L Reunión Anual de la Sociedad Argentina de Biofísica

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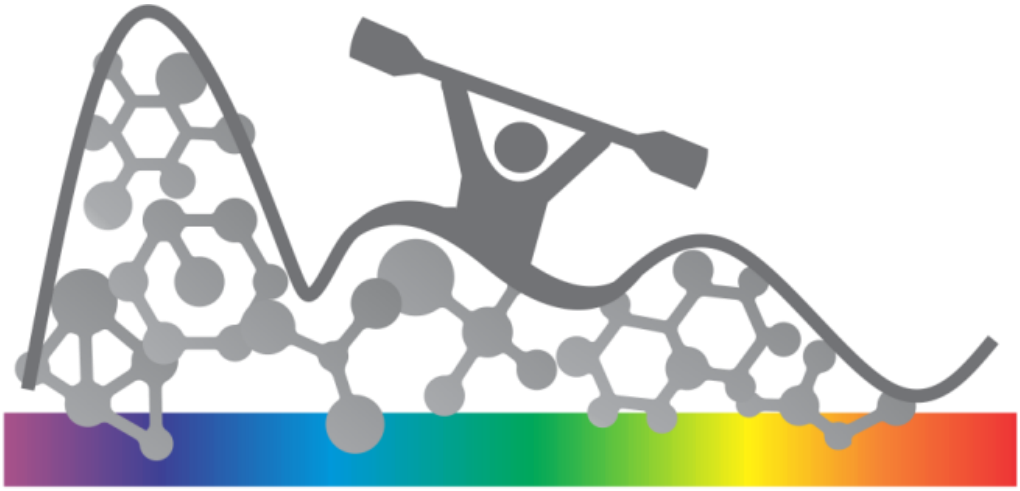

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16-18 Noviembre 2022

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16-18 November 2022

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Cholesterol effects on α7-nAChR embedded in POPC bilayer.

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Nicotinic acetylcholine receptors (nAChRs) are ligand-gated ion channels (LGIC) made up of five transmembrane glycoprotein subunits organized pseudosymmetrically around a central pore or channel. They can adopt three main conformational states, in addition to several other intermediate states: a closed (C) or resting (R) state, an open (O) state that occurs after agonist binding, and a desensitized (D) state that occurs after the continued presence of the agonist. Subtle changes in the lipid environment of the nAChRs have great relevance in their activity, causing significant effects on human biology. Two types of lipid positions can be identified for these lipids: annular and non-annular. Non-annular sites are in close contact with the receptor and have a low replacement rate, while the annular ones are further away, with a higher replacement rate. In this work, we use a receptor model based on a known structure (PDB: 7EKI) inserted in a lipid bilayer composed entirely of 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) lipids. Lipids at annular sites of the membrane were replaced by cholesterols, obtaining different lipid environments for the receptor. Atomistic Molecular Dynamics were performed for the receptor and the membrane with various combinations of these cholesterols. Physicochemical properties of the membrane and the receptor were analyzed and compared with the results obtained for the control system, which lacks cholesterol molecules.

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