



Figure S1. MD simulations of M2TM' in a lipid bilayer. The backbone of the M2TM' protein is shown as a red cartoon, and lipid molecules are represented as sticks (hydrogen not shown), with the bilayer cut at the plane normal to the viewer that intersects the protein. (A), (B) and (C) show the configurations of the M2TM' system with +2 charge, at 0, 4, and 80 ns, respectively. (D), (E) and (F) show the same for the +3 charge. Note that the bundle in (C) and (E), but with its internal structure not altered. In (F), instead, the structure of the bundle is much more similar to the low pH structure of Stouffer *et al* (15) than to the intermediate pH structure of Acharya *et al* (23).