Molecular dynamics simulations of scorpion toxin recognition by the Ca^{2+}-activated potassium channel $K_{Ca}3.1$

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Supporting Material

TABLE S1 The interacting residue pairs in the model structures of the ChTx-K_{Ca}3.1 and OSK1-K_{Ca}3.1 complexes obtained from 30 ns of MD simulations. The average distances over the last 10 ns (500 frames) are given together with standard deviations.

ChTx-K_{Ca}3.1	Distance (Å)	OSK1-K_{Ca}3.1	Distance (Å)
F2 -V231	3.0±1.8	K9 -D255	3.8±1.1
S10-D255	2.8±1.3	I10 -V231	2.6±0.4
K11-D239	5.7±1.8	L15-V231	3.1±1.4
W14-V257	2.4±1.4	R24-E227	2.1±2.9
R25-D239	1.9±2.2	F25-V257	3.4±2.5
K27-Y253	2.0±2.2	K27-Y253	4.8±2.3
M29-D255	2.5±1.8	M29-D255	2.5±1.4
R34-D255	1.9±2.2	N30-D255	3.0±1.3

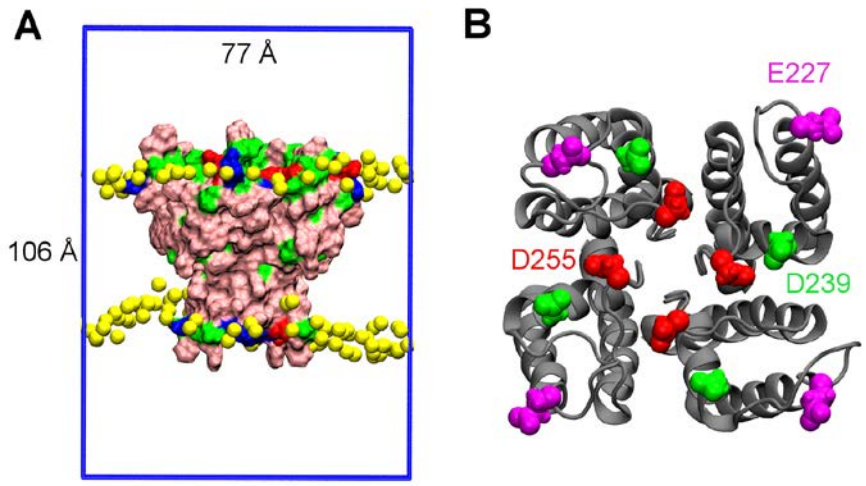

FIGURE S1 (A) The $K_{Ca}3.1$ channel embedded in a lipid bilayer viewed perpendicular to the bilayer normal. Channel residues are colored as: hydrophobic, pink; polar, green; basic, blue; acidic, red. Lipid phosphorus atoms are depicted as yellow spheres. The blue horizontal and vertical lines indicate the boundary of the simulation box. Lipids, water and ions are not shown for clarity. (B) The $K_{Ca}3.1$ channel viewed from the extracellular side along the channel axis. Three rings of acidic residues at positions 227, 239 and 255 are highlighted.

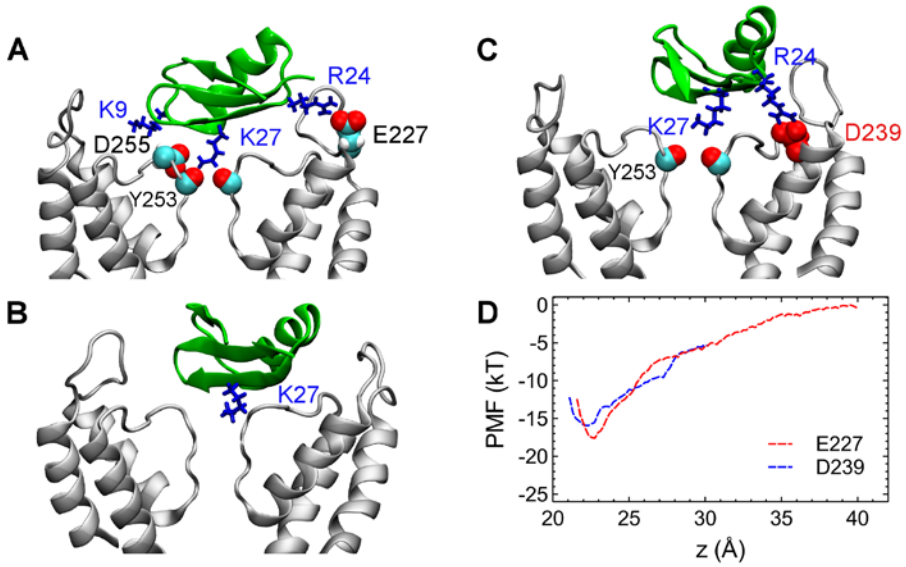

FIGURE S2 Structures of OSK1-K_{Ca}3.1: (A) predicted from a simulation of 2 ns in which a distance restraint is applied to pull the toxin Lys27 into the filter starting from the complex structure of Fig. 5; (B) predicted using the docking program ZDOCK; (C) predicted from a MD simulation of 15 ns, in which a distance restraint is applied to Lys27-Gly252 during the first 5 ns. In (D), the PMF profiles for the two binding modes of OSK1-K_{Ca}3.1 in which Arg24 forms a salt bridge with Glu227 and Asp239 of the channel, respectively, are shown.