

β -BARREL-SURFACTANT STABILIZATION STUDIES BY MOLECULAR DYNAMICS.

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Membrane proteins have been extensively studied due to their potential role as antigens, virulence factors and other important biological relevancies. For decades, the structural determination of membrane proteins (MPs) has been an important challenge in structural biology due to their embedment in the lipid bilayer.¹⁻³ Experimentally, detergents are used to isolate MPs by mimicking the properties of the membrane, allowing even the in vitro refolding of these proteins.⁴ This strategy has recently been used to create biomedical platforms constructed by immobilizing MPs that form channels and pores in matrixes made of synthetic organic polymers.⁵ These are operative composites that regulate the diffusion of alkali ions. Majority of experiments are performed in polar systems but MPs lose their properties in these conditions and require surfactants as protective agents creating an hydrophobic environment surrounding the protein. Then, protein-surfactant interaction plays an important role in the stabilization of the protein in aqueous solution or even in these biologically-uncommon constructions. In this work, molecular dynamics simulations with a β -barrel porin (a MP) in presence of “gentle” non-denaturing alkyl sugar detergent such as dodecyl maltoside.⁶ In order to understand the behavior of the surfactant in the stabilization of MPs, simulations have been performed in systems with different concentration and organization of detergent. Results successfully show how the structure, and therefore the function of the porin, is kept when in contact with surfactants and the protein denaturalizes in absence of them.

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