Supporting information for: Simulating current-voltage relationships for a single-file ion channel using the weighted ensemble method

Joshua L. Adelman*,† and Michael Grabe*,‡

Department of Biological Sciences, University of Pittsburgh, Pittsburgh, PA 15206, and Cardiovascular Research Institute, Department of Pharmaceutical Chemistry, University of California, San Francisco, San Francisco, CA 94158

E-mail: jla65@pitt.edu; michael.grabe@ucsf.edu

*To whom correspondence should be addressed
†University of Pittsburgh
‡University of California, San Francisco

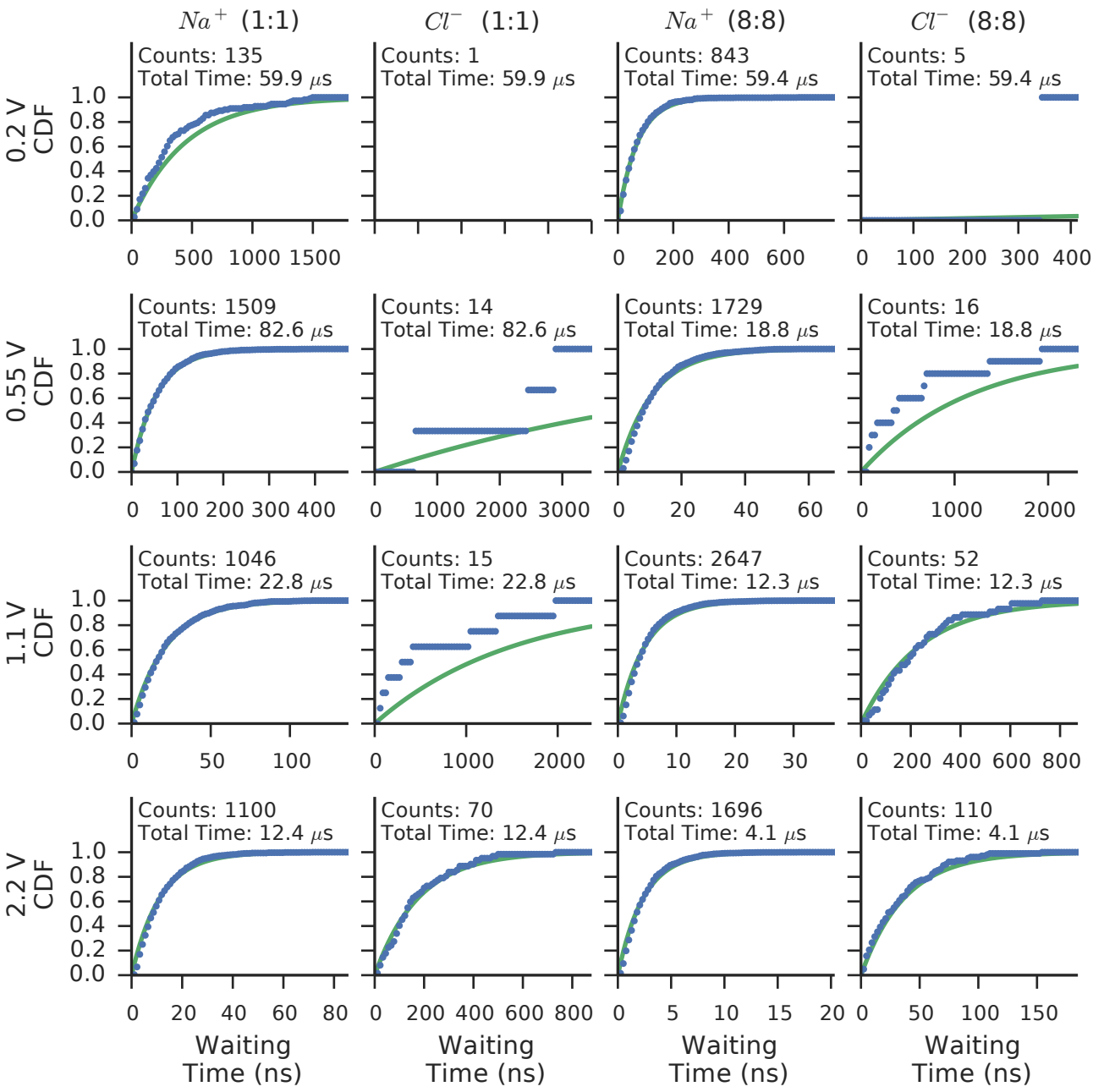

Figure S1: Waiting time distributions from brute force simulations. At each applied voltage, the empirical cumulative distribution function (CDF) for the waiting time between permeation events through the channel observed in the brute force simulations is plotted for the Na^+ and Cl^- ions at both ion concentrations (blue points). The CDF expected from Poisson statistics for a process with characteristic constant, λ, equal to the observed rate is shown as a solid green line. The total number of observed permeation counts and aggregate simulation time noted as inset text.

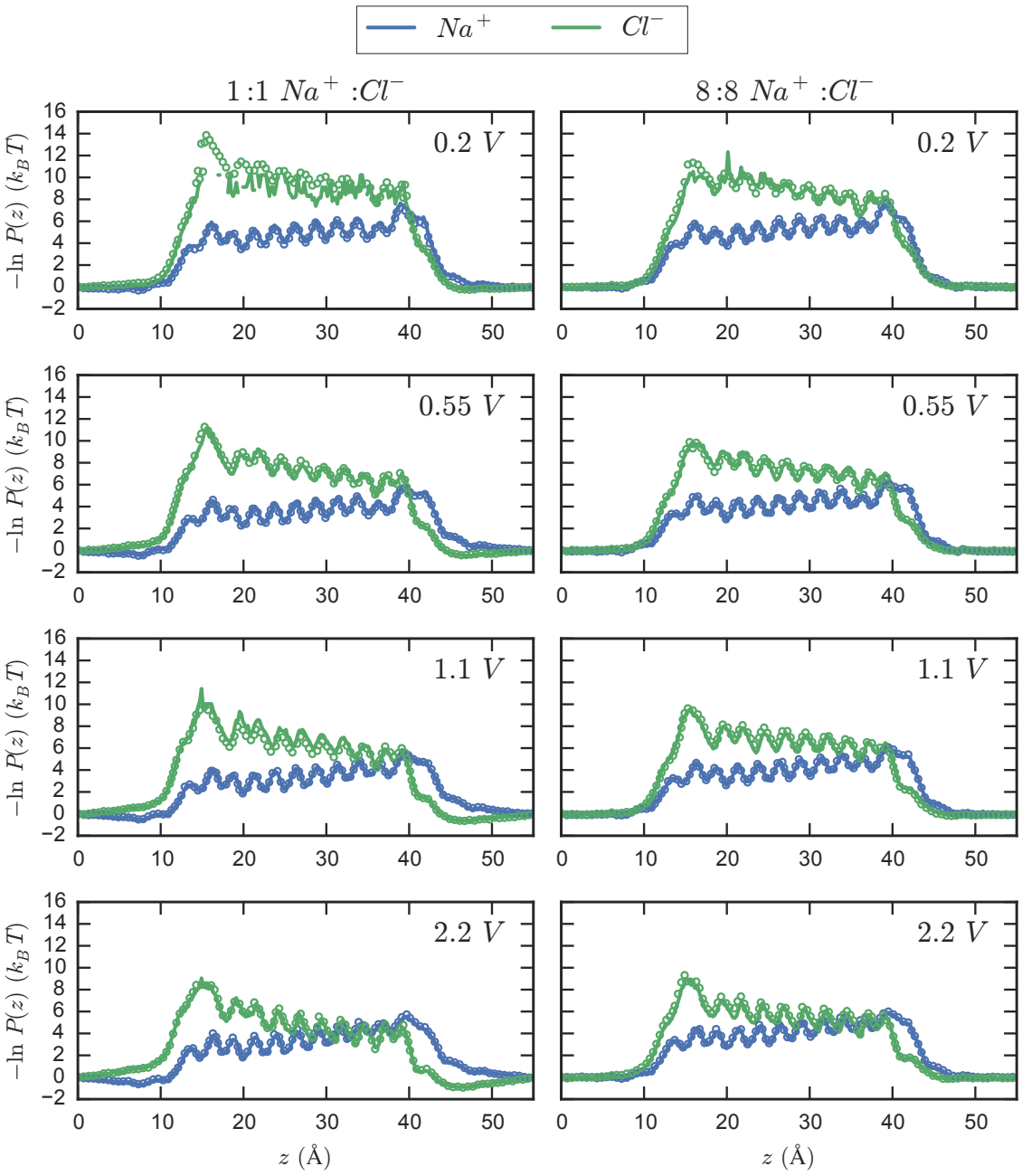

Figure S2: Biased energy profiles for Na^+ and Cl^- as a function of ion position for simulations at all applied voltages calculated from the projection of the steady-state ion distribution onto the z axis of the simulation box. Profiles calculated from brute force trajectories are shown as solid lines and the open circles show the same profiles as calculated from the corresponding WE simulation. The profiles for the WE simulations are calculated from the final 400 iterations. The left and right column of panels are from simulations with the low and high concentration systems, respectively.

Table S1: Summary of brute force simulations

Simulation	t (ns)	Na^+_{up}	Na^+_{down}	Cl^-_{up}	Cl^-_{down}
0.2 V - 1:1 Na^+:Cl^-					
1	2549.0	6	0	0	0
2	2549.8	7	0	0	0
3	2552.5	7	0	0	0
4	2556.9	5	0	0	0
5	2552.2	7	0	0	0
6	2546.6	7	0	0	1
7	2551.0	5	0	0	0
8	2555.5	6	1	0	0
9	2535.2	5	0	0	0
10	2523.7	10	0	0	0
11	2279.5	1	0	0	0
12	2531.7	5	0	0	0
13	2533.5	6	0	0	0
14	2537.1	5	0	0	0
15	2294.8	5	0	0	0
16	2530.2	2	0	0	0
17	2535.1	4	0	0	0
18	2536.3	4	0	0	0
19	2537.4	10	0	0	0
20	2297.5	6	0	0	0
21	2282.4	5	0	0	0
22	2517.2	5	0	0	0
23	2531.4	7	0	0	0
24	2530.1	5	0	0	0
Total:	59946.7	135	1	0	1
0.55 V - 1:1 Na^+:Cl^-					
1	5427.4	99	0	0	2
2	5442.5	92	0	0	1
3	5434.0	95	0	0	0
4	5437.7	109	0	0	1
5	5432.8	106	0	0	1
6	5434.6	87	0	0	1
7	5440.4	88	0	0	1
8	5439.2	103	0	0	3
9	2570.6	43	0	0	0
10	2570.2	46	0	0	1
11	2574.4	53	0	0	0
12	2569.3	44	0	0	0
13	2572.8	41	0	0	1
14	2574.0	47	0	0	0
15	2572.3	48	0	0	0
16	2573.1	44	0	0	1
17	2314.8	50	0	0	1
18	2317.4	43	0	0	0
19	2321.0	38	0	0	0
20	2310.2	43	0	0	0
21	2310.1	48	0	0	0
22	2312.9	49	0	0	0
23	2311.1	52	0	0	0

Simulation	t (ns)	Na^+_{up}	Na^+_{down}	Cl^-_{up}	Cl^-_{down}
24	2318.2	41	0	0	0
Total:	82581.1	1509	0	0	14
1.1 V - 1:1 Na^+:Cl^-					
1	2847.5	137	0	0	4
2	2844.7	133	0	0	0
3	2854.6	133	0	0	1
4	2852.8	147	0	0	3
5	2847.5	138	0	0	1
6	2853.4	123	0	0	1
7	2848.9	110	0	0	3
8	2852.6	125	0	0	2
Total:	22802.0	1046	0	0	15
2.2 V - 1:1 Na^+:Cl^-					
1	1556.1	140	0	0	7
2	1556.9	134	0	0	8
3	1555.7	153	0	0	8
4	1554.6	138	0	0	6
5	1557.6	130	0	0	9
6	1552.0	119	0	0	10
7	1556.9	148	0	0	9
8	1556.6	138	0	0	13
Total:	12446.3	1100	0	0	70
0.2 V - 8:8 Na^+:Cl^-					
1	2529.9	35	0	0	1
2	2530.2	39	0	0	0
3	2277.4	31	0	0	0
4	2536.6	24	0	0	0
5	2535.1	40	0	0	0
6	2533.7	41	0	0	0
7	2532.1	29	0	0	0
8	2529.3	35	0	0	0
9	2266.7	36	0	0	2
10	2517.2	39	1	0	0
11	2524.8	32	0	0	0
12	2518.2	35	0	0	0
13	2285.2	30	0	0	0
14	2519.0	37	0	0	0
15	2273.9	30	0	0	0
16	2519.1	37	0	0	1
17	2520.9	44	0	0	0
18	2519.2	29	0	0	0
19	2518.6	43	0	0	0
20	2287.0	41	0	0	0
21	2520.2	32	0	0	0
22	2525.3	34	0	0	0
23	2517.2	37	0	0	0
24	2514.3	33	0	0	1
Total:	59351.2	843	1	0	5
0.55 V - 8:8 Na^+:Cl^-					
1	2341.2	204	0	0	3
2	2341.7	222	0	0	6
3	2342.1	211	0	0	2
4	2347.9	231	0	0	0

Simulation	t (ns)	Na^+_{up}	Na^+_{down}	Cl^-_{up}	Cl^-_{down}
5	2343.4	199	0	0	1
6	2345.0	221	0	0	2
7	2346.5	228	0	0	0
8	2344.6	213	0	0	2
Total:	18752.4	1729	0	0	16
1.1 V - 8:8 Na^+:Cl^-					
1	1529.5	335	0	0	5
2	1532.7	338	0	0	5
3	1533.6	328	0	0	6
4	1533.4	327	0	0	9
5	1535.2	326	0	0	9
6	1534.9	319	0	0	4
7	1531.5	327	0	0	8
8	1533.1	347	0	0	6
Total:	12263.8	2647	0	0	52
2.2 V - 8:8 Na^+:Cl^-					
1	510.9	208	0	0	16
2	510.4	204	0	0	12
3	511.6	218	0	0	11
4	508.5	200	0	0	13
5	510.9	214	0	0	19
6	512.4	240	0	0	14
7	511.1	215	0	0	10
8	510.7	197	0	0	15
Total:	4086.6	1696	0	0	110