	2	4
A12'_B1'2'[1] ---CaM_Ca_n-CaNAB--> A12_B1'2'	0.037256	8	2	4.9706	2	4
A1'2'_B1'2'[1] ---CaM_Ca_n-CaNAB--> A1'2_B1'2'	0.037256	8	2	4.9706	2	4
A12_B12 ---CaM_Ca_n-CaNAB--> A12_B12'[1]	0.037256	8	2	4.9706	2	4
A12_B12 ---CaM_Ca_n-CaNAB--> A12'_B12[2]	0.037256	8	2	4.9706	2	4
A12_B12'[1] ---CaM_Ca_n-CaNAB--> A12_B12[3]	0.037256	8	2	4.9706	2	4
A12'_B12[2] ---CaM_Ca_n-CaNAB--> A12_B12[3]	0.037256	8	2	4.9706	2	4
A1'2_B12[1] ---CaM_Ca_n-CaNAB--> A1'2_B12'	0.037256	8	2	4.9706	2	4
A1'2_B12[1] ---CaM_Ca_n-CaNAB--> A1'2'_B12	0.037256	8	2	4.9706	2	4
A1'2_B12' ---CaM_Ca_n-CaNAB--> A1'2_B12[5]	0.037256	8	2	4.9706	2	4
A1'2'_B12 ---CaM_Ca_n-CaNAB--> A1'2_B12[5]	0.037256	8	2	4.9706	2	4
A12_B12[2] ---CaM_Ca_n-CaNAB--> A12_B12'[2]	0.037256	8	2	4.9706	2	4
A12_B12[2] ---CaM_Ca_n-CaNAB--> A12'_B12[1]	0.037256	8	2	4.9706	2	4
A12_B12'[2] ---CaM_Ca_n-CaNAB--> A12_B12[6]	0.037256	8	2	4.9706	2	4
A12'_B12[1] ---CaM_Ca_n-CaNAB--> A12_B12[6]	0.037256	8	2	4.9706	2	4
A12_B12[4] ---CaM_Ca_n-CaNAB--> A12_B12'[3]	0.037256	8	2	4.9706	2	4
A12_B12[4] ---CaM_Ca_n-CaNAB--> A12'_B12[3]	0.037256	8	2	4.9706	2	4
A12'_B12[3] ---CaM_Ca_n-CaNAB--> A12_B12[7]	0.037256	8	2	4.9706	2	4
A12_B12'[3] ---CaM_Ca_n-CaNAB--> A12_B12[7]	0.037256	8	2	4.9706	2	4
neurogranin*[1] ---CaM_Ca_n-CaNAB--> neurogranin[1]	0.0061778	2.67	0.67	10.012	0.67	3.9851
CaMKII-thr286-PSD ---tot-CaM-CaMKII-PSD--> CaMKII***-PSD	0.015625	24	6	320	6	4
CaMKII-CaM-PSD ---tot-CaM-CaMKII-PSD--> CaMKII-thr286-CaM-PSD	0.0013021	2	0.5	320	0.5	4
CaMKII-PSD ---tot-CaM-CaMKII-PSD--> CaMKII-thr286-PSD	0.0052083	8	2	320	2	4
CaMKII-thr286 ---tot_CaM_CaMKII--> CaMKII***	0.0024474	24	6	227	6	4
CaMKII-CaM ---tot_CaM_CaMKII--> CaMKII-thr286*-CaM	0.000204	2	0.5	227	0.5	4

CaMKII-thr286 ---tot_autonomous_CaMKII--> CaMKII***	0.0015873	24	6	350	6	4
CaMKII-CaM ---tot_autonomous_CaMKII--> CaMKII-thr286*-CaM	0.0001323	2	0.5	349.99	0.5	4
ATP ---AC1-CaM--> cAMP	0.0013889	18	4.5	300	4.5	4
ATP ---AC2*--> cAMP	0.0006173	8	2	300	2	4
cAMP ---cAMP-PDE--> AMP	0.046667	40	10	19.841	10	4
cAMP ---cAMP-PDE*--> AMP	0.093333	80	20	19.841	20	4
cAMP ---PDE1--> AMP	0.0038889	6.67	1.667	39.7	1.667	4.0012
cAMP ---CaM.PDE1--> AMP	0.023333	40	10	39.683	10	4

Pools

name	CoInit	buffered
CaM-Ca4	0	0
PP1-active	1.8	0
cAMP	0	0
Ca	0.08	0
PKA-active	0	0
CaM-Ca3	0	0
CaM-TR2-Ca2	0	0
PP2A	0.11111	0
CaNAB-Ca4	0	0
CaMKII-thr286-CaM-PSD	0	0
CaMKII-CaM-PSD	0	0
CaMKII-thr286-PSD	0	0
CaMKII-PSD	0	0
CaMKII***-PSD	0	0
CaMKII-thr306-PSD	0	0
tot-auto-PSD	2	0
CaM-TR2-Ca2-PSD	0	0
CaM-Ca3-PSD	0.0025458	0
CaM-Ca4-PSD	0	0
Ca-PSD	0.08	0
286P-PSD	0	0
actCaMKII-PSD	2	0
tot_CaMKII_PSD	2	0
tot_CaMKII_cyt	22	0
PP1-active_PSD	4	0
PKC-active	0.1	0
temp-PIP2	2.5	1
I_845-P	0	0
tot_I_GluR12	0	0
total_Int	0.096296	0
A12_B12	0	0
A12_B12'[1]	0	0
A12'_B12[2]	0	0
A12_B12[3]	0	0
A12_B12[2]	0	0
A12_B12[4]	0	0
A12_B12'[2]	0	0
A12_B12'[3]	0	0
A12'_B12[1]	0	0
A12'_B12[3]	0	0
A12_B12[6]	0	0
A12_B12[7]	0	0
A1'2_B12[1]	0	0
A1'2_B12'	0	0
A1'2'_B12	0	0
A1'2_B12[5]	0	0
Ser845	0	0
Ser845-P	0	0
Ser845-PP	0	0
Ser831	0	0
Ser831-P	0	0
Ser831-PP	0	0
tot_mem_GluR12	0	0
act_CaMKII_cyt	2	0
NMDAR	120	0
CaM_Ca_n-CaNAB	0	0
basal_CaMKII_cyt	2	1
basal_CaMKII_PSD	2	0
PKC-control	0.1	1
Ca_control_cyt	0.08	1
Ca_control_PSD	0.08	1
basal_CaMKII_PSD_control	2	1
Anchor	27.333	0
AMPA_bulk	0.0092593	1
I_845	0	0
I_845_PP	0	0
tot-CaM-CaMKII-PSD	0	0
CaMKII	20	0
CaMKII-CaM	0	0
CaMKII-thr286*-CaM	0	0
CaMKII***	0	0
CaMKII-thr286	0	0
CaMK-thr306	0	0
tot_CaM_CaMKII	0	0

tot_autonomous_CaMKII	2	0
CaM	26.333	0
neurogranin-CaM	0	0
neurogranin*	0	0
neurogranin	10	0
CaM-PSD	26.333	0
neurogranin-CaM[1]	0	0
neurogranin[1]	10	0
neurogranin*[1]	0	0
I1	1.8	0
I1*	0	0
PP1-I1*	0	0
PP1-I1	0	0
CaNAB	1	0
CaNAB-Ca2	0	0
R2C2	0.5	0
R2C2-cAMP	0	0
R2C2-cAMP2	0	0
R2C2-cAMP3	0	0
R2C2-cAMP4	0	0
R2C-cAMP4	0	0
R2-cAMP4	0	0
PKA-inhibitor	0.25926	0
inhibited-PKA	0	0
ATP	2000	1
AC1-CaM	0	0
AC1	0.074074	0
AC2*	0	0
AC2	0.074074	0
AMP	0	0
cAMP-PDE	0.55556	0
cAMP-PDE*	0	0
PDE1	2.5926	0
CaM.PDE1	0	0
cAMP_in_dend	0	0
I1	4	0
I1*	0	0
PP1-I1*	0	0
PP1-I1	0	0
GluR23_M	3.5	0
GluR23_I	0.092593	0
total_mem	3.4667	0
A12_B12'	0	0
A1'2_B12'	0	0
A12_B1'2'	0	0
A1'2_B1'2'	0	0
A12'_B12	0	0
A1'2'_B12	0	0
A12'_B1'2	0	0
A1'2'_B1'2	0	0
A12_B12	0	0
A1'2_B12	0	0
A12_B1'2	0	0
A1'2_B1'2	0	0
A12'_B12'[1]	0	0
A1'2'_B12'[1]	0	0
A12'_B1'2'[1]	0	0
A1'2'_B1'2'[1]	0	0
AMPAR_deg	0	1

Model Parameters for nested bistability model.

Concentration units: uM (micromolar) for rate constants presented as Kf, Kb, Km
#/cell for rate constants presented as kf, kb, k1, k2, k3. This formulation of rates may depend on cellular volume.
Time units: Seconds in all cases.
Total Volume of Synapse = 0.1 femtoliters (fl)
Volume of cytosolic portion = 0.09 fl
Volume of Postsynaptic Density (PSD) = 0.01 fl

The enzyme rates are related as follows:
Km = (k2 + k3)/k1 (after conversion of units)
Kcat = k3.
Ratio = k2/k3

Initial concentrations (CoInit) are mostly zero, except for a few key molecules.
There is a flag for 'buffered' in the molecule concentration table. When this flag is zero the molecule concentrations are computed according to the reaction equations. If the flag is one the molecule concentration is held fixed to its initial concentration.

The entire model scheme is presented as composite tables for molecules, reactions and enzymes.

All equations.
Reactions

Reaction	kf	kb	Kf	Kb
CaMKII-PSD + CaM-Ca4-PSD <===> CaMKII-CaM-PSD	8.3333	0	50	0
CaMKII-CaM + NMDAR <===> CaMKII-CaM-PSD	2.00E-05	0	0.00108	0
CaMKII-thr286*-CaM + NMDAR <===> CaMKII-thr286-CaM-PSD	2.00E-05	0	0.00108	0
CaMKII-PSD <===> CaMKII + NMDAR	0.3	1.00E-05	0.3	6.00E-05
CaMKII-thr306-PSD <===> CaMK-thr306 + NMDAR	0.3	1.00E-05	0.3	6.00E-05
CaMKII-thr286-PSD + CaM-Ca4-PSD <===> CaMKII-thr286-CaM-PSD	166.67	0.1	1000	0.1
CaM-Ca4-PSD <===> CaM-Ca4	540	60	540	60
I1* + PP1-active_PSD <===> PP1-I1*	83.33	0.1	499.98	0.1
CaM-Ca3 + Ca <===> CaM-Ca4	0.0086111	10	0.465	10
GluR23_M <===> GluR23_I	0.00035	0.0014	0.00035	0.0014
CaMKII-CaM-PSD <===> CaM-Ca4-PSD + CaMKII-PSD	5	0	5	0
PKC-control <===> PKC-active	2.5	2.5	2.5	2.5
Ca_control_cyt <===> Ca	100	100	100	100
Ca_control_PSD <===> Ca-PSD	100	100	100	100
basal_CaMKII_PSD_control <===> basal_CaMKII_PSD	1	1	1	1
AMPA_bulk <===> A12_B12	1	1	1	1
CaM-Ca4 + CaMKII <===> CaMKII-CaM	0.92592	5	50	5
CaMKII-thr286 + CaM-Ca4 <===> CaMKII-thr286*-CaM	18.522	0.1	1000.2	0.1
CaM + 2 Ca <===> CaM-TR2-Ca2	0.024691	72	71.999	72
CaM-TR2-Ca2 + Ca <===> CaM-Ca3	0.066667	10	3.6	10
neurogranin + CaM <===> neurogranin-CaM	0.0055556	1	0.3	1
neurogranin* <===> neurogranin	0.005	0	0.005	0
CaM-PSD + 2 Ca-PSD <===> CaM-TR2-Ca2-PSD	2	72	72	72
CaM-TR2-Ca2-PSD + Ca-PSD <===> CaM-Ca3-PSD	0.6	10	3.6	10
CaM-Ca3-PSD + Ca-PSD <===> CaM-Ca4-PSD	0.077502	10	0.46501	10
neurogranin[1] + CaM-PSD <===> neurogranin-CaM[1]	0.05	1	0.3	1
neurogranin*[1] <===> neurogranin[1]	0.005	0	0.005	0
I1* + PP1-active <===> PP1-I1*	9.2589	0.1	499.98	0.1
PP1-I1 <===> PP1-active + I1	1	0	1	0
2 Ca + CaNAB-Ca2 <===> CaNAB-Ca4	0.0012346	1	3.6001	1
CaNAB + 2 Ca <===> CaNAB-Ca2	3.4321	1	10008	1
CaM-Ca4 + CaNAB-Ca4 <===> CaM_Ca_n-CaNAB	11.111	1	599.99	1
R2C2 + cAMP <===> R2C2-cAMP	1	33	54	33
R2C2-cAMP + cAMP <===> R2C2-cAMP2	1	33	54	33
R2C2-cAMP2 + cAMP <===> R2C2-cAMP3	1.3889	110	75.001	110
cAMP + R2C2-cAMP3 <===> R2C2-cAMP4	1.3889	32.5	75.001	32.5
R2C2-cAMP4 <===> PKA-active + R2C-cAMP4	60	0.33333	60	18
R2C-cAMP4 <===> PKA-active + R2-cAMP4	60	0.33333	60	18
PKA-active + PKA-inhibitor <===> inhibited-PKA	1.1111	1	59.999	1
CaM-Ca4 + AC1 <===> AC1-CaM	0.92592	1	50	1
AC2* <===> AC2	0.1	0	0.1	0
cAMP-PDE* <===> cAMP-PDE	0.01	0	0.01	0
PDE1 + CaM-Ca4 <===> CaM.PDE1	13.333	5	719.98	5
cAMP <===> cAMP_in_dend	300	5.4	300	5.4
PP1-I1 <===> I1 + PP1-active_PSD	1	0	1	0
A1'2_B12[5] <===> A1'2_B12 + Anchor	0.0008	0	0.0008	0
A12_B12[6] <===> A12_B1'2 + Anchor	0.0008	0	0.0008	0

A12_B12[7] <===> A1'2_B1'2 + Anchor	0.0008	0	0.0008	0
A1'2'_B12'[1] + Anchor <===> A1'2_B12[1]	0.0002	0.008	0.0108	0.008
A12'_B12'[1] + Anchor <===> A12_B12	0.0002	0.008	0.0108	0.008
A1'2'_B1'2'[1] + Anchor <===> A12_B12[4]	0.0002	0.008	0.0108	0.008
A12_B12[3] <===> A12_B12 + Anchor	0.0008	0	0.0008	0
A12'_B1'2'[1] + Anchor <===> A12_B12[2]	0.0002	0.008	0.0108	0.008
A1'2'_B1'2'[1] <===> AMPAR_deg	3.60E-05	0	3.60E-05	0
A12'_B1'2'[1] <===> AMPAR_deg	3.60E-05	0	3.60E-05	0
A1'2'_B12'[1] <===> AMPAR_deg	3.60E-05	0	3.60E-05	0
A12'_B12'[1] <===> AMPAR_deg	3.60E-05	0	3.60E-05	0

All enzymes

Enzyme-reaction	k1	k2	k3	Km	Vmax	ratio
CaMKII-thr286*-CaM ---PP1-active--> CaMKII-CaM	0.045397	10	2.5	5.099	2.5	4
CaMKII-thr286 ---PP1-active--> CaMKII	0.045397	10	2.5	5.099	2.5	4
CaMKII*** ---PP1-active--> CaMKII-thr286	0.045397	10	2.5	5.099	2.5	4
CaMK-thr306 ---PP1-active--> CaMKII	0.045397	10	2.5	5.099	2.5	4
CaMKII*** ---PP1-active--> CaMK-thr306	0.045397	10	2.5	5.099	2.5	4
cAMP-PDE ---PKA-active--> cAMP-PDE*	0.11111	36	9	7.5001	9	4
I1 ---PKA-active--> I1*	0.11111	36	9	7.5001	9	4
I1 ---PKA-active--> I1*	0.11111	36	9	7.5001	9	4
A12_B12 ---PKA-active--> A12_B12'	0.074072	24	6	7.5002	6	4
A1'2_B12 ---PKA-active--> A1'2_B12'	0.074072	24	6	7.5002	6	4
A12_B1'2 ---PKA-active--> A12_B1'2'	0.074072	24	6	7.5002	6	4
A1'2_B1'2 ---PKA-active--> A1'2_B1'2'	0.074072	24	6	7.5002	6	4
A12_B12 ---PKA-active--> A12'_B12	0.074072	24	6	7.5002	6	4
A1'2_B12 ---PKA-active--> A1'2'_B12	0.074072	24	6	7.5002	6	4
A12_B1'2 ---PKA-active--> A12'_B1'2	0.074072	24	6	7.5002	6	4
A1'2_B1'2 ---PKA-active--> A1'2'_B1'2	0.074072	24	6	7.5002	6	4
A12'_B12 ---PKA-active--> A12'_B12'[1]	0.074072	24	6	7.5002	6	4
A1'2'_B12 ---PKA-active--> A1'2'_B12'[1]	0.074072	24	6	7.5002	6	4
A12'_B1'2 ---PKA-active--> A12'_B1'2'[1]	0.074072	24	6	7.5002	6	4
A1'2'_B1'2 ---PKA-active--> A1'2'_B1'2'[1]	0.074072	24	6	7.5002	6	4
A12_B12' ---PKA-active--> A12'_B12'[1]	0.074072	24	6	7.5002	6	4
A1'2_B12' ---PKA-active--> A1'2'_B12'[1]	0.074072	24	6	7.5002	6	4
A12_B1'2' ---PKA-active--> A12'_B1'2'[1]	0.074072	24	6	7.5002	6	4
A1'2_B1'2' ---PKA-active--> A1'2'_B1'2'[1]	0.074072	24	6	7.5002	6	4
A12_B12'[1] ---PKA-active--> A12_B12	0.074072	24	6	7.5002	6	4
A12'_B12[2] ---PKA-active--> A12_B12	0.074072	24	6	7.5002	6	4
A12_B12[3] ---PKA-active--> A12'_B12[2]	0.074072	24	6	7.5002	6	4
A12_B12[3] ---PKA-active--> A12_B12'[1]	0.074072	24	6	7.5002	6	4
A1'2_B12' ---PKA-active--> A1'2_B12[1]	0.074072	24	6	7.5002	6	4
A1'2'_B12 ---PKA-active--> A1'2_B12[1]	0.074072	24	6	7.5002	6	4
A1'2_B12[5] ---PKA-active--> A1'2_B12'	0.074072	24	6	7.5002	6	4
A1'2_B12[5] ---PKA-active--> A1'2'_B12	0.074072	24	6	7.5002	6	4
A12_B12'[2] ---PKA-active--> A12_B12[2]	0.074072	24	6	7.5002	6	4
A12'_B12[1] ---PKA-active--> A12_B12[2]	0.074072	24	6	7.5002	6	4
A12_B12[6] ---PKA-active--> A12_B12'[2]	0.074072	24	6	7.5002	6	4
A12_B12[6] ---PKA-active--> A12'_B12[1]	0.074072	24	6	7.5002	6	4
A12_B12'[3] ---PKA-active--> A12_B12[4]	0.074072	24	6	7.5002	6	4
A12'_B12[3] ---PKA-active--> A12_B12[4]	0.074072	24	6	7.5002	6	4
A12_B12[7] ---PKA-active--> A12_B12'[3]	0.074072	24	6	7.5002	6	4
A12_B12[7] ---PKA-active--> A12'_B12[3]	0.074072	24	6	7.5002	6	4
I1* ---PP2A--> I1	0.01196	8.3334	2	16	2	4.1667
PP1-I1* ---PP2A--> PP1-I1	0.01196	8.3334	2	16	2	4.1667
I1* ---PP2A--> I1	0.01196	8.3334	2	16	2	4.1667
PP1-I1* ---PP2A--> PP1-I1	0.01196	8.3334	2	16	2	4.1667
I1* ---CaNAB-Ca4--> I1	0.0006333	0.136	0.034	4.9708	0.034	4
I1* ---CaNAB-Ca4--> I1	0.0006333	0.136	0.034	4.9707	0.034	4
CaMKII-thr286-PSD ---tot-auto-PSD--> CaMKII***-PSD	0.01	24	6	500	6	4
CaMKII-CaM-PSD ---tot-auto-PSD--> CaMKII-thr286-CaM-PSD	0.0008333	2	0.5	500	0.5	4
CaMKII-PSD ---tot-auto-PSD--> CaMKII-thr286-PSD	0.0033333	8	2	500.01	2	4
A12_B12 ---actCaMKII-PSD--> A1'2_B12[1]	0.0046296	2	0.5	90.001	0.5	4
A12_B12'[1] ---actCaMKII-PSD--> A1'2_B12'	0.0046296	2	0.5	90.001	0.5	4
A12'_B12[2] ---actCaMKII-PSD--> A1'2'_B12	0.0046296	2	0.5	90.001	0.5	4
A12_B12[3] ---actCaMKII-PSD--> A1'2_B12[5]	0.0046296	2	0.5	90.001	0.5	4
A12_B12 ---actCaMKII-PSD--> A12_B12[2]	0.0046296	2	0.5	90.001	0.5	4
A12_B12'[1] ---actCaMKII-PSD--> A12_B12'[2]	0.0046296	2	0.5	90.001	0.5	4
A12'_B12[2] ---actCaMKII-PSD--> A12'_B12[1]	0.0046296	2	0.5	90.001	0.5	4
A12_B12[3] ---actCaMKII-PSD--> A12_B12[6]	0.0046296	2	0.5	90.001	0.5	4
A12_B12[2] ---actCaMKII-PSD--> A12_B12[4]	0.0046296	2	0.5	90.001	0.5	4
A12_B12'[2] ---actCaMKII-PSD--> A12_B12'[3]	0.0046296	2	0.5	90.001	0.5	4
A12'_B12[1] ---actCaMKII-PSD--> A12'_B12[3]	0.0046296	2	0.5	90.001	0.5	4
A12_B12[6] ---actCaMKII-PSD--> A12_B12[7]	0.0046296	2	0.5	90.001	0.5	4
A1'2_B12[1] ---actCaMKII-PSD--> A12_B12[4]	0.0046296	2	0.5	90.001	0.5	4
A1'2_B12' ---actCaMKII-PSD--> A12_B12'[3]	0.0046296	2	0.5	90.001	0.5	4
A1'2'_B12 ---actCaMKII-PSD--> A12'_B12[3]	0.0046296	2	0.5	90.001	0.5	4
A1'2_B12[5] ---actCaMKII-PSD--> A12_B12[7]	0.0046296	2	0.5	90.001	0.5	4
A12_B12 ---PP1-active_PSD--> A12_B12'[1]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12 ---PP1-active_PSD--> A12'_B12[2]	0.14583	0.68	0.17	0.97145	0.17	4
A12'_B12[2] ---PP1-active_PSD--> A12_B12[3]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12'[1] ---PP1-active_PSD--> A12_B12[3]	0.14583	0.68	0.17	0.97145	0.17	4
A1'2_B12[1] ---PP1-active_PSD--> A1'2_B12'	0.14583	0.68	0.17	0.97145	0.17	4
A1'2_B12[1] ---PP1-active_PSD--> A1'2'_B12	0.14583	0.68	0.17	0.97145	0.17	4
A1'2_B12' ---PP1-active_PSD--> A1'2_B12[5]	0.14583	0.68	0.17	0.97145	0.17	4
A1'2'_B12 ---PP1-active_PSD--> A1'2_B12[5]	0.14583	0.68	0.17	0.97145	0.17	4
A1'2_B12[1] ---PP1-active_PSD--> A12_B12	0.14583	1.4	0.35	2	0.35	4

A1'2_B12' ---PP1-active_PSD--> A12_B12'[1]	0.14583	1.4	0.35	2	0.35	4
A1'2'_B12 ---PP1-active_PSD--> A12'_B12[2]	0.14583	1.4	0.35	2	0.35	4
A1'2_B12[5] ---PP1-active_PSD--> A12_B12[3]	0.14583	1.4	0.35	2	0.35	4
A12_B12[2] ---PP1-active_PSD--> A12_B12'[2]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12[2] ---PP1-active_PSD--> A12'_B12[1]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12'[2] ---PP1-active_PSD--> A12_B12[6]	0.14583	0.68	0.17	0.97145	0.17	4
A12'_B12[1] ---PP1-active_PSD--> A12_B12[6]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12[4] ---PP1-active_PSD--> A12_B12'[3]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12[4] ---PP1-active_PSD--> A12'_B12[3]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12'[3] ---PP1-active_PSD--> A12_B12[7]	0.14583	0.68	0.17	0.97145	0.17	4
A12'_B12[3] ---PP1-active_PSD--> A12_B12[7]	0.14583	0.68	0.17	0.97145	0.17	4
A12_B12'[2] ---PP1-active_PSD--> A12_B12'[1]	0.14583	1.4	0.35	2	0.35	4
A12_B12[2] ---PP1-active_PSD--> A12_B12	0.14583	1.4	0.35	2	0.35	4
A12'_B12[1] ---PP1-active_PSD--> A12'_B12[2]	0.14583	1.4	0.35	2	0.35	4
A12_B12[6] ---PP1-active_PSD--> A12_B12[3]	0.14583	1.4	0.35	2	0.35	4
A12_B12[4] ---PP1-active_PSD--> A12_B12[2]	0.14583	1.4	0.35	2	0.35	4
A12_B12'[3] ---PP1-active_PSD--> A12_B12'[2]	0.14583	1.4	0.35	2	0.35	4
A12'_B12[3] ---PP1-active_PSD--> A12'_B12[1]	0.14583	1.4	0.35	2	0.35	4
A12_B12[7] ---PP1-active_PSD--> A12_B12[6]	0.14583	1.4	0.35	2	0.35	4
A12_B12[4] ---PP1-active_PSD--> A1'2_B12[1]	0.14583	1.4	0.35	2	0.35	4
A12_B12'[3] ---PP1-active_PSD--> A1'2_B12'	0.14583	1.4	0.35	2	0.35	4
A12'_B12[3] ---PP1-active_PSD--> A1'2'_B12	0.14583	1.4	0.35	2	0.35	4
A12_B12[7] ---PP1-active_PSD--> A1'2_B12[5]	0.14583	1.4	0.35	2	0.35	4
neurogranin ---PKC-active--> neurogranin*	0.0018889	2.34	0.58	28.627	0.58	4.0345
neurogranin-CaM ---PKC-active--> CaM + neurogranin*	0.0011333	1.4	0.35	28.596	0.35	4
AC2 ---PKC-active--> AC2*	0.011111	16	4	33.334	4	4
neurogranin-CaM[1] ---PKC-active--> CaM-PSD + neurogranin*[1]	0.0011333	1.4	0.35	28.596	0.35	4
neurogranin[1] ---PKC-active--> neurogranin*[1]	0.0018889	2.34	0.58	28.627	0.58	4.0345
neurogranin* ---CaM_Ca_n-CaNAB--> neurogranin	0.0061778	2.67	0.67	10.012	0.67	3.9851
I1* ---CaM_Ca_n-CaNAB--> I1	0.0063333	1.36	0.34	4.9708	0.34	4
PP1-I1* ---CaM_Ca_n-CaNAB--> PP1-I1	0.0063333	1.36	0.34	4.9708	0.34	4
I1* ---CaM_Ca_n-CaNAB--> I1	0.0063334	1.36	0.34	4.9707	0.34	4
PP1-I1* ---CaM_Ca_n-CaNAB--> PP1-I1	0.0063334	1.36	0.34	4.9707	0.34	4
A12_B12' ---CaM_Ca_n-CaNAB--> A12_B12	0.037256	8	2	4.9706	2	4
A1'2_B12' ---CaM_Ca_n-CaNAB--> A1'2_B12	0.037256	8	2	4.9706	2	4
A12_B1'2' ---CaM_Ca_n-CaNAB--> A12_B1'2	0.037256	8	2	4.9706	2	4
A1'2_B1'2' ---CaM_Ca_n-CaNAB--> A1'2_B1'2	0.037256	8	2	4.9706	2	4
A12'_B12 ---CaM_Ca_n-CaNAB--> A12_B12	0.037256	8	2	4.9706	2	4
A1'2'_B12 ---CaM_Ca_n-CaNAB--> A1'2_B12	0.037256	8	2	4.9706	2	4
A12'_B1'2 ---CaM_Ca_n-CaNAB--> A12_B1'2	0.037256	8	2	4.9706	2	4
A1'2'_B1'2 ---CaM_Ca_n-CaNAB--> A1'2_B1'2	0.037256	8	2	4.9706	2	4
A12'_B12'[1] ---CaM_Ca_n-CaNAB--> A12'_B12	0.037256	8	2	4.9706	2	4
A1'2'_B12'[1] ---CaM_Ca_n-CaNAB--> A1'2'_B12	0.037256	8	2	4.9706	2	4
A12'_B1'2'[1] ---CaM_Ca_n-CaNAB--> A12'_B1'2	0.037256	8	2	4.9706	2	4
A1'2'_B1'2'[1] ---CaM_Ca_n-CaNAB--> A1'2'_B1'2	0.037256	8	2	4.9706	2	4
A12'_B12'[1] ---CaM_Ca_n-CaNAB--> A12_B12'	0.037256	8	2	4.9706	2	4
A1'2'_B12'[1] ---CaM_Ca_n-CaNAB--> A1'2_B12'	0.037256	8	2	4.9706	2	4
A12'_B1'2'[1] ---CaM_Ca_n-CaNAB--> A12_B1'2'	0.037256	8	2	4.9706	2	4
A1'2'_B1'2'[1] ---CaM_Ca_n-CaNAB--> A1'2_B1'2'	0.037256	8	2	4.9706	2	4
A12_B12 ---CaM_Ca_n-CaNAB--> A12_B12'[1]	0.037256	8	2	4.9706	2	4
A12_B12 ---CaM_Ca_n-CaNAB--> A12'_B12[2]	0.037256	8	2	4.9706	2	4
A12_B12'[1] ---CaM_Ca_n-CaNAB--> A12_B12[3]	0.037256	8	2	4.9706	2	4
A12'_B12[2] ---CaM_Ca_n-CaNAB--> A12_B12[3]	0.037256	8	2	4.9706	2	4
A1'2_B12[1] ---CaM_Ca_n-CaNAB--> A1'2_B12'	0.037256	8	2	4.9706	2	4
A1'2_B12[1] ---CaM_Ca_n-CaNAB--> A1'2'_B12	0.037256	8	2	4.9706	2	4
A1'2_B12' ---CaM_Ca_n-CaNAB--> A1'2_B12[5]	0.037256	8	2	4.9706	2	4
A1'2'_B12 ---CaM_Ca_n-CaNAB--> A1'2_B12[5]	0.037256	8	2	4.9706	2	4
A12_B12[2] ---CaM_Ca_n-CaNAB--> A12_B12'[2]	0.037256	8	2	4.9706	2	4
A12_B12[2] ---CaM_Ca_n-CaNAB--> A12'_B12[1]	0.037256	8	2	4.9706	2	4
A12_B12'[2] ---CaM_Ca_n-CaNAB--> A12_B12[6]	0.037256	8	2	4.9706	2	4
A12'_B12[1] ---CaM_Ca_n-CaNAB--> A12_B12[6]	0.037256	8	2	4.9706	2	4
A12_B12[4] ---CaM_Ca_n-CaNAB--> A12_B12'[3]	0.037256	8	2	4.9706	2	4
A12_B12[4] ---CaM_Ca_n-CaNAB--> A12'_B12[3]	0.037256	8	2	4.9706	2	4
A12'_B12[3] ---CaM_Ca_n-CaNAB--> A12_B12[7]	0.037256	8	2	4.9706	2	4
A12_B12'[3] ---CaM_Ca_n-CaNAB--> A12_B12[7]	0.037256	8	2	4.9706	2	4
neurogranin*[1] ---CaM_Ca_n-CaNAB--> neurogranin[1]	0.0061778	2.67	0.67	10.012	0.67	3.9851
CaMKII-thr286-PSD ---tot-CaM-CaMKII-PSD--> CaMKII***-PSD	0.015625	24	6	320	6	4
CaMKII-CaM-PSD ---tot-CaM-CaMKII-PSD--> CaMKII-thr286-CaM-PSD	0.0013021	2	0.5	320	0.5	4
CaMKII-PSD ---tot-CaM-CaMKII-PSD--> CaMKII-thr286-PSD	0.0052083	8	2	320	2	4
CaMKII-thr286-CaM-PSD ---PP1-active_CaMKII_PSD--> CaMKII-CaM-PSD	0.083333	0.8	0.2	2	0.2	4
CaMKII-thr286-PSD ---PP1-active_CaMKII_PSD--> CaMKII-PSD	0.083333	0.8	0.2	2	0.2	4
CaMKII***-PSD ---PP1-active_CaMKII_PSD--> CaMKII-thr286-PSD	0.083333	0.8	0.2	2	0.2	4
CaMKII-thr306-PSD ---PP1-active_CaMKII_PSD--> CaMKII-PSD	0.083333	0.8	0.2	2	0.2	4
CaMKII***-PSD ---PP1-active_CaMKII_PSD--> CaMKII-thr306-PSD	0.083333	0.8	0.2	2	0.2	4
CaMKII-thr286 ---tot_CaM_CaMKII--> CaMKII***	0.0024474	24	6	227	6	4
CaMKII-CaM ---tot_CaM_CaMKII--> CaMKII-thr286*-CaM	0.000204	2	0.5	227	0.5	4

CaMKII-thr286 ---tot_autonomous_CaMKII--> CaMKII***	0.0015873	24	6	350	6	4
CaMKII-CaM ---tot_autonomous_CaMKII--> CaMKII-thr286*-CaM	0.0001323	2	0.5	349.99	0.5	4
ATP ---AC1-CaM--> cAMP	0.0013889	18	4.5	300	4.5	4
ATP ---AC2*--> cAMP	0.0006173	8	2	300	2	4
cAMP ---cAMP-PDE--> AMP	0.046667	40	10	19.841	10	4
cAMP ---cAMP-PDE*--> AMP	0.093333	80	20	19.841	20	4
cAMP ---PDE1--> AMP	0.0038889	6.67	1.667	39.7	1.667	4.0012
cAMP ---CaM.PDE1--> AMP	0.023333	40	10	39.683	10	4

All pools

name	CoInit	buffered
CaM-Ca4	0	0
PP1-active	1.8	0
cAMP	0	0
Ca	0.08	0
PKA-active	0	0
CaM-Ca3	0	0
CaM-TR2-Ca2	0	0
PP2A	0.11111	0
CaNAB-Ca4	0	0
CaMKII-thr286-CaM-PSD	0	0
CaMKII-CaM-PSD	0	0
CaMKII-thr286-PSD	0	0
CaMKII-PSD	0	0
CaMKII***-PSD	0	0
CaMKII-thr306-PSD	0	0
tot-auto-PSD	2	0
CaM-TR2-Ca2-PSD	0	0
CaM-Ca3-PSD	0	0
CaM-Ca4-PSD	0	0
Ca-PSD	0.08	0
286P-PSD	0	0
actCaMKII-PSD	2	0
tot_CaMKII_PSD	2	0
tot_CaMKII_cyt	22	0
PP1-active_PSD	4	0
PKC-active	0.1	0
temp-PIP2	2.5	1
I_845-P	0	0
tot_I_GluR12	0	0
total_Int	0.096296	0
A12_B12	0	0
A12_B12'[1]	0	0
A12'_B12[2]	0	0
A12_B12[3]	0	0
A12_B12[2]	0	0
A12_B12[4]	0	0
A12_B12'[2]	0	0
A12_B12'[3]	0	0
A12'_B12[1]	0	0
A12'_B12[3]	0	0
A12_B12[6]	0	0
A12_B12[7]	0	0
A1'2_B12[1]	0	0
A1'2_B12'	0	0
A1'2'_B12	0	0
A1'2_B12[5]	0	0
Ser845	0	0
Ser845-P	0	0
Ser845-PP	0	0
Ser831	0	0
Ser831-P	0	0
Ser831-PP	0	0
tot_mem_GluR12	0	0
act_CaMKII_cyt	2	0
NMDAR	120	0
CaM_Ca_n-CaNAB	0	0
basal_CaMKII_cyt	2	1
basal_CaMKII_PSD	2	0
PKC-control	0.1	1
Ca_control_cyt	0.08	1
Ca_control_PSD	0.08	1
basal_CaMKII_PSD_control	2	1
Anchor	27.333	0
AMPA_bulk	0.0092593	1
I_845	0	0
I_845_PP	0	0
tot-CaM-CaMKII-PSD	0	0
PP1-active_CaMKII_PSD	2	0
CaMKII	20	0
CaMKII-CaM	0	0
CaMKII-thr286*-CaM	0	0
CaMKII***	0	0
CaMKII-thr286	0	0
CaMK-thr306	0	0

tot_CaM_CaMKII	0	0
tot_autonomous_CaMKII	2	0
CaM	26.333	0
neurogranin-CaM	0	0
neurogranin*	0	0
neurogranin	10	0
CaM-PSD	26.333	0
neurogranin-CaM[1]	0	0
neurogranin[1]	10	0
neurogranin*[1]	0	0
I1	1.8	0
I1*	0	0
PP1-I1*	0	0
PP1-I1	0	0
CaNAB	1	0
CaNAB-Ca2	0	0
R2C2	0.5	0
R2C2-cAMP	0	0
R2C2-cAMP2	0	0
R2C2-cAMP3	0	0
R2C2-cAMP4	0	0
R2C-cAMP4	0	0
R2-cAMP4	0	0
PKA-inhibitor	0.25926	0
inhibited-PKA	0	0
ATP	2000	1
AC1-CaM	0	0
AC1	0.074074	0
AC2*	0	0
AC2	0.074074	0
AMP	0	0
cAMP-PDE	0.55556	0
cAMP-PDE*	0	0
PDE1	2.5926	0
CaM.PDE1	0	0
cAMP_in_dend	0	0
I1	4	0
I1*	0	0
PP1-I1*	0	0
PP1-I1	0	0
GluR23_M	3.5	0
GluR23_I	0.092593	0
total_mem	3.4667	0
A12_B12'	0	0
A1'2_B12'	0	0
A12_B1'2'	0	0
A1'2_B1'2'	0	0
A12'_B12	0	0
A1'2'_B12	0	0
A12'_B1'2	0	0
A1'2'_B1'2	0	0
A12_B12	0	0
A1'2_B12	0	0
A12_B1'2	0	0
A1'2_B1'2	0	0
A12'_B12'[1]	0	0
A1'2'_B12'[1]	0	0
A12'_B1'2'[1]	0	0
A1'2'_B1'2'[1]	0	0
AMPAR_deg	0	1