Selectivity and Mechanism of Fengycin, an Antimicrobial Lipopeptide from Molecular Dynamics

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Supplementary Information

Figure S1 shows that in the initial simulation time the probability of finding fengycins at a distance of 10Åwas higher in PC rather than in PE:PG. But initially there was also a chance of finding fengycins at longer distance (20 Å) in PE:PG but not in PC. This suggests that from early on fengycins has the inherent tendency to find each other in PC due to lack of electrostatic interactions with lipid head groups. On the other hand, fengycin's charged groups can be stabilized in PE:PG due to the abundance of hydrogen bond forming entities in the lipid head groups. Over time, the likelihood of finding another fengycin at 20Åalso increases even in PC which could be due to larger number of aggregates or occasionally displaced fengycin monomer from the aggregate.

Figure S2A is a plot of the average lifetime of a trimer (3-mer,three fengycins in an aggregate), pentamer (5-mer), and octamer(8-mer) in the two lipid systems (PC and PE:PG) and it is evident that 3-mers decay rapidly irrespective of the membrane system. However larger aggregates behave differently in the two membranes. According to Figure S2B, five-

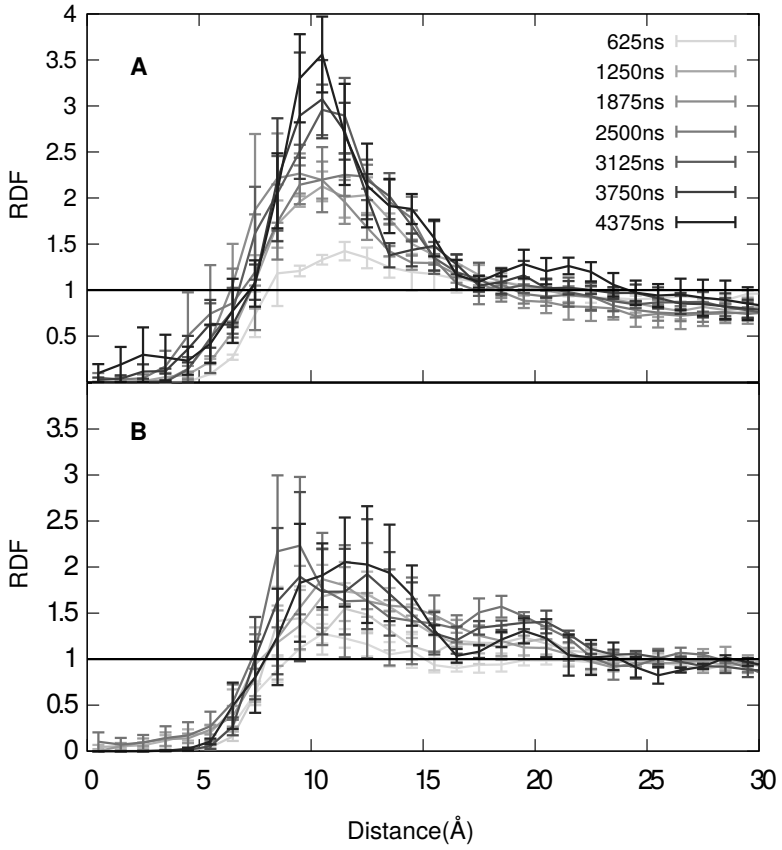

Figure S1: Time evolution of lateral radial distribution function between fengycins in (A)PC and (B)PE:PG. Distance between the lipopeptides is the x-axis, while the y-axis is probability density. The straight line at 1 represents the RDF value for a random distribution.

mers remain as an aggregate for a longer period of time in PC while they decay rapidly in PE:PG systems. Eight-mers found in PE:PG have a tendency to disintergrate fast as evident in S2C compared to the same in PC Another indication that larger aggregates have more stability in PC compared to PE:PG.

In addition, the variance in PC is high for the correlation coefficient of fengycin- aggregate disintegration while for PE:PG system, the same is low. This could be due to dislodging of one or two fengycins from the larger sized aggregates.

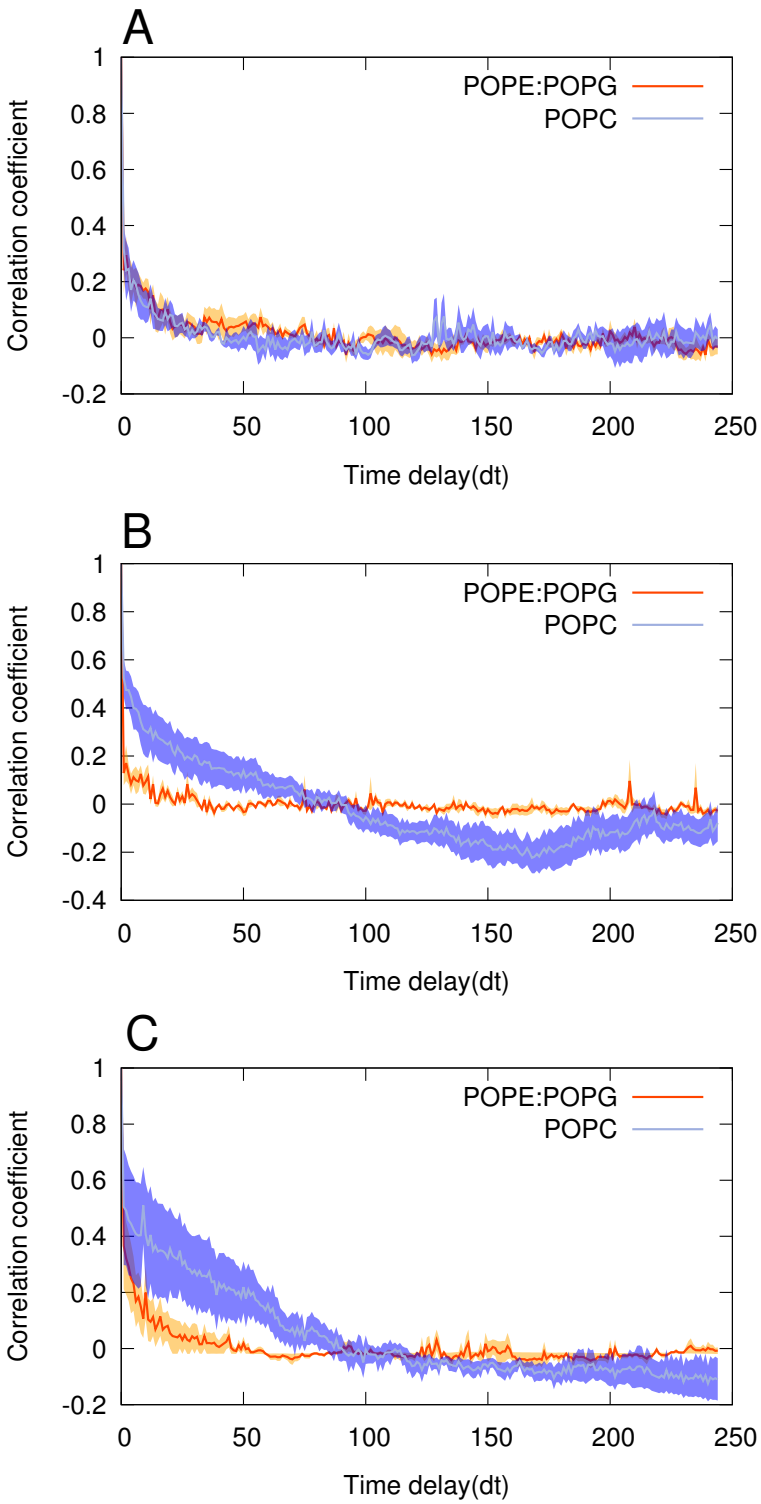

Figure S2: Lifetime of (A)3-mer (B)5-mer and (C)8-mer in the two membrane systems. Time delay is along the x-axis while auto-correlation coefficient is along the y-axis. The error bars represent the standard error by treating each replicate as a single measurement. Dark blue represents standard error in PC system while yellow represents the standard error in PE:PG.