Supplementary material

Comparative analysis of a POPC bilayer and a DPC micelle comprising an interfacial anchored peptide using all-atom MD simulations

Nahuel PERROT,¹ Adriana ISVORAN,*² Pierre NÉDELLEC,^{3,4} Nadège JAMIN³ AND Veronica BESWICK,^{3,4}

¹Department of Medicine, Division of Hematology/Oncology, Beth Israel Deaconess Medical Center, Boston, USA

²Department of Biology - Chemistry and Advanced Environmental Research Laboratories, Faculty of Chemistry, Biology, Geography, West University of Timisoara, Timisoara, Romania

³Institute for Integrative Biology of the Cell (I2BC), CEA, CNRS, Université Paris-Saclay, F-91191 Gif-sur-Yvette cedex, France

⁴ University of Evry-val-d'Essonne, Department of Physics, F-91025 Evry, France

*To whom correspondence should be addressed: adriana.isvoran@e-uvt.ro

Figure S1: Chemical structure and numbering of DPC (dodecylphosphocholine) (a) and POPC (1-palmitoyl-2-oleoyl-*sn*-glycero-3-phosphatidylcholine) (b) heteroatoms and the atomic representations of the DPC (c), micelle (d), POPC (e) and flat-bilayer (f).









d



e



Figure S2: Radial distributions of different atoms of DPC molecules over the course of the simulation. The nitrogen, the two carbons (C11 and C12) and the phosphorus atoms of the head group are presented as well as the different carbons of the acyl chain.



Figure S3: 2-dimensional contact maps between peptide side chains and DPC. A) DPC nitrogen atom. B) DPC phosphorus atom. C) DPC first acyl chain segment (C21-C26). D) DPC second acyl chain segment (C25-C210). E) DPC third acyl chain segment (C29-C212).

*Lifetime is correlated to the number of consecutive frames for which the distance criteria is satisfied (See Methods for its definition).





Figure S4: 2-dimensional contact maps between peptide side chains and POPC. A) POPC nitrogen atom. B) POPC phosphorus atom. C) POPC glycerol atoms (C1, C2 and C3). D) POPC first palmitoyl chain segment (C31-C37). E) POPC second palmitoyl chain segment (C36-C312). F) POPC third palmitoyl chain segment (C311-C316). G) POPC first oleoyl chain segment (C21-C27). H) POPC second oleoyl chain segment (C26-C212). I) POPC third oleoyl chain segment (C211-C218).

*Lifetime is correlated to the number of consecutive frames for which the distance criteria is satisfied (See Methods for its definition).



