

Supplementary Information

Inhibitory effect of hydrophobic fullerenes on the β -sheet-rich oligomers of hydrophilic GNNQQNY peptide revealed by atomistic simulations

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This material contains six supplemental figures.

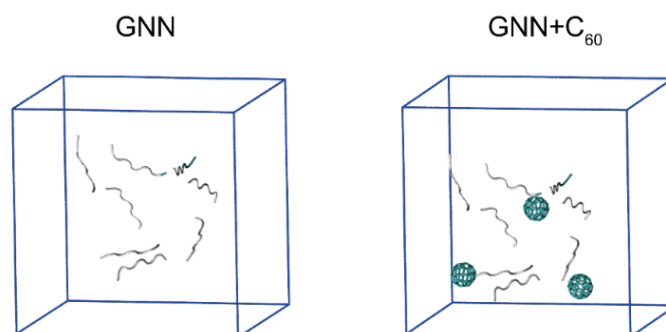


Figure S1. The initiating state for the GNN and GNN+C₆₀ systems.

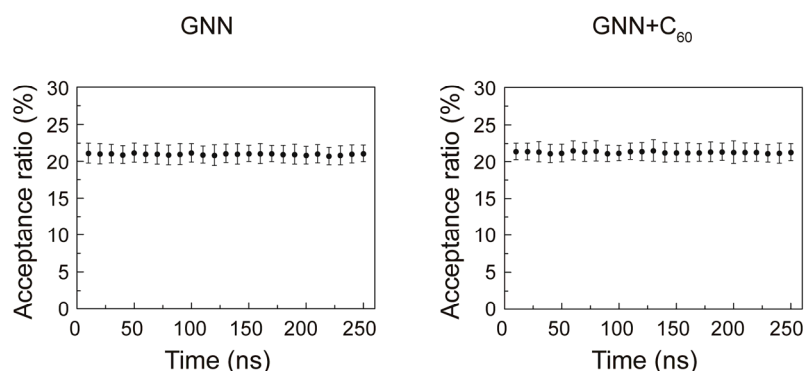


Figure S2. Average acceptance ratio of the REMD simulation for the GNN and GNN+C₆₀ systems. The acceptance ratios are $\sim 21\%$ for both GNN and GNN+C₆₀ systems.

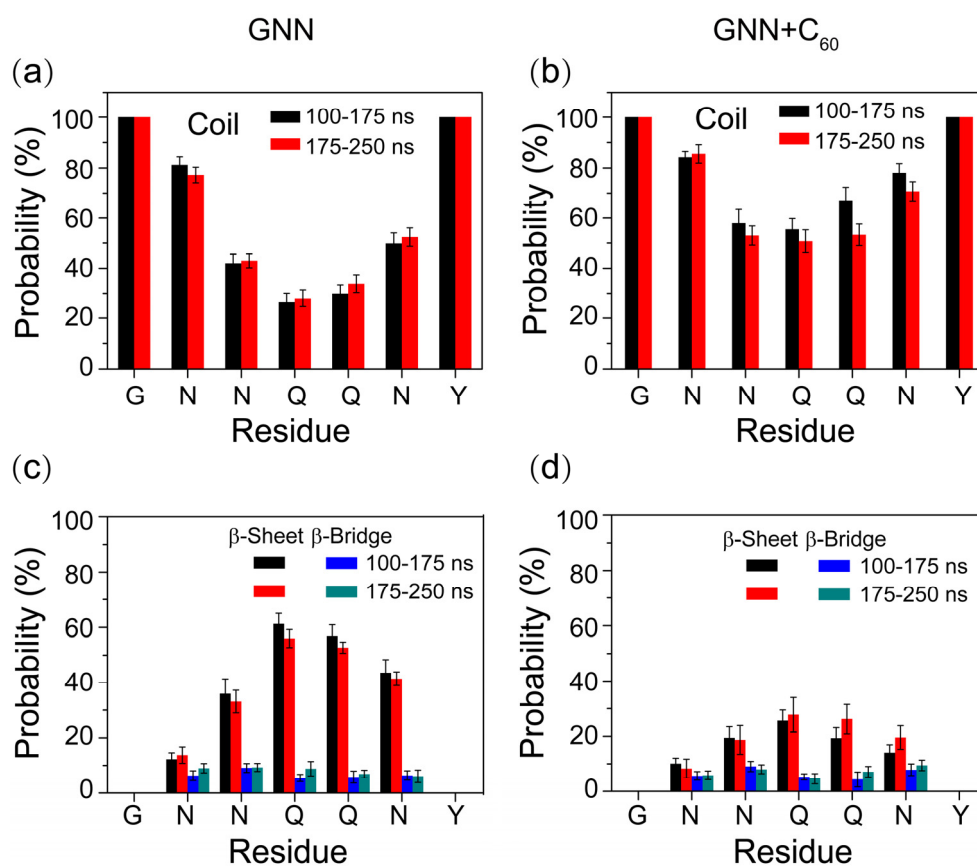


Figure S3. Secondary structure (coil (a, b), β -sheet and β -bridge (c, d)) probability of each residue calculated using the 100-175 ns and 175-250 ns REMD data for GNN and GNN+C₆₀ systems.

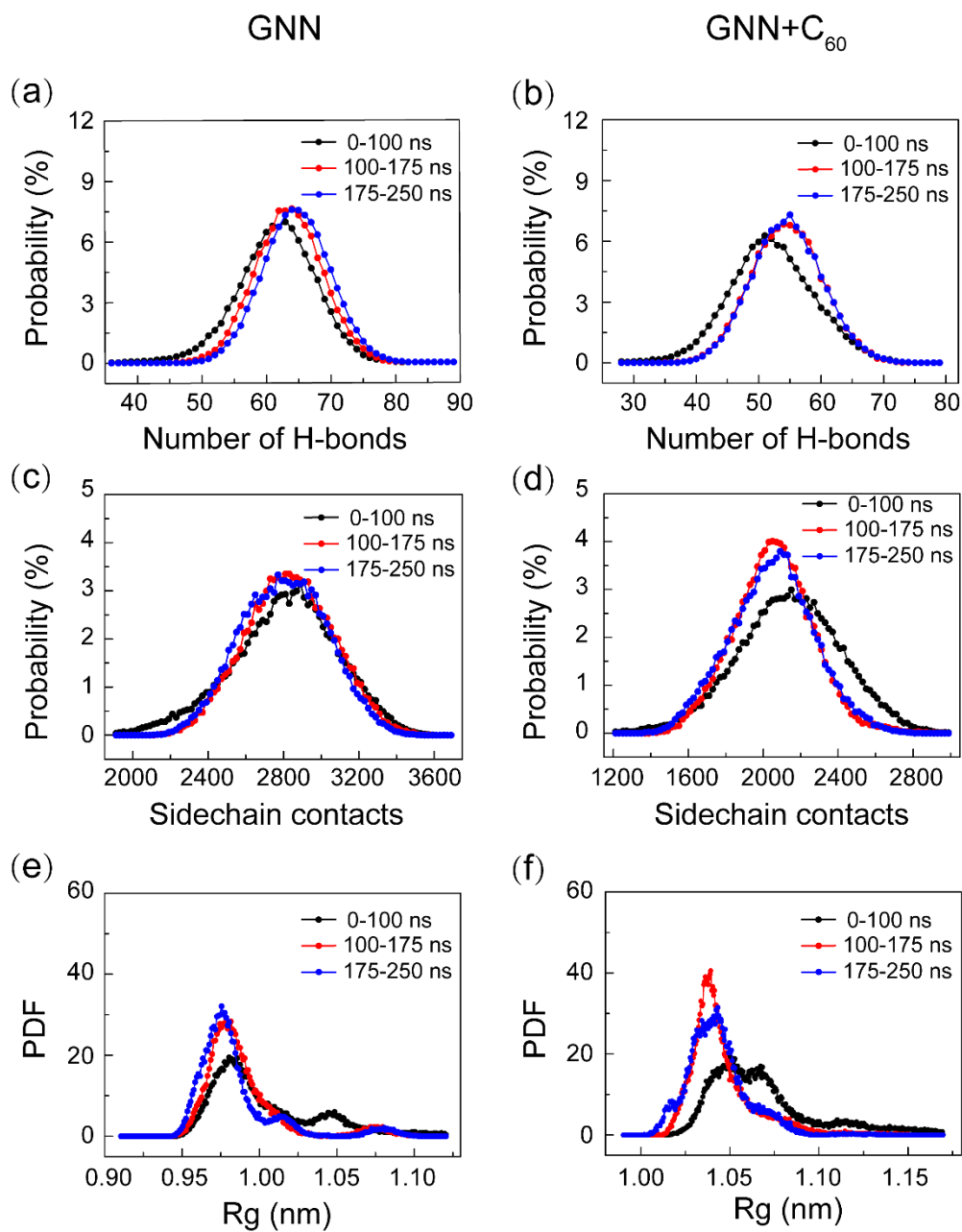


Figure S4. The distribution of total number of H-bonds (a, b), sidechain contact number (c, d) and radius of gyration (e, f) of the octamers within two different time intervals using the 150-200 ns and 200-250 ns data for GNN and GNN+C₆₀ systems. For comparison, we also added the results using the first 100 ns data.

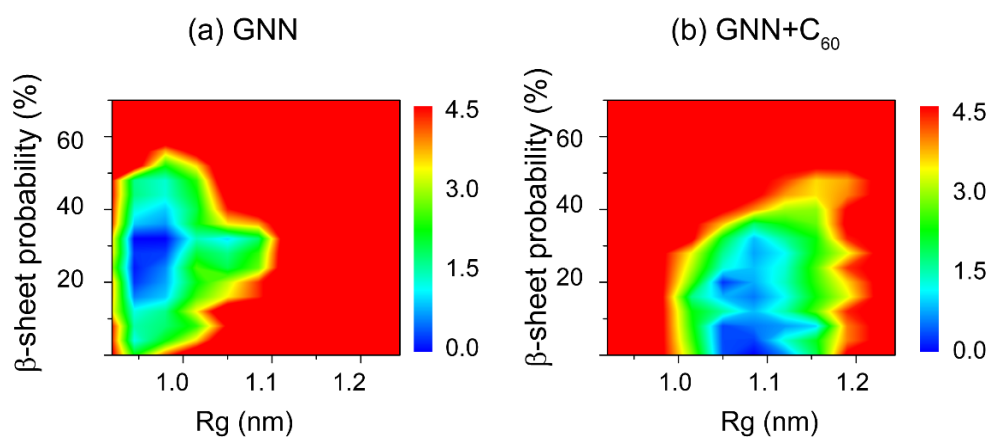


Figure S5. Potential of mean force (PMF) of GNNQQNY octamers in the absence and presence of fullerenes. The PMF (in kcal/mol) was plotted as a function of Rg and β -sheet probability of GNNQQNY octamer in GNN (a) and GNN+C₆₀ (b) systems.

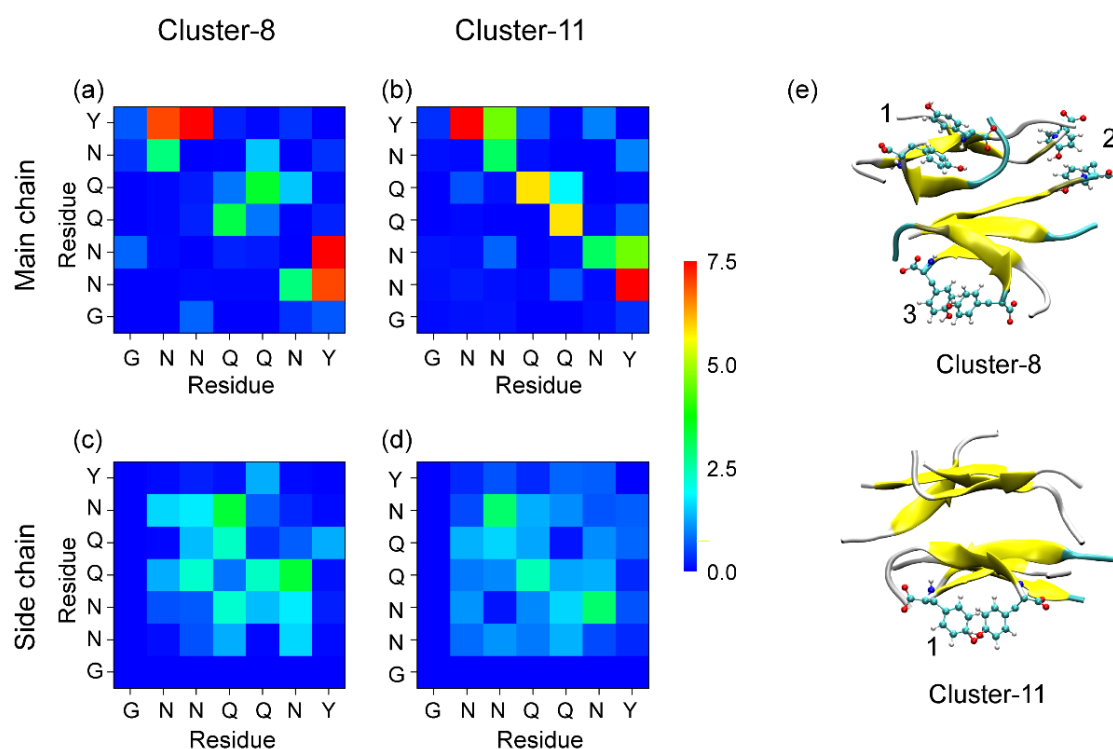


Figure S6. Structural analyses of the conformations in Cluster-8 and Cluster-11. Main-chain - main-chain and side-chain - side-chain H-bond formation probability for Cluster-8 (a, c) and Cluster-11 (b, d). (e) The snapshots of the center structures in the two clusters. Residues Tyr that display π - π stacking interactions are shown in ball-and-stick representation.