A basic model of calcium homeostasis in non-excitable cells

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Supporting Information S7 Program

Calculations leading to Figs 10-12

Description of Fig 10 calculations

The folder `fig10` contains the subfolders `gnuplot-fig10A` and `fortran-fig10B`.

The folder `gnuplot-fig10A` contains the following files:
i) `I_SOCC_vs_Ca_lum_Luik_et_al.txt`: This file contains the extracted data of Figure 1c from Ref. [1] in TEXT format. The extraction was done using the program `GraphClick, https://macdownload.informer.com/graphclick/`

ii) `graph_Luik_vSOCC.pl`: This is a Perl script, which calls gnuplot and fits Eq 14 to the data in file `I_SOCC_vs_Ca_lum_Luik_et_al.txt`. To execute the script direct the `Terminal` (Mac), or `Command Prompt` (Win) to the location of `graph_Luik_vSOCC.pl`, and write:

```
perl graph_Luik_vSOCC.pl
```

This creates the remaining two files:
iii) `graph_jSOCC.pdf`, which is a pdf version of Fig 10A
and
iv) `fit.log`, which contains, among other information, the number of iterations and the final set of parameters with Asymptotic Standard Errors.

The folder `fortran-fig10B` contains the following files:
`CAREG65a.f`: Fortran source file.
`careg65a`, `careg65a.exe`: precompiled binaries for Mac OSX and Windows.
`CAREG65a.INP`: input file.
`copy_input.pl`: Perl script copying input file with run-id in name of copied file.
`graph_jSOCC-Ca_lum.pl`: Perl script to make graph using gnuplot.
`careg65a.sh`, `careg65a.cmd`: Mac and Win scripts to automate calculation.
`CAREG65a-19_jSOCC-Ca_lum.txt`: data file for plotting.
`CAREG65a-19_jSOCC-Ca_lum.pdf`: plot in pdf format.
`CAREG65a-19_summary.txt`: Copy of output in Terminal or Command Prompt.
`libV77.a`: 64-bits library for Mac OSX.
`vms.lib`: 64-bits library for Windows.
`tmp`: temporary file for plot annotation.

To automatically execute the precompiled binaries `careg65a` (Mac) or `careg65a.exe` (Win) and to make the plot of Fig 10B do the following:

Win: Write in Command Prompt window: `careg65a.cmd` and press RETURN.
Mac: Write in Terminal window: `./careg65a.sh` and press RETURN.

If you should get `Permission denied` when using a Mac, write in Terminal window:
`chmod 755 careg65a`

and

`chmod 755 careg65a.sh`.
This will give execution rights to the files `careg65a.sh` and `careg65a`.

During execution, the Terminal or the Command Prompt will show the content of the file `CAREG65a-19_summary.txt` as the the calculation progresses, and will finally show the plot `CAREG65a-19_jSOCC-Ca_lum.pdf`.

The 64-bits binaries were created with `Absoft Pro Fortran` compilers for Mac OSX and Windows, by using the commands:

for Mac: `f77 -o careg65a -m64 -O2 CAREG65a.f libV77.a`
for Win: `f77 -o careg65a -m64 -O2 CAREG65a.f vms.lib`

What the program does:
By using Eq 17 and varying k_{20} (k_{21}=1.0 μM/s) the program starts with a Ca_{lum} steady state concentration of 500 μM and successively decreases the steady state concentration by 20 μM by step-wise reducing k_{20}. The cooperativity n (see Eqs 28 and 29 in S1 Text; Fortran variable `COOP` in `CAREG65a.f`) starts with n=1.3 and decreases by 0.0208 for each 20 μM reduction in the Ca_{lum} steady state concentration. For each changed Ca_{lum} steady state concentration and n the program calculates j_{SOCC} after a certain time. This time starts with 1×10^4 s for n=1.3 and $Ca_{lum,ss}$=500 μM and increases by 1×10^4 s for each reduction in $Ca_{lum,ss}$ and n (see `CAREG65a-19_summary.txt`). Other parameter values are given in the input file `CAREG65a.INP`.

Description of Fig 11 calculations

The folder `fig11` contains the following files:
`CAREG65.f`: Fortran source file.
`careg65`, `careg65.exe`: precompiled binaries for Mac OSX and Windows.
`CAREG65.INP`: input file.
`CAREG65-112.INP`: copy of input file with run-id in file name.
`copy_input.pl`: Perl script copying input file with run-id in file name.
`graph_jSOCC.pl`: Perl script to make graph using gnuplot.
`graph_Ca_ER.pl`: Perl script to make graph using gnuplot.
`careg65.sh`, `careg65.cmd`: Mac and Win scripts to automate calculation.
`CAREG65-112.txt`: data file for plotting Ca_{ER}.
`CAREG65-112_fluxes.txt`: data file for plotting j_{SOCC}.
`CAREG65-112_jSOCC.pdf`: plot in pdf format.
`CAREG65-112_Ca_ER.pdf`: plot in pdf format.
`CAREG65-112_summary.txt`: copy of Terminal or Command Prompt output.
`libV77.a`: 64-bits library for Mac OSX.

`vms.lib`: 64-bits library for Windows.
`tmp`: temporary file used for plot title/annotation.

The 64-bits binaries were created with `Absoft Pro Fortran` compilers for Mac OSX and Windows, by using the commands:

for Mac: `f77 -o careg65 -m64 -O2 CAREG65.f libV77.a`
for Win: `f77 -o careg65 -m64 -O2 CAREG65.f vms.lib`

To automatically execute the precompiled binaries `careg65` (Mac) or `careg65.exe` (Win) and to make the plots in Fig 11 do the following:

Win: Write in Command Prompt window: `careg65.cmd` and press RETURN.
Mac: Write in Terminal window: `./careg65.sh` and press RETURN.

If you should get `Permission denied` when using `careg65.sh`, write in Terminal window:
`chmod 755 careg65`

and

`chmod 755 careg65.sh`.
This will give execution rights to the files `careg65.sh` and `careg65`.

In case you wish to use another plotting program the locations of the plot data are:
File `CAREG65-112.txt`:
column 1: time (s)
column 34: Ca_{ER} (μM)

File `CAREG65-112_fluxes.txt`:
column 1: time (s)
column 16: j_{SOCC} (μM/s)

Description of Fig 12 calculations

The folder `fig12` contains the following files:
`CAREG65.f`: Fortran source file.
`careg65`, `careg65.exe`: precompiled binaries for Mac OSX and Windows.
`CAREG65.INP`: input file.
`CAREG65-173.INP`: copy of input file with run-id in file name.
`copy_input.pl`: Perl script copying input file with run-id in file name.
`graph_jSOCC.pl`: Perl script to make graph using gnuplot.
`graph_jPMCA.pl`: Perl script to make graph using gnuplot.
`graph_NCX.pl`: Perl script to make graph using gnuplot.
`graph_Ca_cyt.pl`: Perl script to make graph using gnuplot.
`CAREG65-173_jSOCC.pdf`: plot in pdf format.
`CAREG65-173_jPMCA.pdf`: plot in pdf format.
`CAREG65-173_NCX.pdf`: plot in pdf format.
`CAREG65-173_Ca_cyt.pdf`: plot in pdf format.
`careg65.sh`, `careg65.cmd`: Mac and Win scripts to automate calculation.
`CAREG65-173.txt`: data file for plotting concentrations.
`CAREG65-173_fluxes.txt`: data file for plotting fluxes.
`CAREG65-173_summary.txt`: copy of Terminal or Command Prompt output.

`libV77.a`: 64-bits library for Mac OSX.
`vms.lib`: 64-bits library for Windows.
`tmp`: temporary file used for plot title/annotation.

The 64-bits binaries were created with `Absoft Pro Fortran` compilers for Mac OSX and Windows, by using the commands:

for Mac: `f77 -o careg65 -m64 -O2 CAREG65.f libV77.a`
for Win: `f77 -o careg65 -m64 -O2 CAREG65.f vms.lib`

To automatically execute the precompiled binaries `careg65` (Mac) or `careg65.exe` (Win) and to make the plots in Fig 11 do the following:

Win: Write in Command Prompt window: `careg65.cmd` and press RETURN.
Mac: Write in Terminal window: `./careg65.sh` and press RETURN.

If you should get `Permission denied` when using `careg65.sh`, write in Terminal window:
`chmod 755 careg65`

and

`chmod 755 careg65.sh`.
This will give execution rights to the files `careg65.sh` and `careg65`.

In case you wish to use another plotting program the locations of the plot data are:
File `CAREG65-173.txt`:
column 1: time (s)
column 2: Ca_{cyt} (μM)
column 10: $Ca_{cyt,set}$ (PMCA) (μM)
column 35: $Ca_{cyt,set}$ (NCX) (μM)

File `CAREG65-173_fluxes.txt`:
column 1: time (s)
column 4: j_{PMCA} (μM/s)
column 14: j_{NCX} (μM/s)
column 16: j_{SOCC} (μM/s)

References

1. Luik RM, Wang B, Prakriya M, Wu MM, Lewis RS. Oligomerization of STIM1 couples ER calcium depletion to CRAC channel activation. Nature. 2008;454(7203):538–542.