Inducing nonlinear conductance and emergent memristance in open pores using blockers

Supplementary Information

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OmpF Sigle channel conductance calculation/approximation from literature:

The following values of single channel conductance of OmpF were extraced/approximated (using WebPlotDigitizer) from Ionescu et al[1]: ~0.96 nS for +100 mV for p-OmpF (orientation of OmpF which leads to higher value of current at positive potential) and ~0.713 nS for +100 mV for n-OmpF (orientation of OmpF which leads to higher value of current at negative potential).

However, voltage direction in that study was opposite in comparison to our study as in the previous study OmpF was added to the cis-side and voltage applied through the trans-side. In contrast, we have added OmpF to the same droplet which was attached to the source electrode. Hence, our negative potential of -100 mV corresponds to their +100 mV.

Since we were unable to calculate the exact proportion of two orientations, we assumed an equal proportion of both orientation was present in the membrane. This assumption was based on the possibility of OmpF insertion in a membrane in either orientation is 50:50[1]

Hence, conductance at -100 mV (corresponding to +100 mV of the cited literature) was assumed to be ~ (0.96 + 0.713)/2 = 0.84 nS (for the trimer) and thus for a single pore, assumed conductance was ~0.84/3 = 0.28 nS

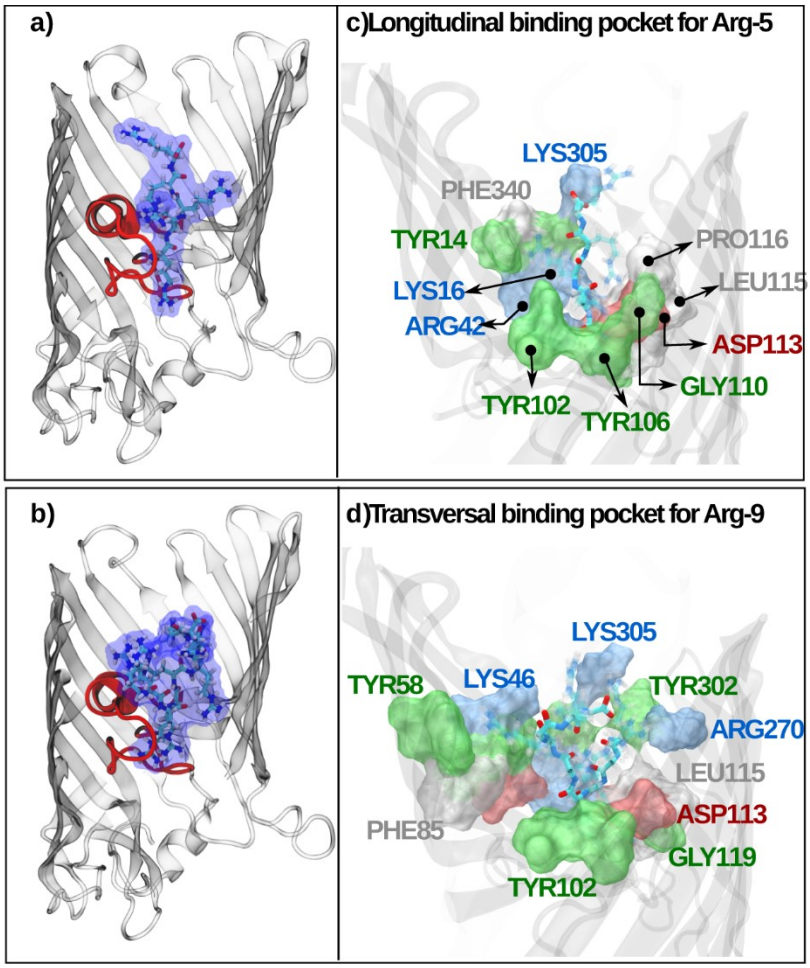

Figure S1 Arg-5 and Arg-9 adopt distinct yet complementary binding modes within the OmpF lumen, governed by a combination of electrostatic, hydrogen-bonding, and cation–π interactions. (a,b) Representative snapshots of Arg-5 (top) and Arg-9 (bottom) bound within the OmpF pore, highlighting peptide orientation relative to the β-barrel lumen. (c,d) Residue-resolved binding pockets stabilizing Arg-5 and Arg-9, respectively. Positively charged residues lining the lumen (blue; e.g., ARG270, LYS305, LYS46) stabilize both peptides through electrostatic interactions with their backbone carbonyl oxygens. Aromatic residues such as PHE85 contribute via cation–π interactions with arginine side chains (e.g., PHE85 with Arg-9 ARG7). Tyrosine residues (TYR14, TYR58, TYR102, TYR106, TYR302) further stabilize binding through hydrogen bonding mediated by their phenolic OH groups, imparting directional specificity to peptide orientation. The longitudinal configuration of Arg-5 primarily engages TYR14, TYR102, and TYR106, whereas the more globular Arg-9 additionally recruits TYR58 and TYR302. Acidic residues such as ASP113 interact via their terminal carboxylate (COO^-) groups, reinforcing electrostatic complementarity. Backbone-mediated contacts involving GLY and LEU residues arise from interactions between their carbonyl oxygens and the peptide. Together, these interactions define peptide recognition within OmpF, with peptide length modulating orientation and contact distribution in the lumen.

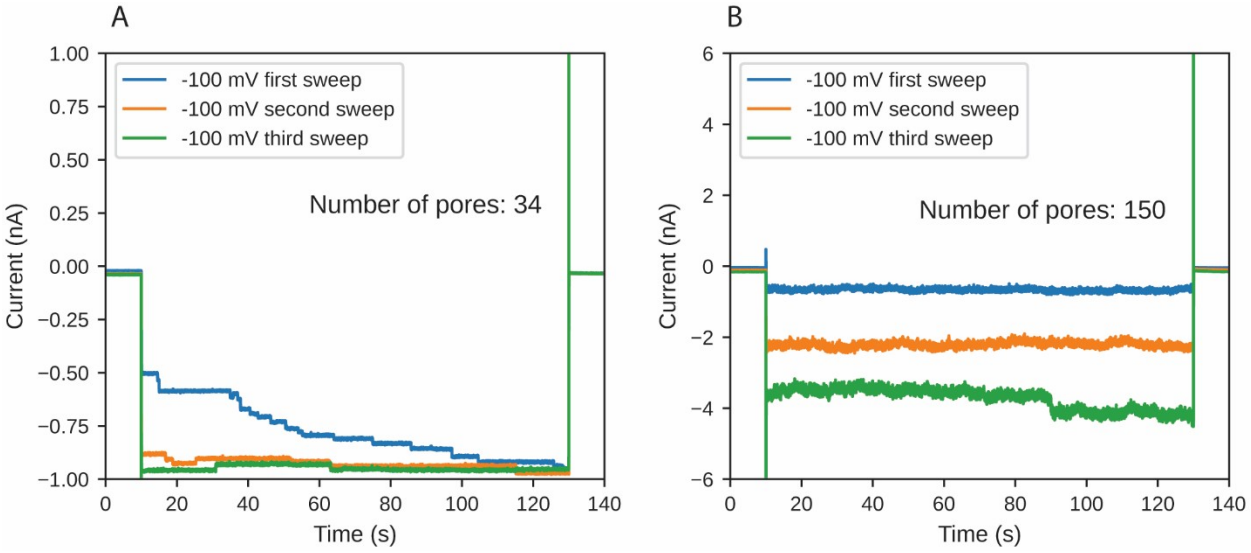

Figure S2 Current response to the three consecutive -100 mV sweeps (with wait time of 5 mins in between) for OmpF insertion corresponding to Figure 3. Number of pores inserted were calculated by calculating the total conductance during the last 5 seconds (125 to 130 sec in the plot) of 3rd -100 mV sweep and and then dividing this value by single channel OmpF conductance calculated as mentioned above. A. Pore insertion sweeps and number of pores in DIB system with OmpF. B. Pore insertion sweeps and number of pores of DIB system with OmpF and Arg-9 blocker molecules

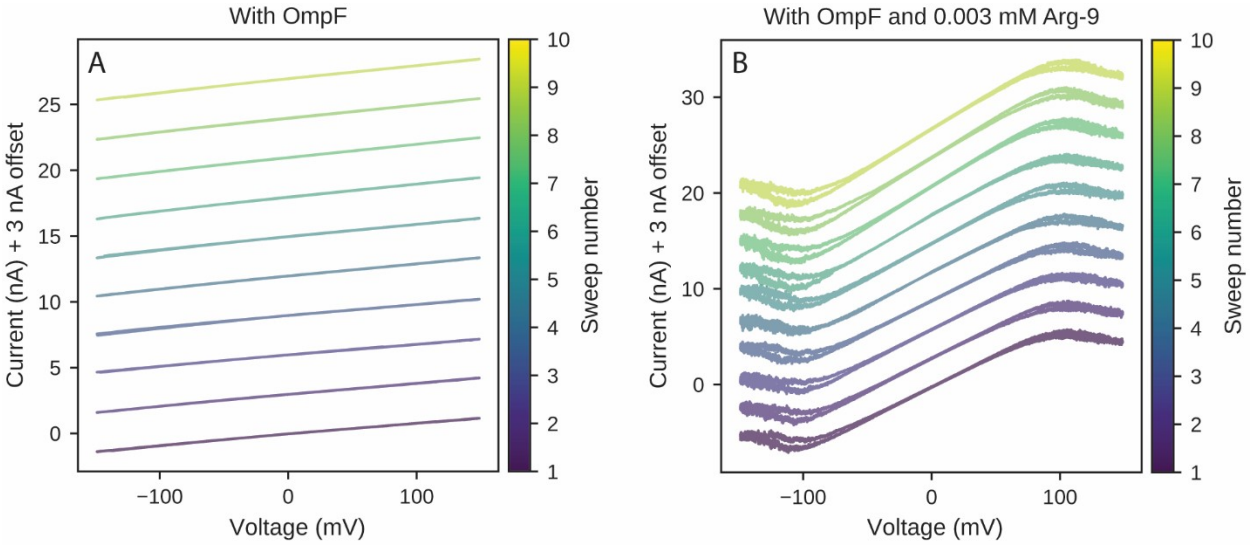

Figure S3 Sweep-wise variation in IV plot with zero-mean triangular voltage input for DIB system with A. OmpF alone, and B. OmpF and 0.003 mM Arg-9 indicating the consistent presence of pinched hysteresis in the presence of 0.003 mM Arg-9 molecules.

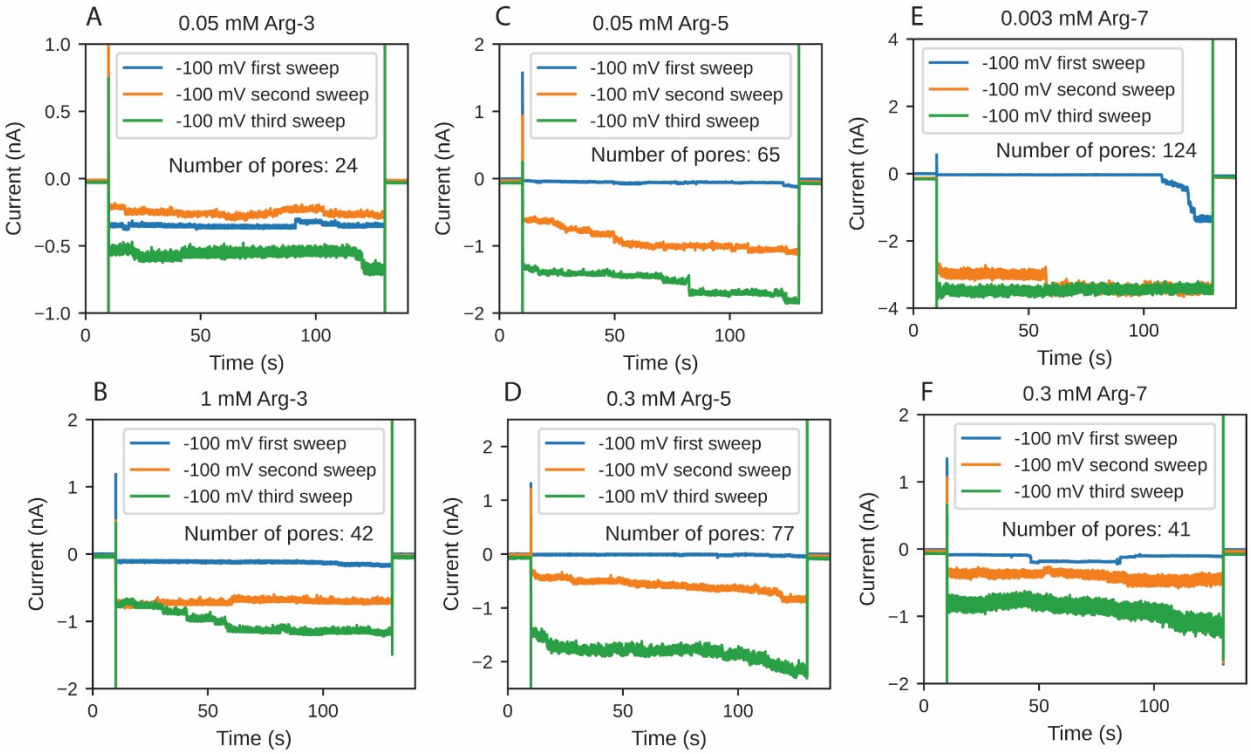

Figure S4 Current response to the three consecutive volage sweeps, where each sweep is 0 mV for 10 sec, -100 mV for 120 sec, and then 0 mV for 10 sec (with wait time of 5 mins in between each sweep) for OmpF insertion corresponding to Figure 4. Number of pores inserted were calculated as mentioned above. Pore insertion sweeps and number of pores in DIB membrane with OmpF and A. 0.05 mM Arg-3, B. 1 mM Arg-3, C. 0.05 mM Arg-5, D. 0.3 mM Arg-5, E. 0.003 mM Arg-7, F. 0.3 mM Arg-7

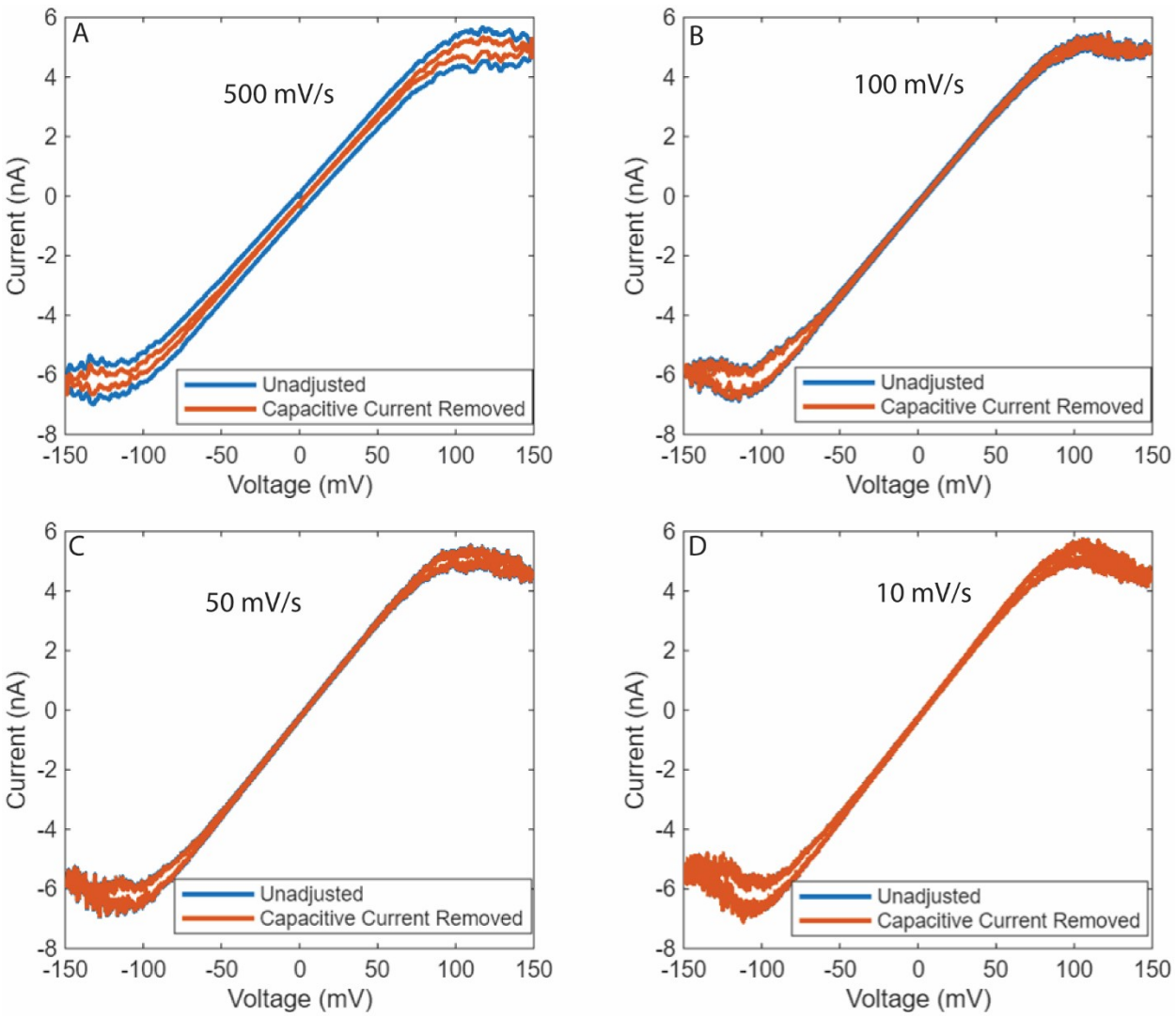

Figure 5 I-V sweeps with different sweep rates with 0.003 mM Arg-9. Both the total current (unadjusted) and the resistive current (capacitive current removed) are shown for each sweep rate. A. Sweep rate of 500 mV/s, B. Sweep rate of 100 mV/s, C. Sweep rate of 50 mV/s, D. Sweep rate of 10 mV/s

References:

(1) Ionescu, S. A.; Lee, S.; Housden, N. G.; Kaminska, R.; Kleanthous, C.; Bayley, H. Orientation of the OmpF Porin in Planar Lipid Bilayers. *ChemBioChem* **2017**, *18* (6), 554-562.