Supporting Information

Soft Wall Ion Channel in Continuum Representation with Application to Modeling Ion Currents in α-Hemolysin

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Table S1. Parameter set for soft repulsion between protein atoms and mobile ions calculated from all-atom MD simulations (SR-MD).

	K^+		Cl^-			K^+		Cl^-			K^+		Cl^-	
	A, Å	η	A, Å	η		A, Å	η	A, Å	η		A, Å	η	A, Å	η
Standard Backbone					MET					ASN				
N	4.33	7.77	3.18	33.21	CB	4.42	7.38	3.88	22.14	CG	3.20	14.63	3.90	18.11
C	3.45	24.17	4.12	17.75	CG	4.06	12.57	3.80	20.40	CB	4.47	6.91	3.70	11.85
O	2.51	36.48	4.49	8.53	SD	3.01	21.49	4.20	14.37	OD1	2.50	36.25	3.94	15.79
CA	4.41	6.93	3.65	23.55	CE	4.01	7.69	3.84	12.61	ND2	3.47	9.01	3.20	18.46
ACE					SER					GLN				
CH3	3.81	11.31	3.72	18.18	CB	3.40	18.57	3.69	21.49	CB	4.47	6.91	3.70	11.85
NME					OG	2.53	43.46	3.05	33.36	CG	4.20	6.71	3.80	12.20
CH3	3.81	11.31	3.72	18.18	THR					CD	3.20	14.63	3.90	18.11
N-TERM					CB	3.46	15.91	3.76	23.33	OE1	2.50	36.25	3.94	15.79
N	3.96	17.31	3.1	24.74	OG1	2.51	49.72	3.04	49.14	NE2	3.47	9.01	3.20	18.46
CA	4.86	5.93	3.6	13.63	CG2	3.55	13.32	3.77	17.56	PRO				
C	3.45	24.17	3.7	15.44	PHE					CB	4.37	7.53	3.63	35.22
O	2.51	36.48	3.5	13.21	CG,CZ	3.18	19.40	4.17	14.87	CG	3.94	10.38	3.92	20.33
C-TERM					CD*,CE*	3.18	19.40	4.17	14.87	CD	4.60	6.46	4.01	13.41
N	3.60	9.90	4.70	7.03	TYR					GLU				
CA	3.44	9.60	4.45	15.63	CB	4.40	7.28	3.79	20.53	N	3.60	9.90	4.70	7.03
C	3.10	16.23	4.45	15.63	CG	4.54	4.85	4.76	8.58	CA,CB,CG	3.44	9.60	4.45	15.63
O	2.58	18.78	4.22	25.13	CD*	3.82	25.91	3.82	25.91	CD	3.10	16.23	4.45	15.63
OXT	2.58	18.78	4.22	25.13	CE*	3.30	20.60	3.76	21.13	OE*	2.58	18.78	4.22	25.13
GLY					CZ	3.05	27.06	3.84	25.56	ASP				
ALA					OH	2.53	43.22	2.99	36.38	N	3.60	9.90	4.70	7.03
CB	3.83	10.69	3.77	19.19	TRP					CA	3.44	9.60	4.45	15.63
VAL					CB	4.57	5.87	3.76	22.55	CB	3.44	9.60	4.45	15.63
CA	4.41	6.93	3.65	23.55	CG	3.42	23.07	4.45	14.09	CG	3.10	16.23	4.45	15.63
CB	4.47	9.99	4.12	13.67	CD1	3.06	17.60	3.83	19.97	OD*	2.58	18.78	4.22	25.13
CG*	3.83	10.69	3.77	19.19	CD2	3.24	29.62	4.76	9.62	ARG				
LEU					NE1	2.82	28.13	3.04	49.04	O	2.51	36.48	4.10	8.89
CB	5.00	6.44	4.10	10.03	CE2	3.05	43.57	3.88	31.54	CA	4.00	15.29	3.65	23.55
CG	5.00	6.44	4.80	6.13	CE3	3.83	8.57	3.92	20.15	CB,CG,CD	4.81	6.43	3.60	18.61
CD*	3.83	10.69	3.77	19.19	CZ2	3.71	8.85	3.95	12.96	NE	4.00	9.75	3.10	23.99
ILE					CZ3	3.91	8.11	3.83	19.46	CZ	4.70	6.46	3.55	23.94
CB	5.00	6.44	4.10	10.03	CH2	3.92	7.99	3.94	12.89	NH*	4.00	9.75	3.10	23.99
CG1	5.00	3.58	4.80	3.81	HIS					LYS				
CG2,CD1	3.83	10.69	3.77	19.19	CB	4.11	7.49	3.99	14.22	CB,CD,CE	4.86	5.93	3.60	13.63
CYS					CG	5.00	3.74	4.11	22.50	CG	4.86	5.93	3.70	14.04
CA	4.41	6.93	3.78	13.84	ND1	4.66	4.27	3.20	17.22	NZ	3.96	17.31	3.10	24.74
CB	4.23	9.07	3.78	13.84	CD2	3.56	16.57	3.55	22.41					
SG	3.10	16.80	3.75	17.90	CE1	3.24	15.63	3.74	18.67					
					NE2	2.64	26.45	4.05	13.42					

Table S2. Average and standard deviation of current upon channel rotations and different grid scales. The current was calculated with applied potential of 80 mV.

Current calculation method	Current, pA	
	Grid scale, grids/Å	
	1.0	2.0
PNP-HR	18.97±0.26	20.31±0.04
PNP-SR-MD	21.40±0.20	22.53±0.07
PNP-SR-LJ	22.13±0.15	22.86±0.09

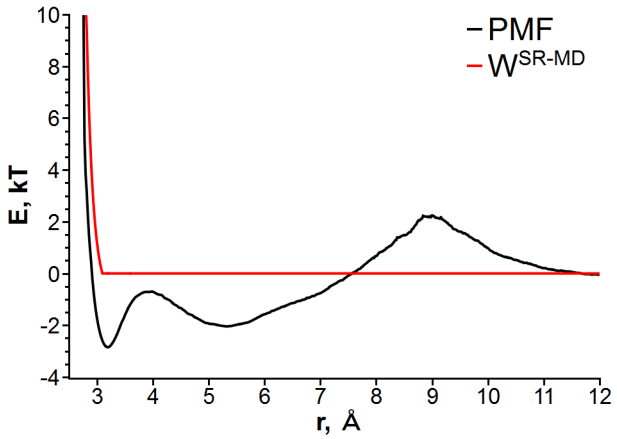

Figure S1. Comparison of repulsive part of PMF ($W^{SR\text{-}MD}$) calculated using SR-MD with complete PMF calculated from all atom MD simulation between N_ζ atom of Lys and Cl^-. Note that $W^{SR\text{-}MD}$ is slightly above of complete PMF because it is decouple from electrostatic attraction.

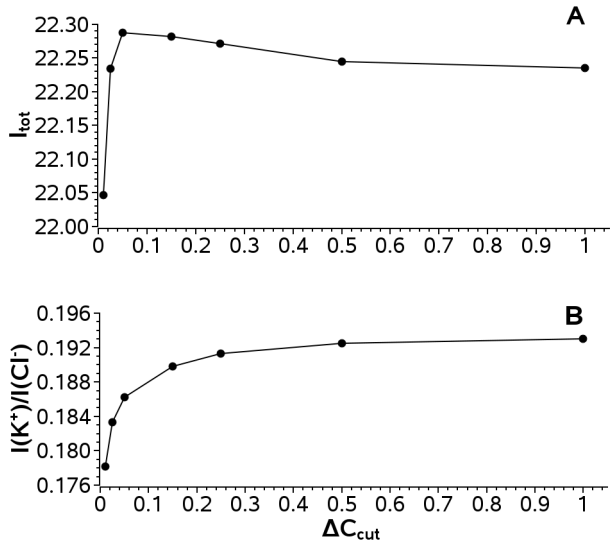

Figure S2. Dependency of total current (**A**) and selectivity of the channel as ration of K^+/Cl^- currents (**B**) on the choice of ΔC_{cut} during IAV determination procedure.

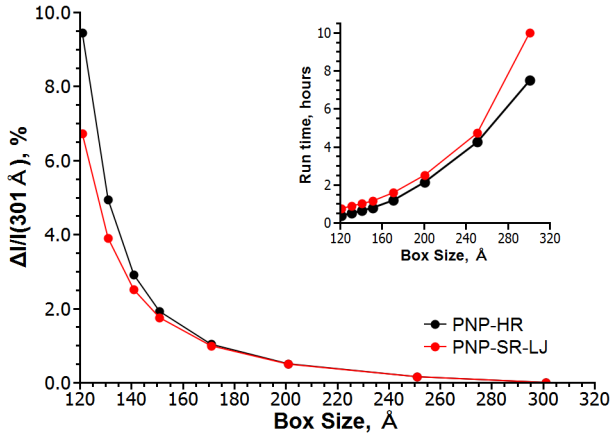

Figure S3. Dependency of calculated current and calculation run time (inset) on the size of simulation box; box size corresponds to each side of simulation box. Calculation was done using two CPU's core on desktop with Intel Pentium D 830 CPU.

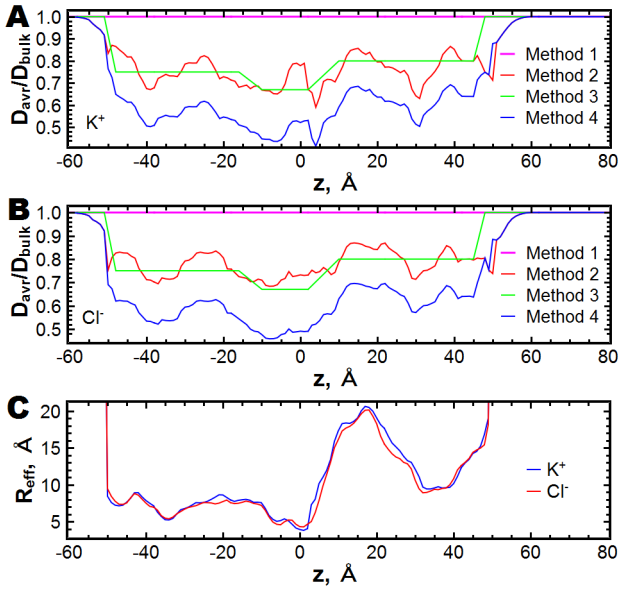

Figure S4. Average diffusion coefficient and effective pore radius along z-axis for PNP-SR-MD calculations. (**A**) and (**B**) – diffusion coefficients for K^+ and Cl^- respectively, the diffusion coefficients are averaged over the pore's cross section perpendicular to z-axis. (**C**) Effective pore radius for K^+ and Cl^-; effective radius is calculated as square root of cross section accessible by ions over π.