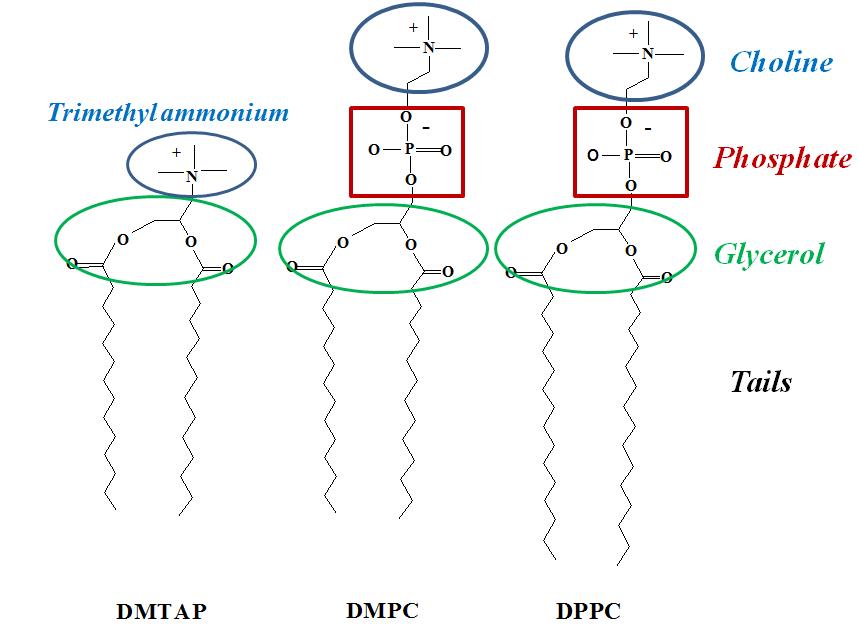
Supporting information

**Molecular insight into the mutual interactions of two transmembrane domains of Human Glycine Receptor (TM23-GlyR), with the lipid bilayers**

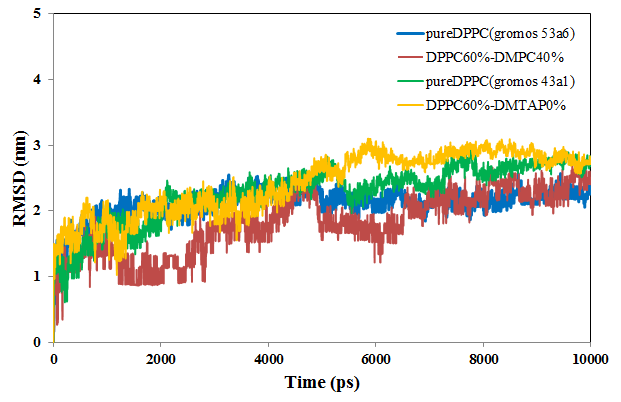
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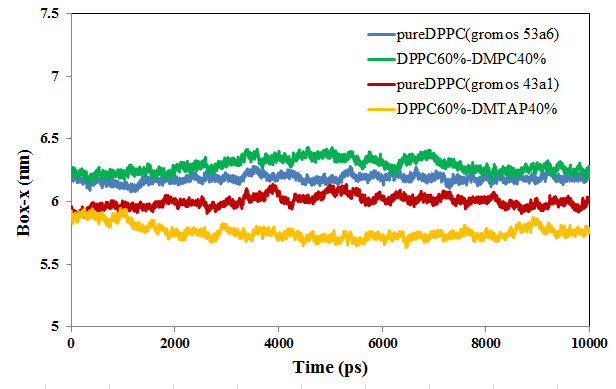
**Email** : [d\_aghaie@sutech.ac.ir](mailto:d_aghaie@sutech.ac.ir)

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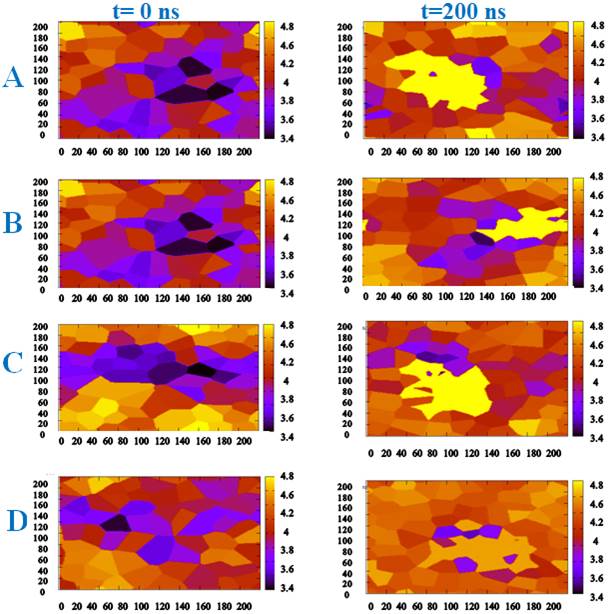
**Figure S1**. Chemical structures of the three studied lipids. Oxygen atoms in the phosphate and glycerol regions are the hydrogen bond acceptor sites.



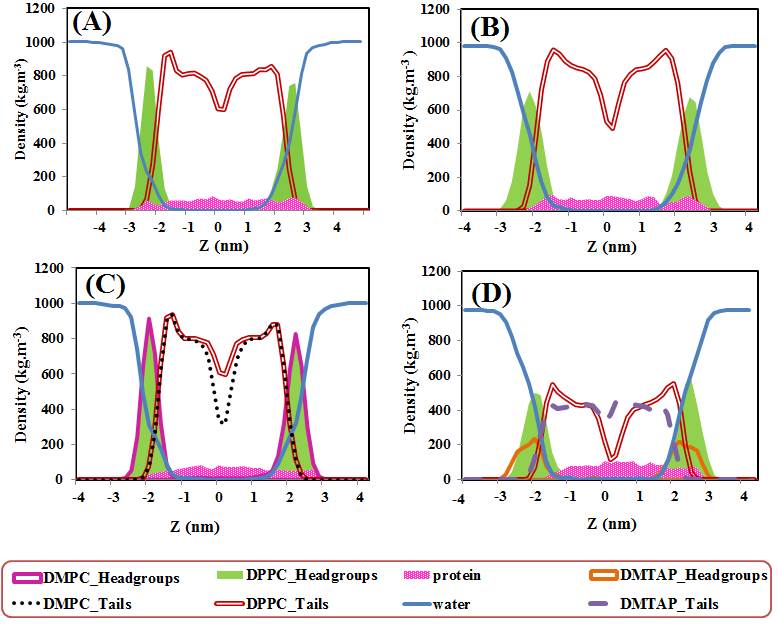
**Figure S2.** RMSD plots of DPPC molecules for systems, **1:** pure DPPC (GROMOS 53A6), **2**: pure DPPC (GROMOS 43A1), **3:** (DPPC60%-DMPC40%) and **4:** (DPPC60%-DMTAP40%).



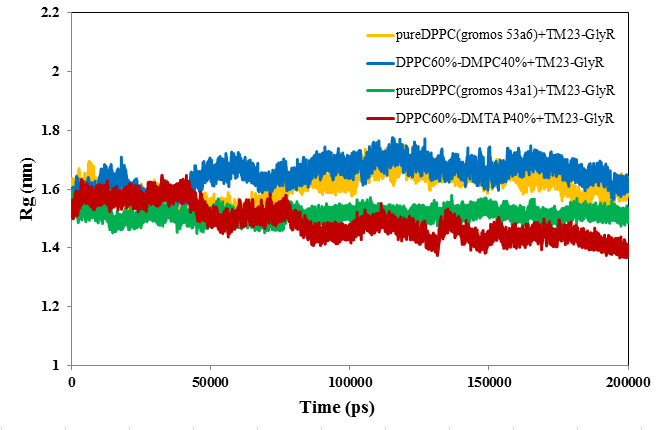
**Figure S3.** Box-x length of the simulation box for systems, **1:** pure DPPC (GROMOS 53A6), **2:** pure DPPC (GROMOS 43A1), **3:** (DPPC60%-DMPC40%) and **4:** (DPPC60%-DMTAP40%).

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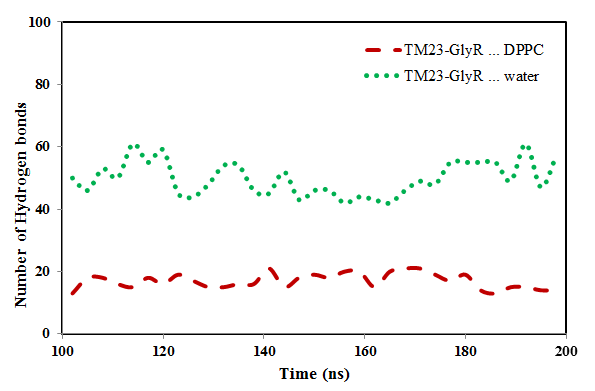
**Figure S4.** Membrane Thickness contour plots of protein-containing systems, **A**) **System** **5**, Pure DPPC (GROMOS 53A6) + TM23-GlyR, **B**) **System** **6**, Pure DPPC (GROMOS 43A1) + TM23-GlyR, **C**) **System** **7**, (DPPC60%-DMPC40% + TM23-GlyR), **D**) **System** **8**, (DPPC60%-DMTAP40% + TM23-GlyR), at the beginning (t=0 ns) and end (t=200 ns) of simulation runs. The legend shows bilayer thickness (nm), mapped to the corresponding colors.

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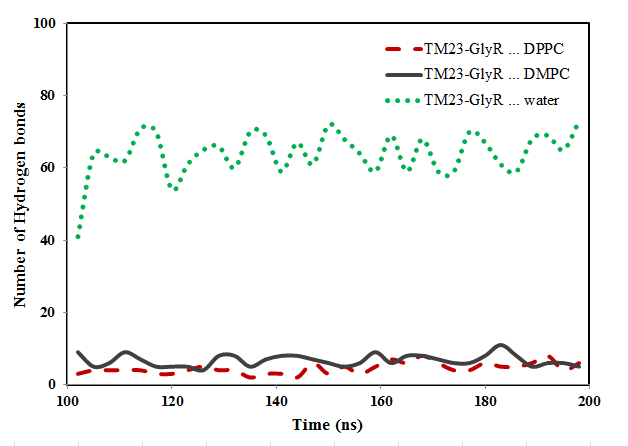
**Figure S5.** Density profiles of membrane components, along the membrane normal direction, obtained from the trajectories of protein containing systems, **A**) **System** **5**, Pure DPPC (GROMOS 53A6) + TM23-GlyR, **B**) **System 6**, Pure DPPC (GROMOS 43A1) + TM23-GlyR, **C) System** **7**, (DPPC60%-DMPC40%+TM23-GlyR), **D) System** **8**, (DPPC60%-DMTAP40% + TM23-GlyR).



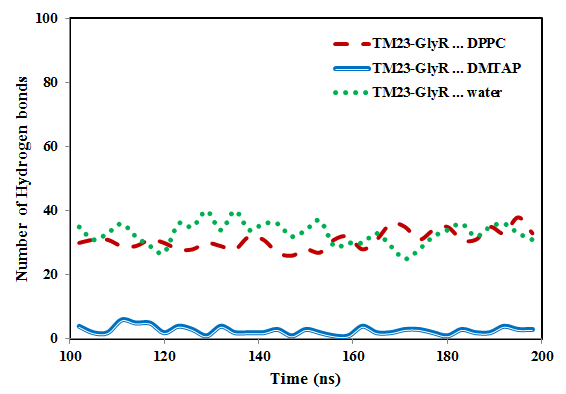
**Figure S6.** The Rg plots of TM23-GlyR membrane protein in systems: **5**, [Pure DPPC (GROMOS 53A6) + TM23-GlyR], **6**, [Pure DPPC (GROMOS 43A1) + TM23-GlyR], **7**, [DPPC60%-DMPC40% + TM23-GlyR], and **8**, [DPPC60%-DMTAP40% + TM23-GlyR], over 200 ns simulation time.



**Figure S7.** Number of hydrogen bonds of DPPC and water molecules with TM23-GlyR, in system 5, [pure DPPC (GROMOS 53A6) + TM23-GlyR] over last 100 ns.



**Figure S8.** Number of hydrogen bonds of DPPC, DMPC and water molecules with TM23-GlyR, in system 7, [DPPC60%-DMPC40%+TM23-GlyR] over last 100 ns.



**Figure S9.** Number of hydrogen bonds of DPPC, DMTAP and water molecules with TM23-GlyR, in system **8**, [DPPC60%-DMTAP40%+TM23-GlyR] over last 100 ns.