Potential Anti-Alzheimer Agents From Guanidinyl Tryptophan Derivatives with Activities of Membrane Adhesion and Conformational Transition Inhibitions

Supplementary Materials

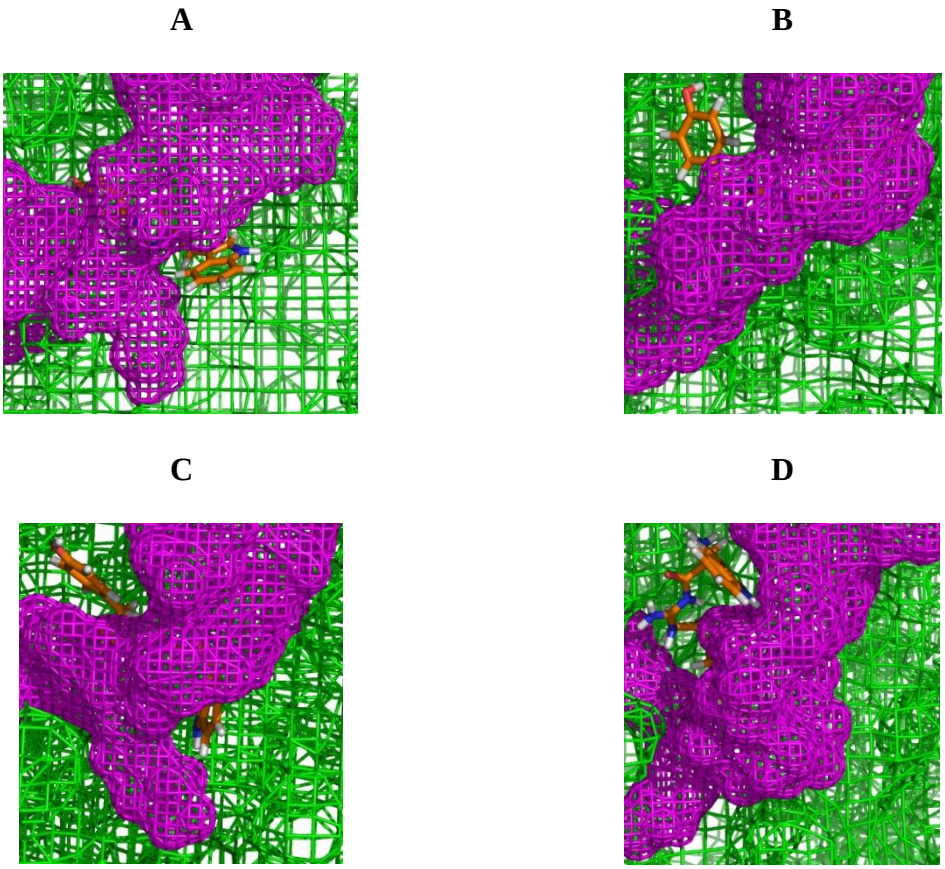

Figure S1. Closed views of the complexes of $A\beta_{1-42}$ monomers and (A) TGN1, (B) TGN2, (C) TGN3, and (D) TGN4 on the upper-layer surfaces of the POPC membranes. The $A\beta_{1-42}$ monomers, ligands, and POPC membranes are shown in magenta-mesh, orange-stick, and green-mesh representations, respectively.

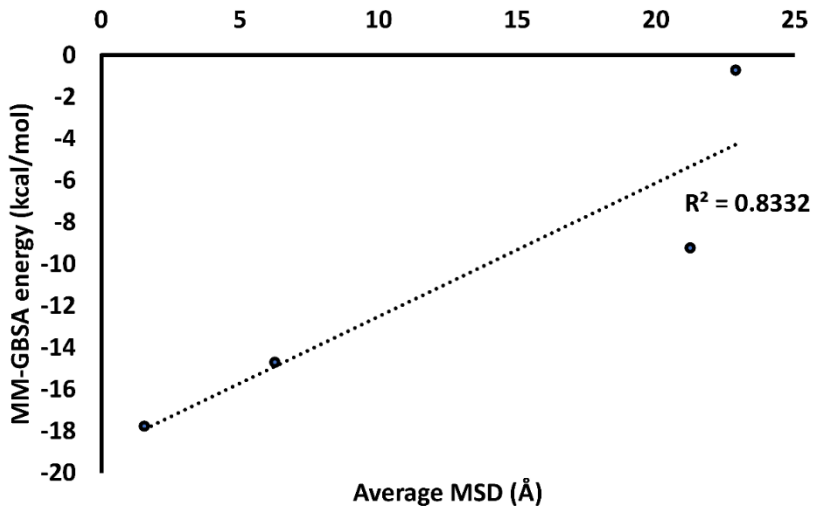

Figure S2. Correlation between the MM-GBSA scores and the MSD values of TGN1, TGN2, TGN3, and TGN4.

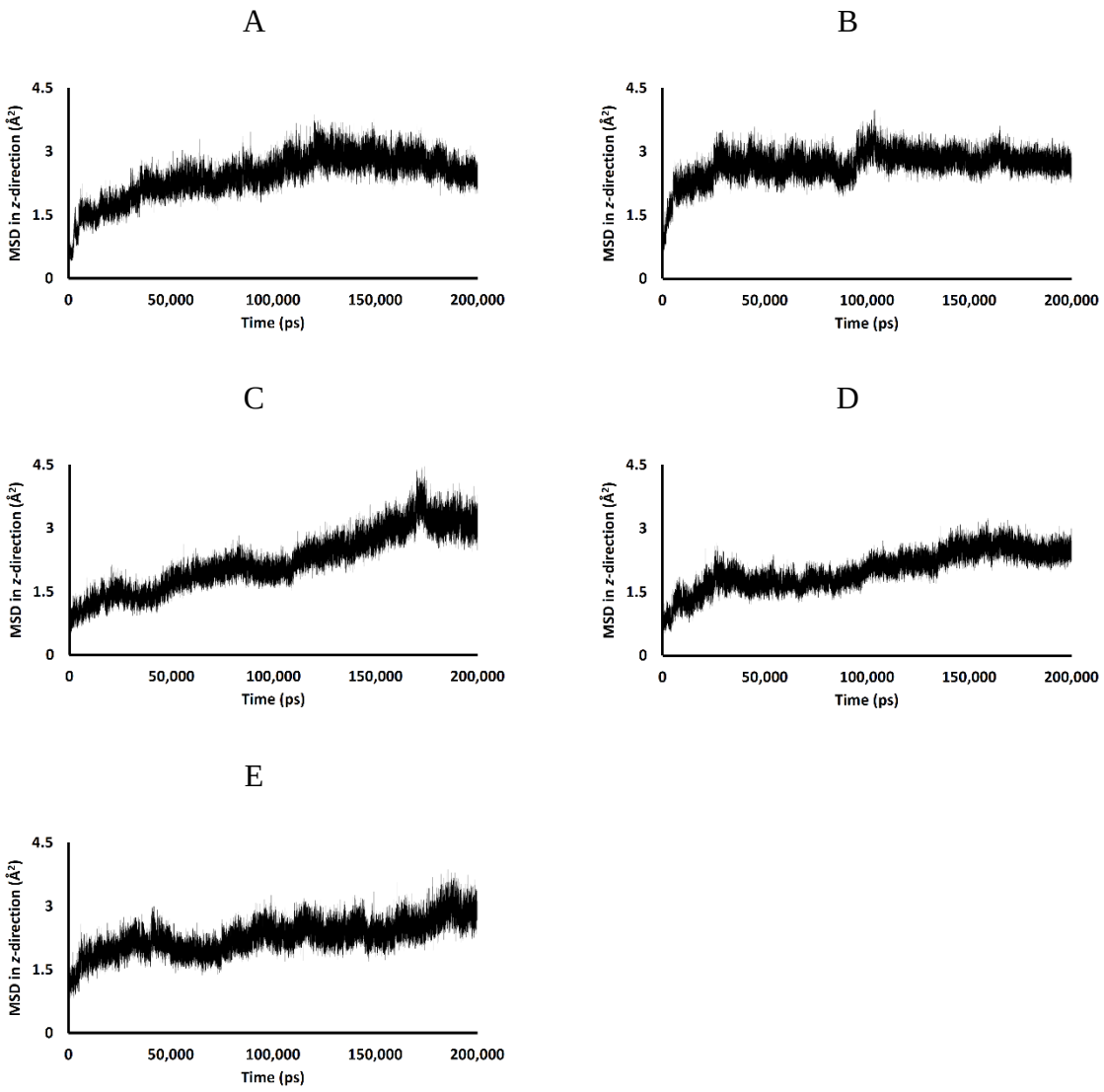

Figure S3. The mobilities in the z-direction of the $A\beta_{1\text{-}42}$ monomer structures in (A) TGN1, (B) TGN2, (C) TGN3, (D) TGN4, and (E) no ligand (only monomer) models in the POPC membranes are shown as MSD on the ps timescale.