**Solvated Influenza A protein structures**

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Proton conduction in the M2 protein in the influenza viruses plays a major role in viral replication. Exploring the Protein Data Bank for the AM2 protein, the protein sequence in entry, 1NYJ, is chosen. Four configurations are generated in correspondence to the pH level based on Stouffer's work[1]. This work[1] identifies the open-state protein channel formed by replicating helix A as a good starting point for the low pH dominant equilibrium structure and the closed-state protein channel comprised of four rotated copies of helix D as a good candidate for the high pH dominant equilibrium structure. At neutral pH, the tetrameric bundles are made up of either helix B or C. VMD[2] and NAMD[3] programs let us visualize the M2 protein structures and perform molecular dynamics simulation using CHARMM36[4] force field. Water is added to the protein systems and modelled using TIP3P[5] in order to resemble the aqueous environment. Molecular dynamics is performed to find the equilibrium distribution of water molecules within the channels. In the future, we will analyze the equilibrium distribution of waters in the channels for hydrogen bonding.

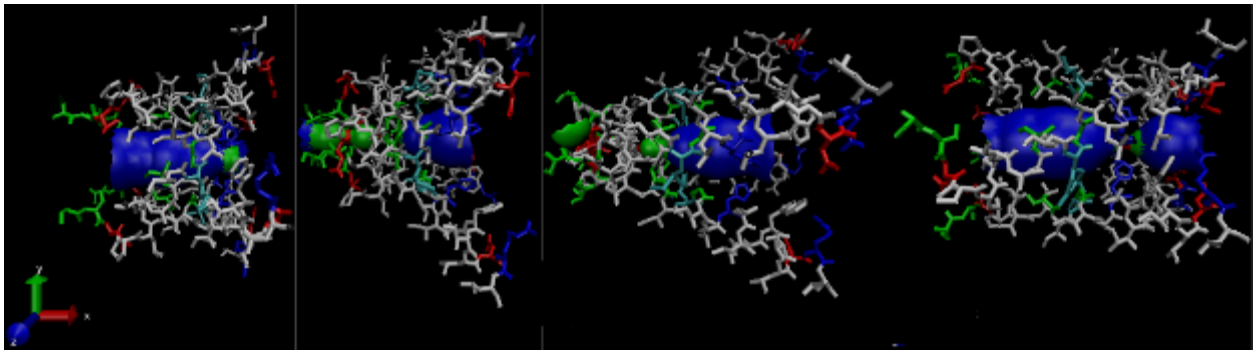

Figure 1: Four configurations of AM2 protein structure. From left to right, the pore channels are depicted from its open state to closed state corresponding to increasing pH

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