

Supplementary Information

Figure S1. The secondary structure profile of the pHLIP in the MD runs of (a) S (acidic) and (b) S (basic).

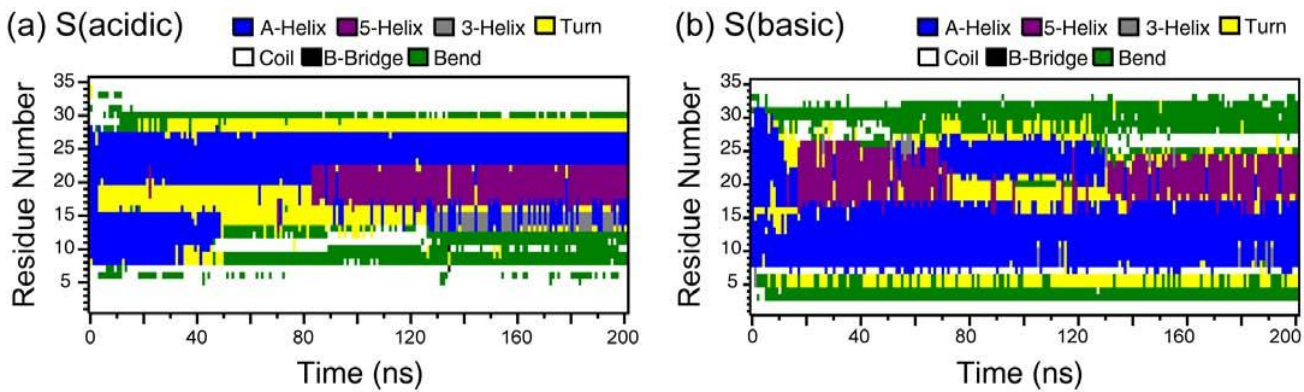


Figure S2. The secondary structure profile of the pHLIP in the MD runs of (a) P (acidic) and (b) P(basic).

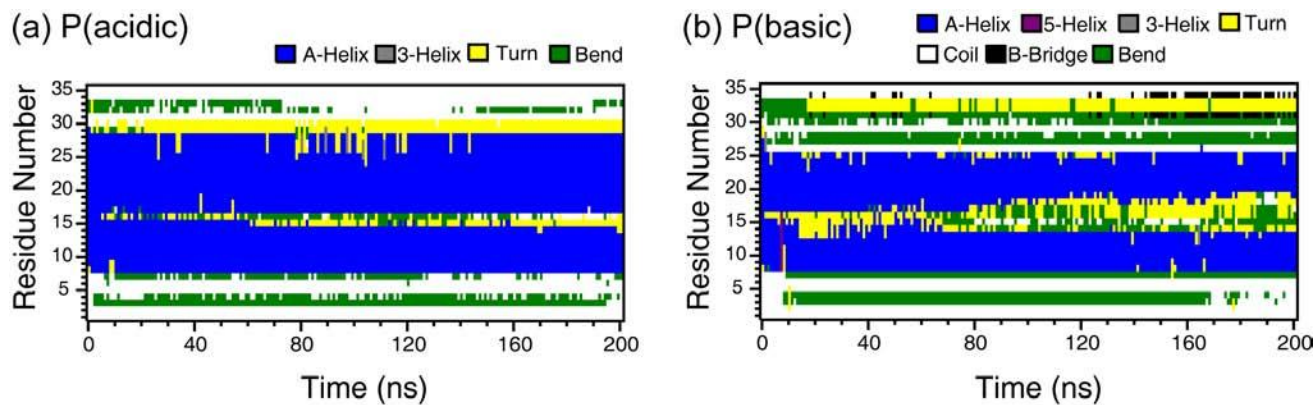


Figure S3. Characterization of the ordering of POPC bilayer in F system. (a) Time evolution of area per lipid and bilayer thickness in simulation F (acidic) (upper panel) and F (basic) (lower panel); (b) Time-averaged order parameter S_{CD} of sn-1 chain of POPC lipids over the last 50-ns of MD runs P (acidic) and P (basic). For comparison, the S_{CD} of sn-1 chain obtained from a 20 ns MD run for pure POPC lipid bilayer is also presented.

