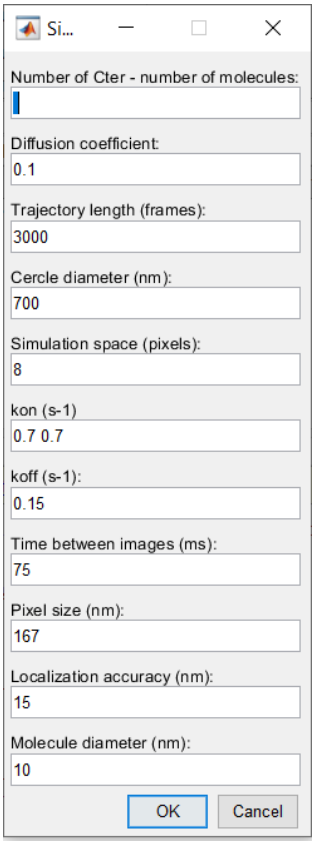
DiffuTrapKv2

Simulation of diffusion and trapping of a tetramer of size “molecule diameter” onto fixed interaction sites. In the tetramer there are “Cter” number of interacting subunits.

Reference: Paupiah et al (2025) *Epileptic encephalopathy-related Kv2.1 mutants impair channel clustering and membrane distribution but not neuronal excitability* bioRxiv https://doi.org/10.1101/2025.10.13.681825

Enter the parameters in the pop up window:



Number of Cter – number of molecules:

Enter the number of subunits bearing the entire Cter (with a PRC domain) and the number of molecules with these characteristics (two numbers, separated by a space):

Example: 2 100 -> means a simulation with 100 molecules (tetramers) with 2 PRC domains.

If you combine two groups, enter the values for one after the other:

Example: 2 100 4 100

Diffusion coefficient:

In µm2/s (mean value of a gaussian distribution of D).

Trajectory length:

Duration of the simulation, in “SPT” frames.

Circle diameter:

Circular space, in the middle of the simulation space, where interactions may occur.

Simulation space: Size of the bounding box where molecules diffuse.

Kon and koff: Effective constants for the scaffolding interaction (each PRC acting independently).

Time between images, Pixel size, Localization accuracy: The same than the SPT experiment that the simulation wants to reproduce.

Molecule diameter: Size of the diffusing molecule (circle).

<u>Output :</u>

- SPT-like trajectory files (.trc, a txt file), in \trc folder with:

molecule #	time (frame)	x position	y position	group # (# Cter)
1.0000000e+00	3.0000000e+00	5.9697640e+00	6.5621707e+00	1.0000000e+00
1.0000000e+00	4.0000000e+00	5.3354033e+00	6.8361045e+00	1.0000000e+00
1.0000000e+00	5.0000000e+00	4.6893458e+00	7.0009205e+00	1.0000000e+00
1.0000000e+00	8.0000000e+00	4.2023057e+00	6.8358916e+00	1.0000000e+00
1.0000000e+00	9.0000000e+00	4.3780341e+00	5.5166036e+00	1.0000000e+00
1.0000000e+00	1.0000000e+01	4.8763509e+00	4.4509895e+00	1.0000000e+00
1.0000000e+00	1.1000000e+01	5.7165512e+00	3.9205467e+00	1.0000000e+00

Files **cter***group#-simulation#***.trc** : trajectories of each group separately

Files **sim-***simulation#***-all.trc :** all groups together

- A report file with the parameters (main folder)