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Computational Simulations of POPG Aggregates in presence of the Antimicrobial Peptide LL37

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Abstract: The antimicrobial peptide LL37 is the first amphipathic alpha-helical peptide isolated from human cells. It is part of the first line of defense against local infection and systemic invasion of pathogens at sites of inflammation. LL37 has antibacterial and anti-biofilm activities, being also significantly resistant to proteolytic degradation in solution. Preliminary SAXS data suggest that LL37 destabilizes 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoglycerol (POPG) bilayers and induce the formation of a different aggregate structure. We have performed MD simulations at the coarse-grained level of the antimicrobial of LL37 in POPG bilayers and vesicles to investigate potential POPG aggregate arrangements. These data are further mapped back into atomistic models and compared the SAXS measurements. The MARTINI force-field [1,2] was used in conjunction with the GROMACS v4.6.7 software package.[3] The CG membrane bilayer was built with the INSANE script [4] and the CG vesicle with the PACKMOL software.[5] The systems were energy-minimized and solvated with CG water molecules and 150 mM of NaCl, followed by a second round of energy minimization and equilibration for 2 μs under *NpT* conditions. We analyze and discuss structural properties derived from these simulations to argue in support of one given aggregate arrangement.

Key-words: phase transition, membrane hydration, diffusion coefficients

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