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Exploring 3D structure of human gonadotropin hormone receptor at antagonist state using homology modeling, molecular dynamic simulation, and cross-docking studies

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Human gonadotropin hormone receptor, a G-protein coupled receptor, is the target of many medications used in fertility disorders. Obtaining more structural information about the receptor could be useful in many studies related to drug design. In this study, the structure of human gonadotropin receptor was subjected to homology modeling studies and molecular dynamic simulation within a DPPC lipid bilayer for 100 ns. Several frames were thereafter extracted from simulation trajectories representing the receptor at different states. In order to find a proper model of the receptor at the antagonist state, all frames were subjected to cross-docking studies of some antagonists with known experimental values (Ki). Frame 194 revealed a reasonable correlation between docking calculated energy scores and experimental activity values ($|r|=0.91$). The obtained correlation was validated by means of stratum-specific likelihood ratios (SSLR) and showed the presence of no chance correlation for the obtained model. Different structural features reported for the receptor, such as two disulfide bridges and ionic lock between GLU90 and LYS 121 were also investigated in the final model.

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