Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The Interactions of Aβ Protofibril with Cholesterol Enriched Membrane and Involvement of Neuroprotective Cabazolium Based Substances

Hedayat Karimi,[1] Maryam Heydari Dokoohaki,[1] Amin Reza Zolghadr[1]*, Mohammad Hadi Ghatee[1]

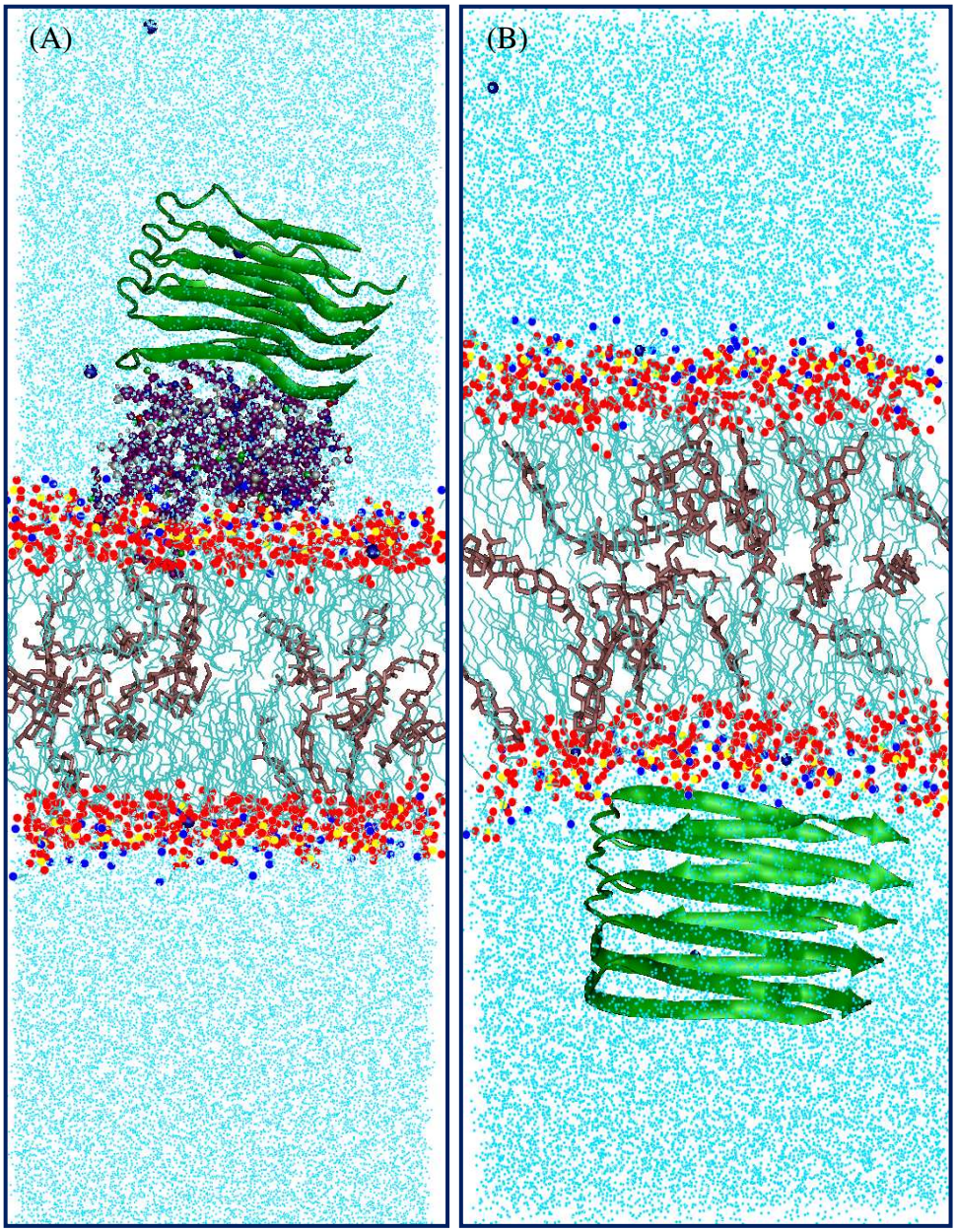

Fig. S1. The snapshot of two independent simulations A) Aβ peptide on lipid bilayer and B) Aβ peptide and P7C3-S243 on lipid bilayer.

1 *Department of Chemistry, Shiraz University, Shiraz, 71946-84795, Iran*

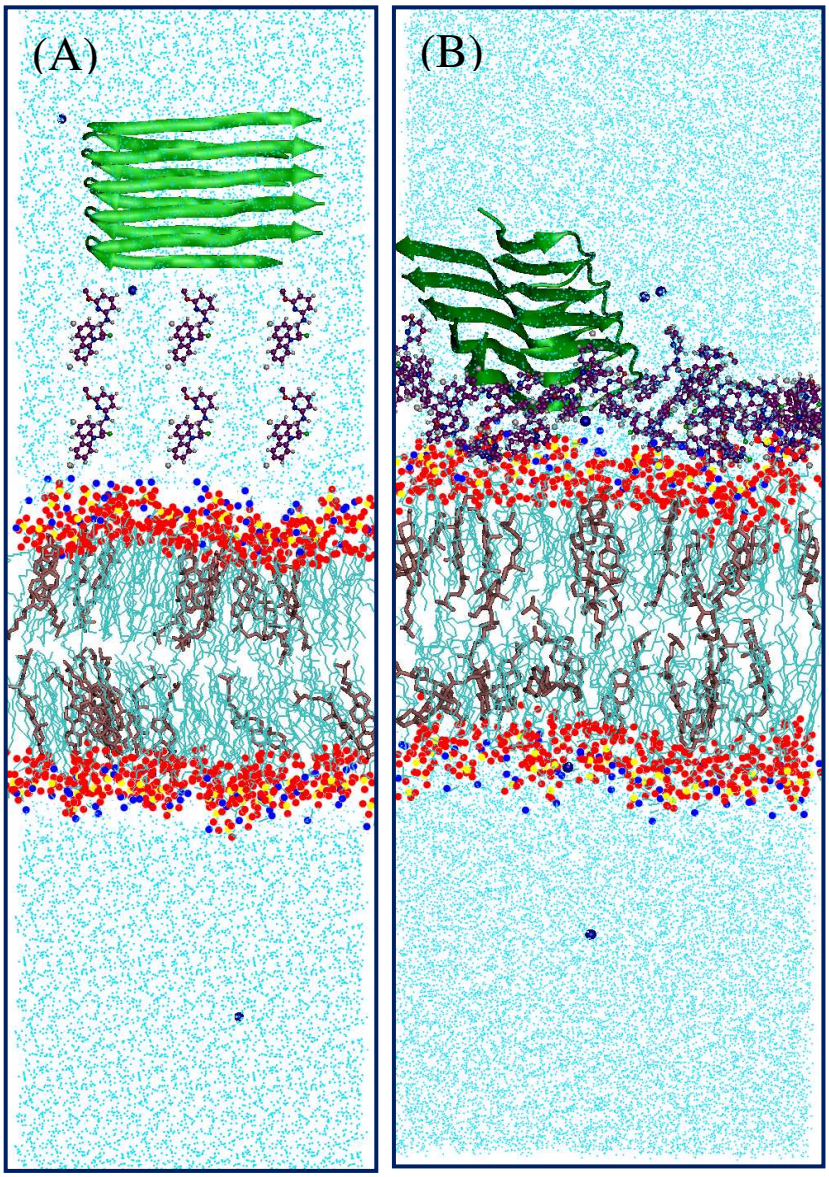

Fig. S2. Snapshot of a simulation with another orientation of the drug candidate. A) initial structure and B) equilibrated structure.

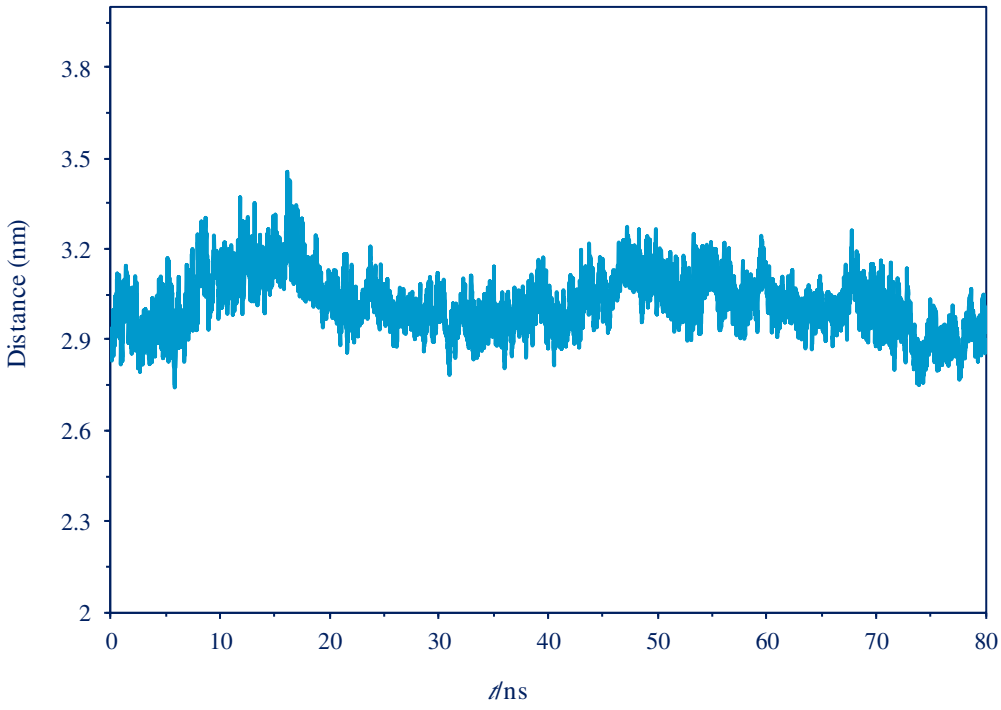

Fig. S3. The evolution of distance between the center of down leaflet of bilayer and Aβ amyloid (down zone) in the last of 80 ns of the simulation.

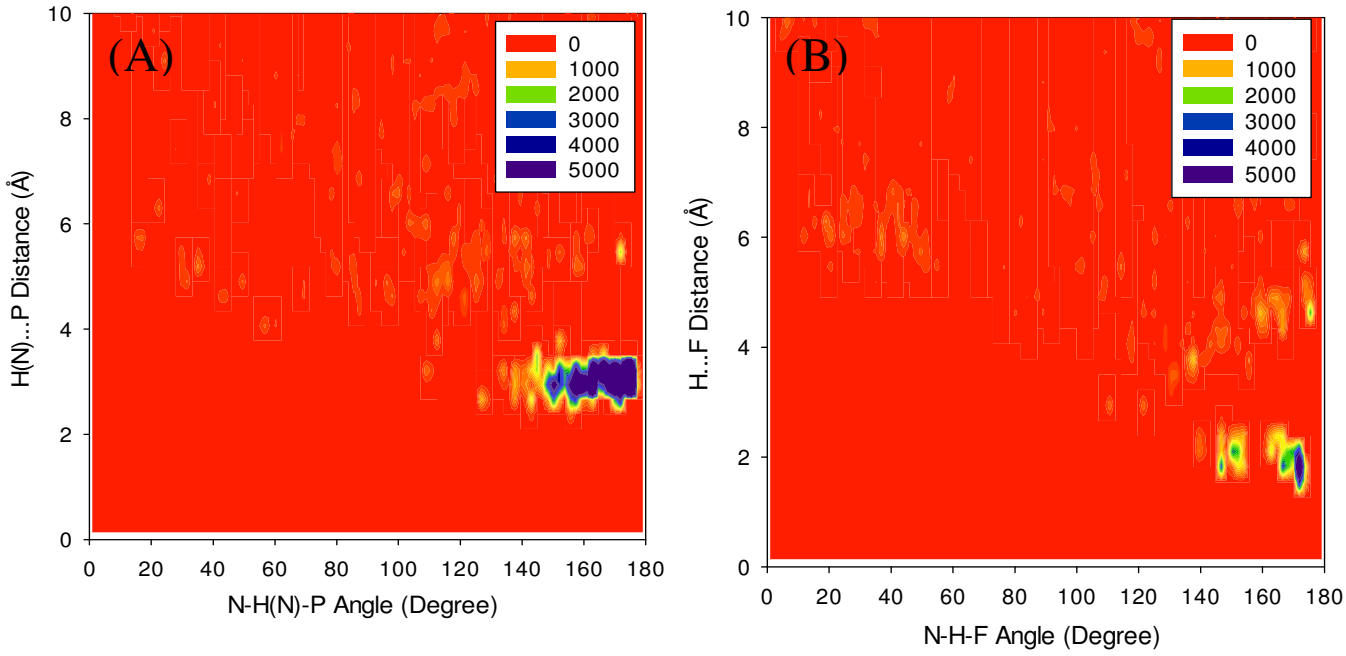

Fig. S4. The combined radial/angular distribution functions of the drug candidate with (A) POPC, and (B) oligomer.

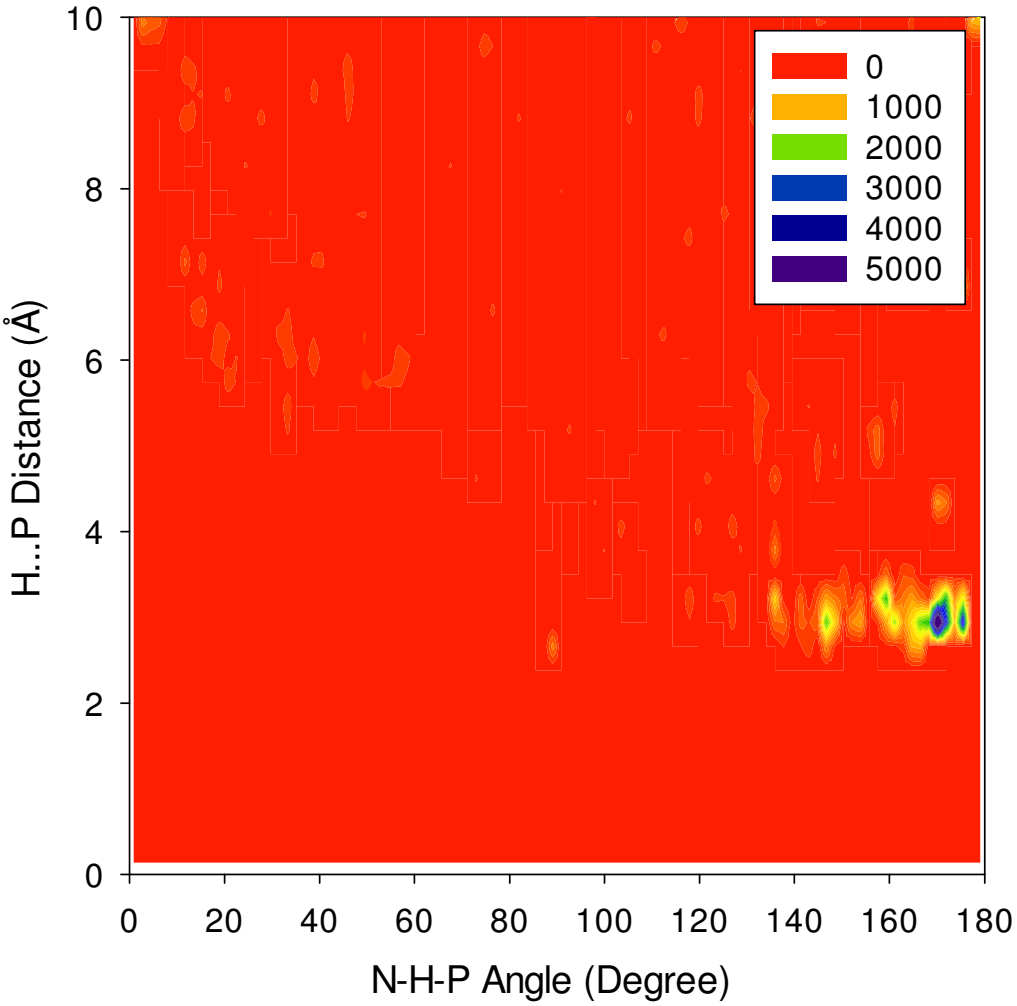

Fig. S5. Combined radial/angular distribution functions for investigation of interactions between Aβ amyloid oligomer and the lipid bilayer in the presence of drug candidate (upper leaflet).