Electronic Supplementary Material (ESI) for Soft Matter.

Towards designing globular antimicrobial peptide mimics: role of polar functional groups in biomimetic ternary antimicrobial polymers

Garima Rani[a,b], Kenichi Kuroda[c], and Satyavani Vemparala[a,b]

[a]The Institute of Mathematical Sciences, CIT Campus, Taramani, Chennai, India;
[b]Homi Bhabha National Institute, Training School Complex, Anushaktinagar, Mumbai 400094, India;
[c]Department of Biologic and Materials Sciences, School of Dentistry, University of Michigan, Ann Arbor, Michigan 48109, United States

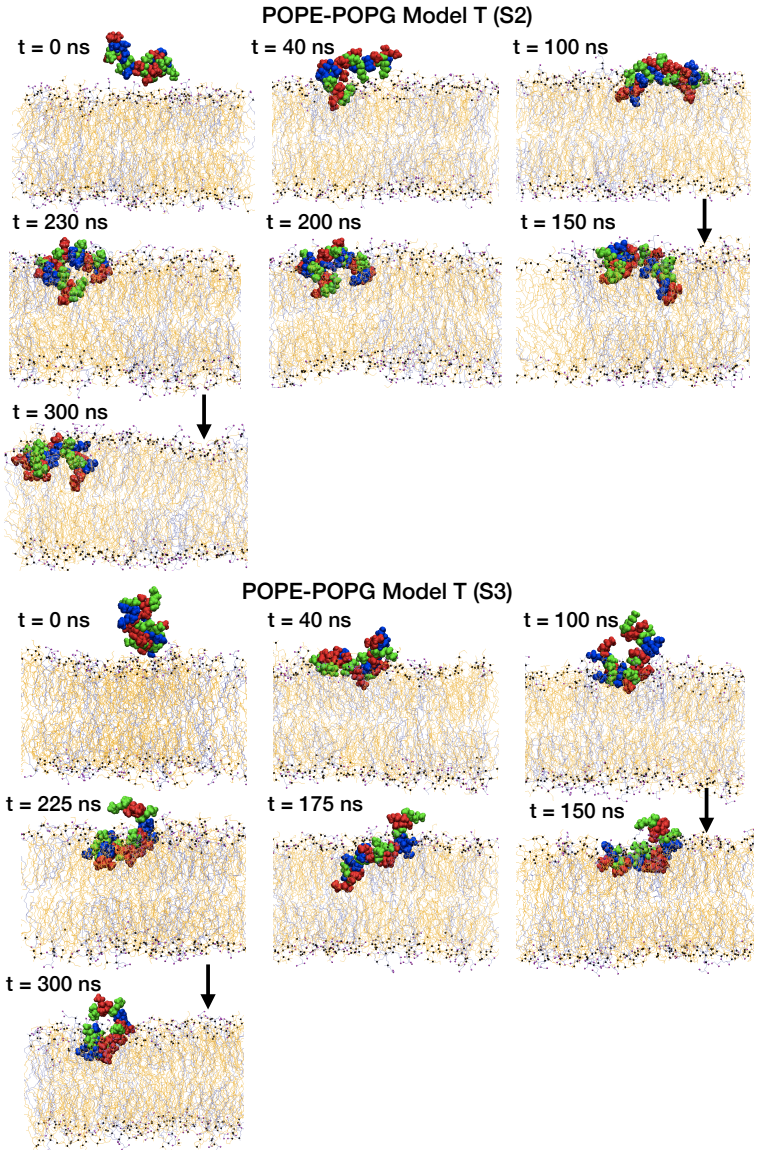

Figure 1: Representative snapshots of model T, interacting with the bacterial bilayer (systems S2 and S3). The POPE lipids are coloured orange and POPG lipids are shown in ice-blue colour; the lipid head groups are oxygen (magenta), nitrogen (cyan) and Phosphate (black). The cationic, hydrophobic and polar groups of the model polymers are shown in green, red and blue colour respectively.

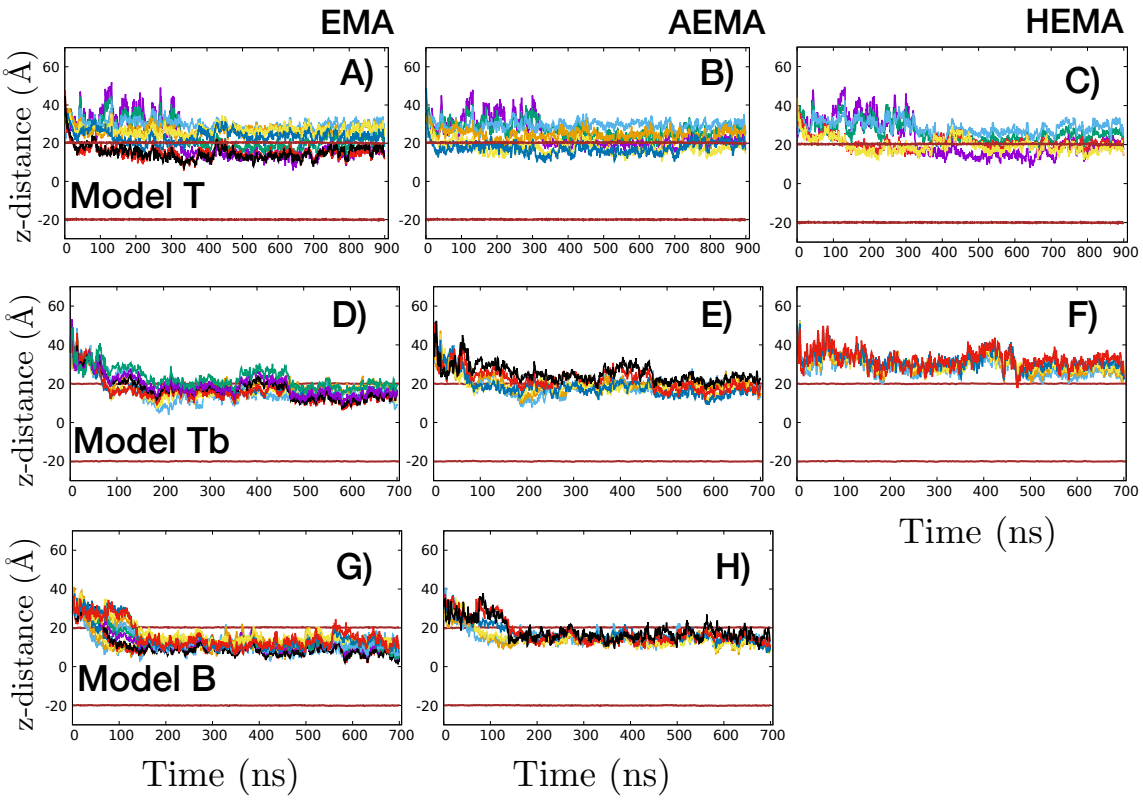

Figure 2: Evolution of center of mass (z-component) of hydrophobic, cationic and neutral polar groups for the three model polymers models - T (A, B,C), Tb (D, E, F) and B (G ,H). Brown lines denote the bilayer phosphate atoms. We note that here the different colors used each figure denote the different monomers of each functional group (for instance, the 8 different colors used in A denote the 8 different EMA monomers in the model T polymer).

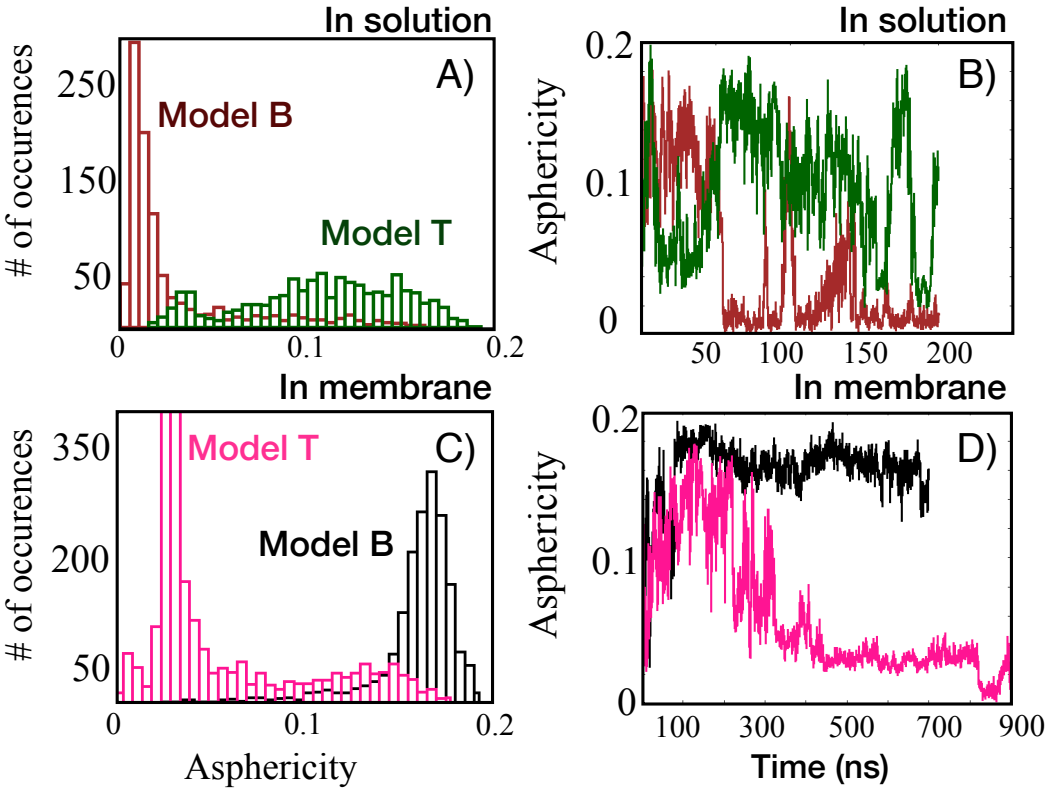

Figure 3: A) Distribution of asphericity (Δ), with data sampled over the entire trajectory, for polymer models T and B is shown in solution phase. B) Time evolution of Δ is shown for both the polymers in solution phase. C) Distribution of asphericity (Δ) for polymer models T and B is shown in membrane phase. D) Time evolution of Δ is shown for both the polymers in membrane phase.

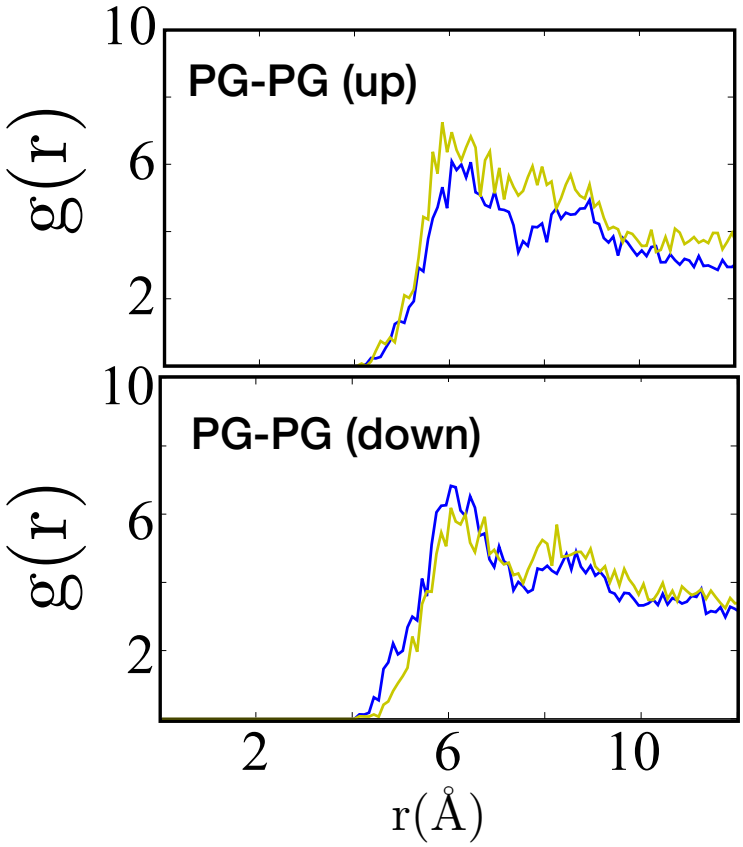

Figure 4: g(r) values measured between the phosphate groups of POPG-POPG lipids, averaged over 50 ns (650-700 ns) for the upper (denoted up) and lower leaflets (denoted down) of the model Tb polymer-membrane systems (yellow colour). For comparison, g(r) for membrane only system is shown in blue colour.