

Identification of Electric-Field-Dependent Steps in the Na⁺,K⁺-Pump Cycle

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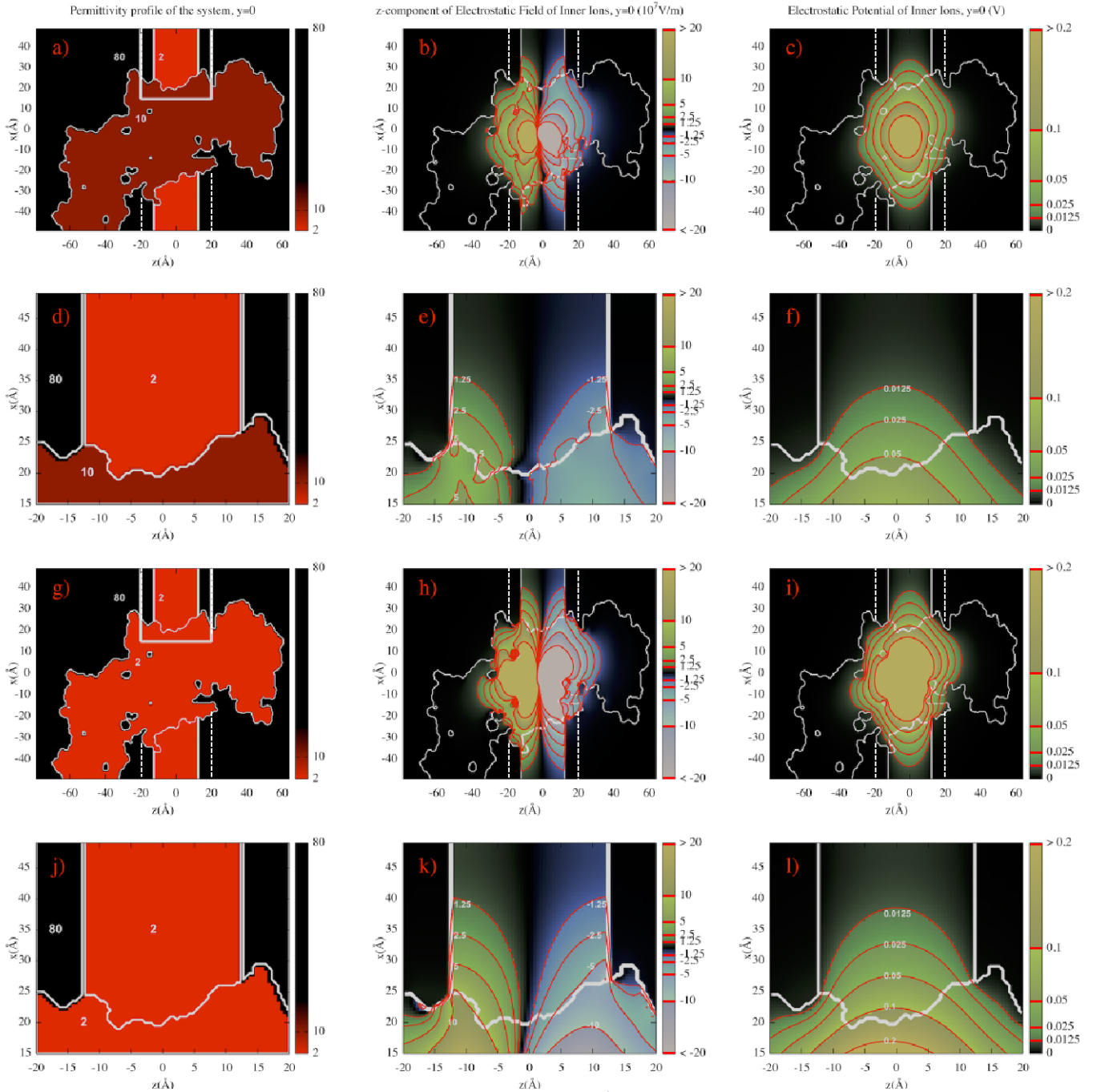


Figure S1. Electrostatics due to the binding of 2 K^+ ions to the for the 2ZX structure. Projections (in the plane, $y=0$) of the dielectric constant (relative permittivity), electric field and electrostatic potential are shown in the first, second and third columns, respectively. Panels a, b and c show values computed for $\epsilon_p = 10$, while panels g, h and i show results for $\epsilon_p = 2$. Rows 2 and 4 are zoomed views of rows 1 and 3, respectively. Contours are not evenly spaced but correspond to the tick marks on the right hand colour bars. Values for the electric field are limited to the range $-20:20 \text{ } 10^7 \text{ V/m}$, with lower values lower shown as -20 and higher values as 20 . Values for the electrostatic potential are truncated to 200mV , with higher values shown as 0.2V .

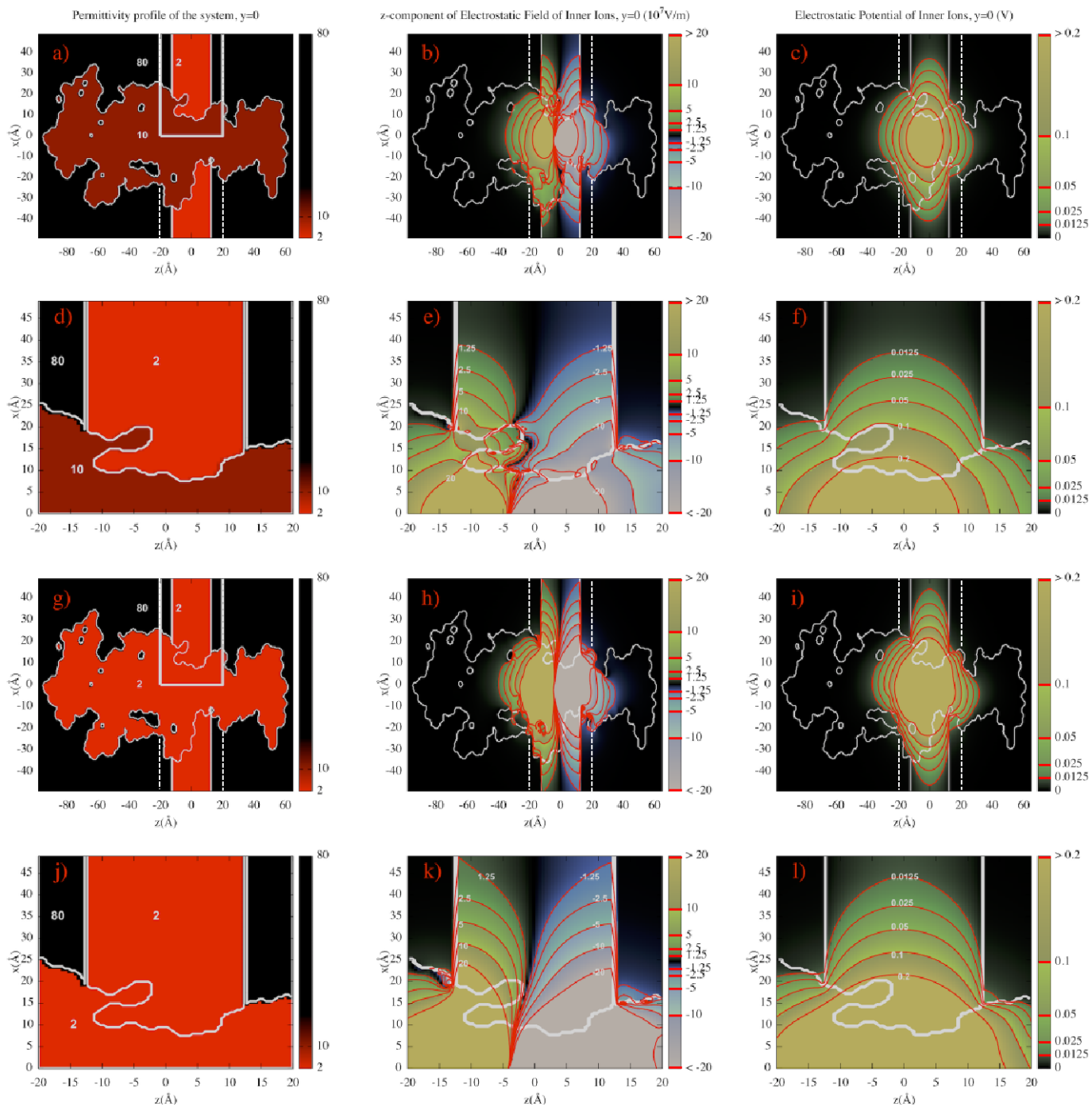


Figure S2. Electrostatics due to the binding of 3 Na^+ ions to the for the 3WGU structure, with details as in Fig.S1.

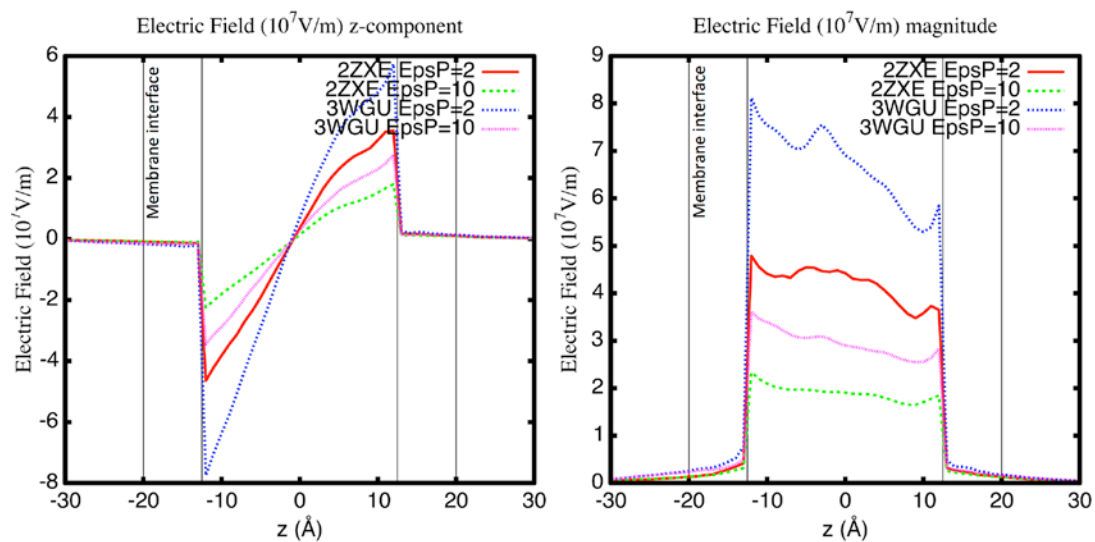


Figure S3. Average value of the electric field across the membrane outside the protein. Results are shown for the z -component (left) and the magnitude of electric field (right) as a function of z . The two curves per system correspond to the two different values of ϵ_p (EpsP) used. Vertical lines indicate the boundaries of the membrane interfacial region.