The description of data set used for figures in the paper

"Changes in ion selectivity following asymmetrical addition of charge to the selectivity filter of bacterial sodium channels"

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1 Shared Data Directory

1.1 Selectivity Filter Occupancy

The following data files contain the time evolution of the number of Na^+ and Ca^{2+} ions in the Selectivity Filter of wild type (Q_f=-4e) and mutant NavMs (Q_f=-5e) in our equilibrium Molecular Dynamics simulations.

`Occup_NavMs_Qf4_Ca.dat` : Wild type NavMs, simulation in 0.1 M $CaCl_2$. Data used in Supporting Figure 5A.

`Occup_NavMs_Qf5_Ca.dat` : Mutant NavMs, simulation in 0.1 M $CaCl_2$. Data used in Supporting Figure 5B.

`Occup_NavMs_Qf4_Na.dat` : Wild type NavMs, simulation in 0.14 M NaCl. Data used in Supporting Figure 4A.

`Occup_NavMs_Qf5_Na.dat` : Mutant NavMs, simulation in 0.14 M NaCl. Data used in Supporting Figure 4B.

The file is organized in 3 columns whose meaning is the following:

Col 1: Time (ns)

Col 2: Frame index

Col 3: Number of Na^+ or Ca^{2+} ions in Selectivity Filter.

1.2 Potential of Mean Force

The following data files contain the Potential of Mean Force of Na^+ and Ca^{2+} ions along the axis of the channel of wild type (Q_f=-4e) and mutant NavMs (Q_f=-5e) in our equilibrium Molecular Dynamics simulations.

`Free_Ene_NavMs_Qf4_Ca.dat` : Wild type NavMs, simulation in 0.1 M $CaCl_2$. Data used in Figure 4A.

`Free_Ene_NavMs_Qf5_Ca.dat` : Mutant NavMs, simulation in 0.1 M $CaCl_2$. Data used in Figure 4B.

`Free_Ene_NavMs_Qf4_Na.dat` : Wild type NavMs, simulation in 0.14 M NaCl. Data used in Figure 3A.

`Free_Ene_NavMs_Qf5_Na.dat` : Mutant NavMs, simulation in 0.14 M NaCl. Data used in Figure 3B.

The file is organized in 2 columns whose meaning is the following:

Col 1: Axial position (Å)

Col 2: Potential of Mean Force (kcal/mol)

1.3 Ion coordination

The following data files contain the number of coordinating oxygens per Na^+ or Ca^{2+} ion in axial bins with a width of 2.0 Å. The data refer to equilibrium Molecular Dynamics simulations in 0.1 M $CaCl_2$ and 0.14 M NaCl.

`Coord_NavMs_Qf4_Ca.dat` : Wild type NavMs, simulation in 0.1 M $CaCl_2$. Data used in Figure 4C.

`Coord_NavMs_Qf5_Ca.dat` : Mutant NavMs, simulation in 0.1 M $CaCl_2$. Data used in Figure 4D.

`Coord_NavMs_Qf4_Na.dat` : Wild type NavMs, simulation in 0.14 M NaCl. Data used in Figure 3C.

`Coord_NavMs_Qf5_Na.dat` : Mutant NavMs, simulation in 0.14 M NaCl. Data used in Figure 3D.

The file is organized in 6 columns whose meaning is the following:

Col 1: Axial position (Å).

Col 2: Number of coordinating water oxygens per Na^+ or Ca^{2+} ion.

Col 3: Number of coordinating oxygens provided by protein residues other than Aspartates or Glutamates.

Col 4: Number of coordinating oxygens provided by Aspartates and Glutamates.

Col 5: Total number of coordinating oxygens per Na^+ or Ca^{2+} ion.

Col 6: Number of coordinating Chlorides per Na^+ or Ca^{2+} ion.

1.4 Current calculation with collective diffusion model

The following data files contain the current-voltage plots estimated using Linear response Theory in equilibrium Molecular Dynamics simulations of wild type NavMs and its mutant with charge Q_f=-5e in 0.1 M $CaCl_2$ and 0.14 M NaCl.

`NavMs_Qf4_Ca_Lin-Resp-Th_IVplot.dat` : Wild type NavMs, simulation in 0.1 M $CaCl_2$. Data used in Table 2.

`NavMs_Qf5_Ca_Lin-Resp-Th_IVplot.dat` : Mutant NavMs, simulation in 0.1 M $CaCl_2$. Data used in Table 2.

`NavMs_Qf4_Na_Lin-Resp-Th_IVplot.dat` : Wild type NavMs, simulation in 0.14 M NaCl. Data used in Table 2.

`NavMs_Qf5_Na_Lin-Resp-Th_IVplot.dat` : Mutant NavMs, simulation in 0.14 M NaCl. Data used in Table 2.

The files are organized as follows.

Line 1: Diffusion coefficient of charge D_Q (e^2/ps).

Line 2: Thermal fluctuation energy k_BT (eV).

Line 3: Conductance (pS).

Lines 4-24 contain the current-voltage plot and they are organized in 2 columns.

Col 1: Voltage (mV).

Col 2: Current (pA).

1.5 Experimental data on heterotetramer mixtures

This data file, NaChBac_MIX.xlsx, contains current-voltage plots for the different heterotetramer mixtures. These data have been used in Fig 1, Supp. Table 3, and Supp. Fig 1. The file contains the following sheets corresponding to the following systems:

1. Summary
2. LESWAS-LASWAS 1:3 mixture
3. LESWAS-LASWAS 3:1 mixture
4. LESWAS-LASWAS 1:1 mixture
5. Pure LESWAS
6. LESWAS-LEDWAS 3:1 mixture
7. LESWAS-LEDWAS 1:1 mixture

8. LESWAS-LEDWAS 1:3 mixture
9. Pure LEDWAS
10. LESWAS with L226P mutation

Each sheet contains 3 main blocks of data. The first block shows whole cell sodium current curves as a function of the voltage. Voltages are expressed in mV while currents are expressed in pA. Below this block there is a line showing values of membrane capacitance (pF). The ratio of the currents of the first block and the values of the capacitance yields current densities (pA/pF) that are tabulated in the second block of data. Similarly, the third block contains whole cell calcium currents (pA) as a function of the voltage (mV) that are converted into current densities (pA/pF; fourth block) dividing by a line of values of membrane capacitance. The fifth and last block contains normalized calcium currents. Each block of data is organized in a number of columns.

Col 1: Voltage (mV).

Col 2-$n+1$: There are n columns (one for each independent experiment) reporting whole cell currents (pA), current densities (pA/pF) or normalized currents (pure numbers).

Col $n+2$: This column shows the number n of independent experiments.

Col $n+3$: This column contains the average of the currents listed in columns 2-$n+1$.

Col $n+3$: This column contains the Standard Error of the Mean (SEM).

The Summary sheet also contains two blocks of data, the former corresponding to whole cell currents (pA) and the latter to current densities (pA/pF). The currents shown in the summary page are peak currents, so that voltages are not shown. Each block is further split in two sub-blocks referring to sodium and calcium currents. In each sub-block the first column indicates a formal charge that identifies a mixture. For instance mixture LESWAS-LEDWAS 3:1 is obtained mixing LESWAS subunits havibg SF charge -1e with LEDWAS subunits carrying a charge -2e in ratio 3:1. A concatenamer containing exactly 3 LESWAS and 1 LEDWAS subunit would have charge 3*(-1)+(-2)=-5. This charge is used to identify the mixture even if subunits are expected to assemble following a binomial distribution. The remaining three columns of each sub-block report the mean, standard error of the mean and number of independent experiments.

1.6 Experimental data on NavMs concatenamers

This Excel spreadsheet, NavMS_concat.xlsx, contains current-voltage curves for the NavMs concatenamers (the wild type and the mutants carrying the S179D mutation in either repeat I, mutant DI, or repeat II, mutant DII). These data have been used in Fig 2 and Supp. Table 2.

The file contains the following sheets corresponding to the following systems:

1. Summary
2. Wild type NavMs (Q_f=-4e)
3. Mutant DI (Q_f=-5e)
4. Mutant DII (Q_f=-5e)

All the sheets except for the Summary contain whole cell currents (pA) as a function of the voltage (mV). There are two main blocks of data corresponding to sodium and calcium currents respectively, each followed by a line of values of membrane capacitance (pF) that are used to compute the average current densities (pA/pF) shown in the Summary page. Both the sodium and the calcium blocks comprize a first column of volvatges followed by a number of current columns corresponding to the number of independent experiments.

The Summary page also contains two blocks of data referring to sodium and calcium currents. Each block is composed by 7 columns:

Col 1: Voltage (mV).

Col 2: Average current density (pA/pF) of wild type NavMs.

Col 3: Standard Error of the Mean of wild type NavMs current.

Col 4: Average current density (pA/pF) of NavMs DI mutant.

Col 5: Standard Error of the Mean of the current of NavMs DI mutant.

Col 6: Average current density (pA/pF) of NavMs DII mutant.

Col 7: Standard Error of the Mean of the current of NavMs DII mutant.

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