**Supplementary Material**

Chemical model: Reduced MAPK system. All volumes are initial reference volumes, and are rescaled to actual volumes defined by detailed morphology of simulated neuron and subsequent spatial discretization for solving PDEs.

|  |  |  |  |
| --- | --- | --- | --- |
| PSD | Vol = 0.01 fl |  |  |
| Reactions | Kf | Kb |  |
| Ca\_input <===> Ca | 500 s^-1 | 10 s^-1 |  |
| CaM-Ca3 + Ca <===> CaM-Ca4 | 1.8 uM^-1.s^-1 | 10 s^-1 |  |
| CaM + Ca <===> CaM-Ca | 8.4846 uM^-1.s^-1 | 8.4853 s^-1 |  |
| CaM-Ca2 + Ca <===> CaM-Ca3 | 3.6001 uM^-1.s^-1 | 10 s^-1 |  |
| CaM-Ca + Ca <===> CaM-Ca2 | 8.4846 uM^-1.s^-1 | 8.4853 s^-1 |  |
|  |  |  |  |
| Pools |  |  |  |
| name | Initial Concen | buffered | D (m^2/s) |
| Ca | 0.1 uM | No | 100 |
| Ca\_input | 0.08 uM | Yes | 0 |
| CaM | 40 uM | No | 0.5 |
| CaM-Ca3 | 0 uM | No | 1 |
| CaM-Ca2 | 0 uM | No | 1 |
| CaM-Ca | 0 uM | No | 1 |
| CaM-Ca4 | 0 uM | No | 1 |
|  |  |  |  |
| Spine Head | Vol = 0.09 fl |  |  |
| Reactions | Kf | Kb |  |
| CaM-Ca3 + Ca <===> CaM-Ca4 | 1.8 uM^-1.s^-1 | 10 s^-1 |  |
| CaM + Ca <===> CaM-Ca | 8.4845 uM^-1.s^-1 | 8.4853 s^-1 |  |
| CaM-Ca2 + Ca <===> CaM-Ca3 | 3.6001 uM^-1.s^-1 | 10 s^-1 |  |
| CaM-Ca + Ca <===> CaM-Ca2 | 8.4845 uM^-1.s^-1 | 8.4853 s^-1 |  |
| CaM <===> CaM\_xchange | 1 s^-1 | 100 s^-1 |  |
|  |  |  |  |
| Pools |  |  |  |
| name | InitialConc | buffered | D (m^2/s) |
| Ca | 0.11111 uM | No | 100 |
| CaM | 40 uM | No | 0.5 |
| CaM-Ca3 | 0 uM | No | 1 |
| CaM-Ca2 | 0 uM | No | 1 |
| CaM-Ca | 0 uM | No | 1 |
| CaM-Ca4 | 0 uM | No | 1 |
| CaM\_xchange | 0 uM | No | 20 |
|  |  |  |  |
| Dendrite | Vol = 1 fl |  |  |
| Reactions | Kf | Kb |  |
| AA <===> APC | 0.4 s^-1 | 0.01 s^-1 |  |
| 2 Ca + Raf <===> act\_Raf | 12 uM^-2.s^-1 | 4 s^-1 |  |
| K\_A\_p <===> K\_A | 0.05 s^-1 | 0 s^-1 |  |
| 2 AA + PKC <===> act\_PKC | 1 uM^-2.s^-1 | 2 s^-1 |  |
| Ca\_input <===> Ca | 500 s^-1 | 10 s^-1 |  |
| reg\_phosphatase <===> inact\_phosphatase | 0.03 s^-1 | 0 s^-1 |  |
| CaM-Ca3 + Ca <===> CaM-Ca4 | 1.8 uM^-1.s^-1 | 10 s^-1 |  |
| CaM + Ca <===> CaM-Ca | 8.4846 uM^-1.s^-1 | 8.4853 s^-1 |  |
| CaM-Ca2 + Ca <===> CaM-Ca3 | 3.6 uM^-1.s^-1 | 10 s^-1 |  |
| CaM-Ca + Ca <===> CaM-Ca2 | 8.4846 uM^-1.s^-1 | 8.4853 s^-1 |  |
| CaM <===> CaM\_xchange | 10 s^-1 | 10 s^-1 |  |
|  |  |  |  |
| Enzyme-reactions | Km | kcat | ratio |
| P\_MAPK ---phosphatase--> MAPK | 0.02 uM | 1 s^-1 | 4 |
| APC ---P\_MAPK--> AA | 5 uM | 10 s^-1 | 4 |
| K\_A ---P\_MAPK--> K\_A\_p | 10 uM | 10 s^-1 | 4 |
| inact\_phosphatase ---P\_MAPK--> reg\_phosphatase | 1 uM | 0.1 s^-1 | 4 |
| MAPK ---act\_PKC--> P\_MAPK | 5 uM | 10 s^-1 | 4 |
| MAPK ---act\_Raf--> P\_MAPK | 20.001 uM | 10 s^-1 | 4 |
| P\_MAPK ---reg\_phosphatase--> MAPK | 0.099998 uM | 2 s^-1 | 4 |
|  |  |  |  |
| Pools |  |  |  |
| name | Initial Concen | buffered | D (m^2/s) |
| phosphatase | 0.4 uM | No | 1 |
| P\_MAPK | 0 uM | No | 1 |
| MAPK | 2 uM | No | 1 |
| AA | 0 uM | No | 1 |
| act\_PKC | 0 uM | No | 0 |
| PKC | 1 uM | No | 1 |
| APC | 1 uM | Yes | 0 |
| K\_A | 1 uM | No | 0 |
| Raf | 1.4 uM | No | 0 |
| act\_Raf | 0 uM | No | 0 |
| Ca | 0.08 uM | No | 100 |
| Ca\_input | 0.08 uM | Yes | 0 |
| K\_A\_p | 0 uM | No | 0 |
| inact\_phosphatase | 1 uM | No | 1 |
| reg\_phosphatase | 0 uM | No | 1 |
| CaM | 2 uM | No | 0.5 |
| CaM-Ca3 | 0 uM | No | 1 |
| CaM-Ca2 | 0 uM | No | 1 |
| CaM-Ca | 0 uM | No | 1 |
| CaM-Ca4 | 0 uM | No | 1 |
| CaM\_xchange | 0 uM | No | 20 |
|  |  |  |  |

Electrical model: V in mV, referenced to resting potential. Time in ms.

Ion channel definitions, mostly from Traub, Wong, Miles, and Richardson. 1991. J. Neurophysiol 66:635-650.

gCa = gmaxCa.s2r ECa = 140

s-gate:

r-gate for :

r-gate for :

gNa = gmaxNa.m2h ENa = 115

m-gate:

h-gate:

gKDR = gmaxKDR.n EKDR = -15

n-gate:

gKAHP – gmaxKAHP.q EKAHP = -15

q-gate:

gKA = gmaxKA.ab EKA = -15

a\_gate:

b-gate:

gKC = gmaxKC.c EKC = -15

c\_gate for V <= 50:

c\_gate for V > -50:

where

A = normalization constant such that gGluR = gmaxGluR at peak, and

1 = 2 2 = 9

where

A = normalization constant such that gGABAR = gmaxGABAR at peak, and

1 = 4 2 = 9

where

 = 20

 = 0.28  = 62

where

 F = 96485 sA/mol

z = 2 R = 8.314 J/(K.mol)

T = 300 Kelvin Cafrac= fraction of current carried at 0 mV by Ca = 0.02

[Ca\_out] = 1.5mM [Ca\_in] = 0.08 M

Calcium pools:

d[Ca]/dt = (ICa + CaNMDA) –[Ca]/13.33

Passive properties

RM = 1.0 Ω.m2 RA = 1.0 Ω.m CM = 0.01 F/m2

Erest = -60 mV.

Channel distributions

|  |  |  |
| --- | --- | --- |
| Channel | Zone | Distribution, i.e., Gmax. (S/m2) |
| Ca | Basal + Apical | 0.0 Also tested 4.0 |
| Ca | Soma | 40 |
| Na | Basal | 60 |
| Na | Apical | 40+40exp(-p/200) |
| Na | Soma | 600 |
| K\_DR | Basal | (p<400)\*200 |
| K\_DR | Apical | 60+40exp(p<125) |
| K\_DR | Soma | 250 |
| K\_AHP | All | 8 |
| K\_C | Basal + Apical | 50+150exp(-p/200) |
| K\_C | Soma | 100 |
| K\_A | Basal + Apical | 50(1+2/(dia+0.1)) |
| K\_A | Soma | 50 |
| GABA | All | 10+30(p < 125) |
| GluR | Spine Heads | 4000 |
| NMDAR | Spine Heads | 800 (Tested wide range) |

Where p = path length measured along dendrite, from soma to specified point on dendritic tree, and

dia = diameter of dendrite at specified point on dendritic tree.