sciendo

DOI: 10.2478/auoc-2023-0016

Ovidius University Annals of Chemistry Volume 34, Number 2, pp. 121 - 131, 2023

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 NÉDELEC,[3,4] Nadége JAMIN,[3] and Veronica BESWICK[3,4]

[1]*Department of Medicine, Division of Hematology / Oncology, Beth Israel Deaconess Medical Center, Boston, USA*
[2]*Department of Biology-Chemistry and Advanced Environmental Research Laboratories, West University of Timisoara, Timisoara, Romania*
[3]*Institute 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*

Abstract. Biological membranes are complex systems due to their composition and dynamics. Therefore, membrane mimetics are widely used to investigate lipid properties and interactions between molecules and membrane lipids. Using all-atom molecular dynamics simulations, within this study two systems composed of different membrane mimetics are compared: a 1-palmitoyl-2-oleoyl-3-glycero-phosphatidylcholine (POPC) bilayer or a dodecylphosphocholine (DPC) micelle and a nonapeptide (V94-T-K-Y-W-F-Y-R-L102). Previous ^{1}H-NMR experiments have demonstrated that, in the presence of DPC micelles, this peptide folds as a stable amphipathic helix located in the polar head group region with the tryptophan residue pointing toward the inside of the micelle. The present comparison reveals a hydrophobic surface twice as large for the micelle as for the bilayer and a different arrangement of the acyl chains. The peptide secondary structure is not strongly affected by the membrane mimetics whereas the peptide is more deeply inserted in the bilayer than in the micelle. The contacts between the peptide and the DPC or POPC molecules are analysed and although the distances and lifetimes of these contacts are very different in the micelle and the bilayer, similar specific interactions were found that mainly involved the side chains of the residues R101 and L102.

***Keywords*:** membrane; interactions peptide-lipids; secondary structure; dynamics.

[*] Corresponding author. *E-mail address:* adriana.isvoran@e-uvt.ro (Adriana Isvoran)