Unilateral Access Regulation: Ground State Dynamics of the

Pseudomonas aeruginosa Outer Membrane Efflux Duct OprM

SUPPLEMENTAL MATERIAL

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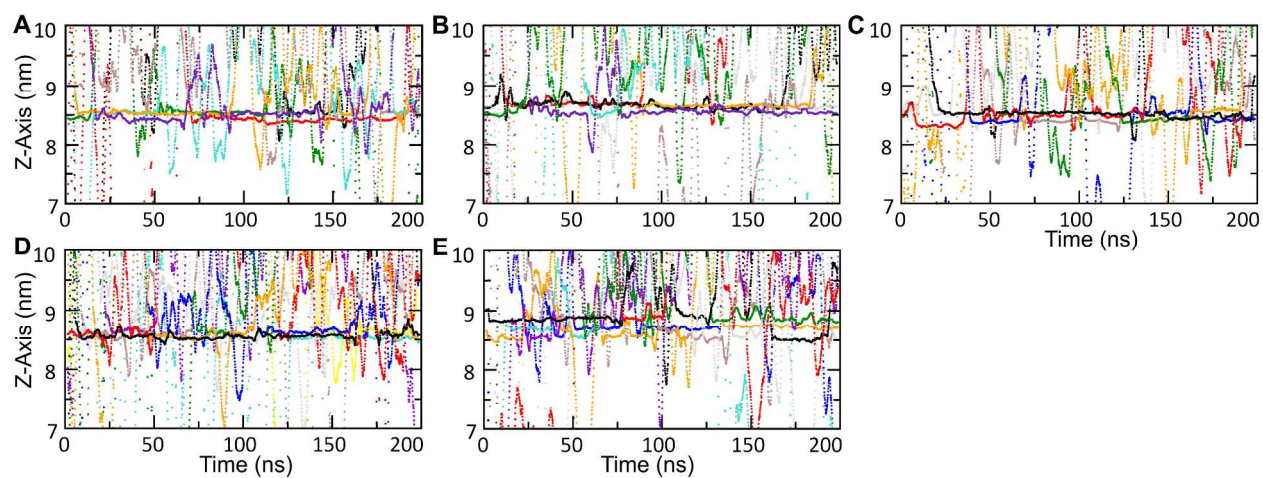
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Running title: OprM Gating

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Supplemental figure 1: Z trajectories of the sodium ions occupying the observed Asp171/Asp230 Na^+ binding sites in each OprM monomer. Once initial sodium binding has occurred during the first 40 ns, in all five independent runs (A-E) the binding sites remain occupied for the rest of the simulation time albeit individual sodium ions do exchange. Vertical gaps between the sodium traces in (E) are due to a slightly tilted orientation OprM adopts in this simulation.