Supplementary Information

Amphiphilic Surface Chemistry of Fullerenols Is Necessary for Inhibiting the Amyloid Aggregation of Alpha-Synuclein NACore

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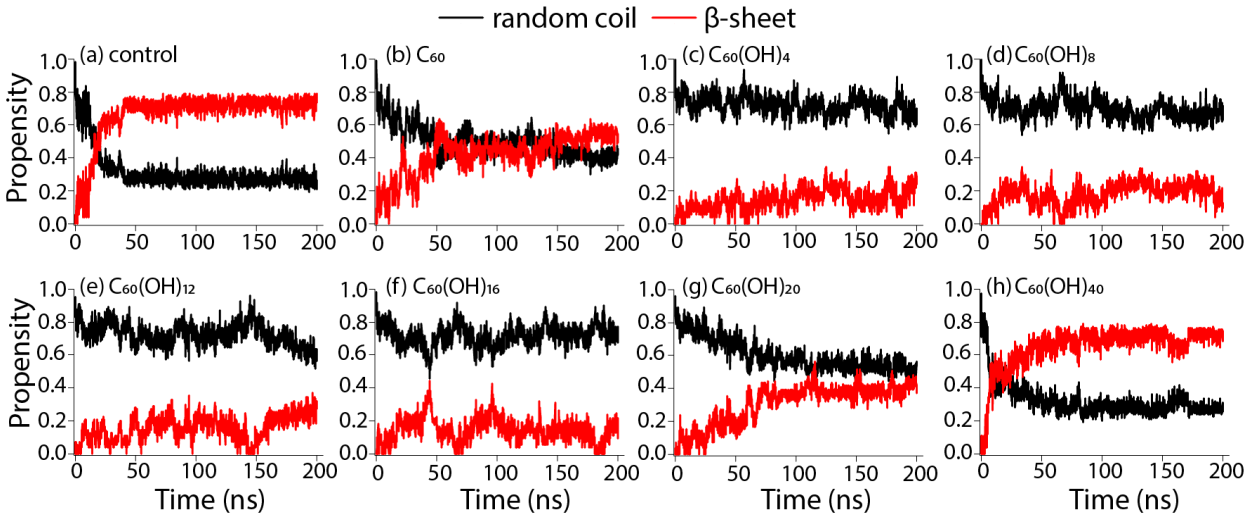

Figure S1. Time evolution of primary secondary structure contents in term of random coil (black) and β-sheet (red) of NACore peptides in each molecular system, suggesting the equilibration of DMD simulations in the last 100 ns. For each system, one randomly selected trajectory out of twenty independent DMD simulations was shown.

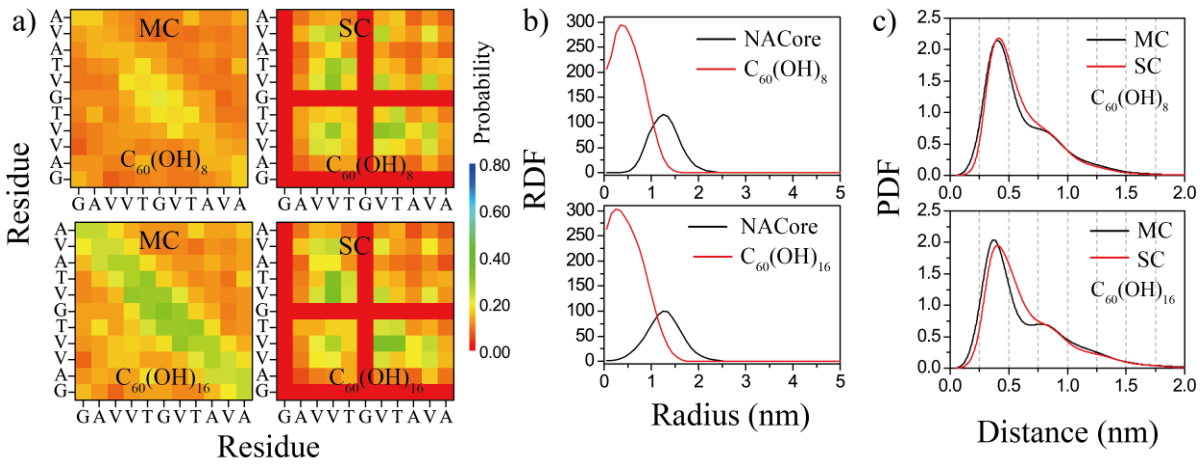

Figure S2. Inter-peptide interactions and structural analyses of nanoparticle-peptide complexes. (a) Per residue inter-peptide contact probabilities computed between main-chain (MC) and side-chain (SC) atoms for each molecular system. (b) Radial distribution function (RDF) for both NACore and nanoparticle atoms in nanoparticle-peptide complexes. (c) Probability distribution (PDF) of peptide backbone or side-chain atoms as a function of their distances to nanoparticles or nanoparticle assemblies, defined as the minimum distance of a peptide atom to any nanoparticle atoms.

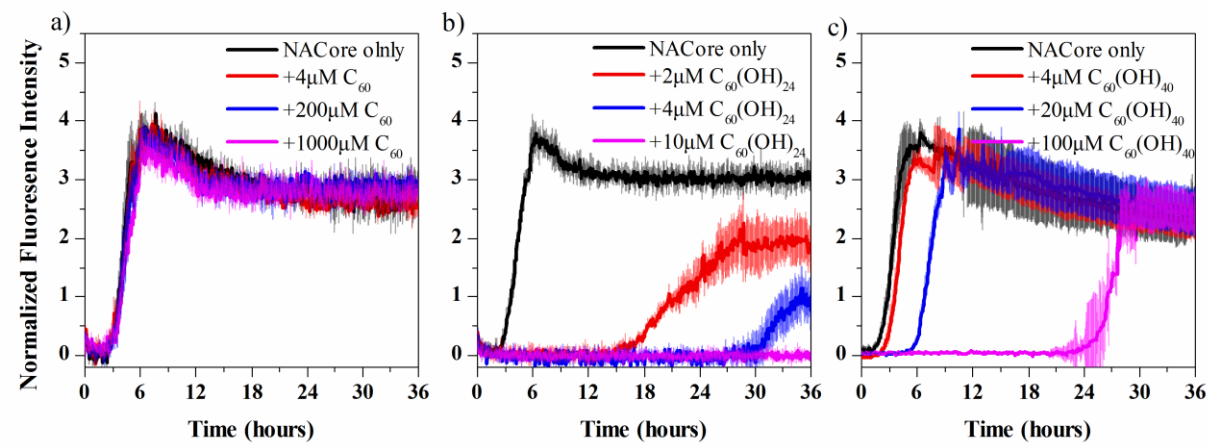

Figure S3. ThT fluorescence intensity of NACore aggregation (10 μM) as a function of time in the absence and presence of fullerene/fullerenol nanoparticles at different concentrations.

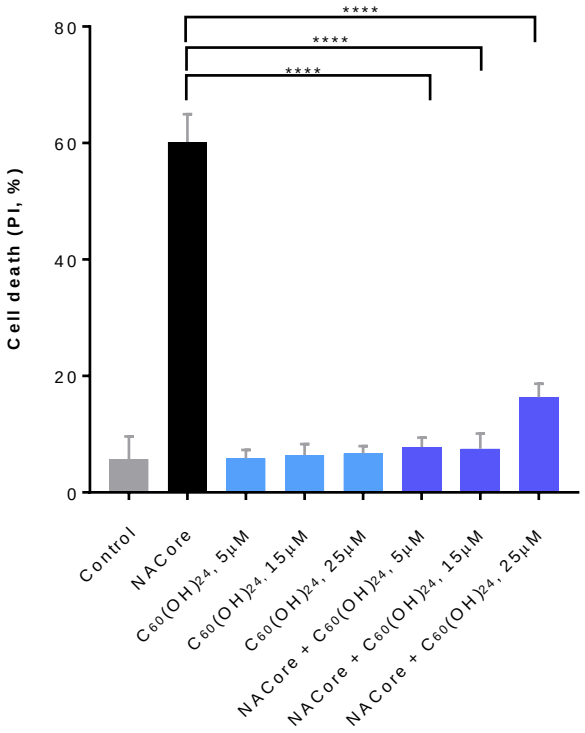

Figure S4. Viability of SH-SY5Y neuronal cells exposed to NACore with or without $C_{60}(OH)_{24}$ of 5, 15 and 25 μM. Exposure time: 24 h. Consistent with the simulation result, $C_{60}(OH)_{24}$ was effective in reducing the NACore toxicity, indicating a strong binding affinity with NACore. PI: propidium iodide. The experiments were carried out in triplicate and error bars show standard deviations (****: $P \leqslant 0.0001$). NACore concentration: 100 μM.

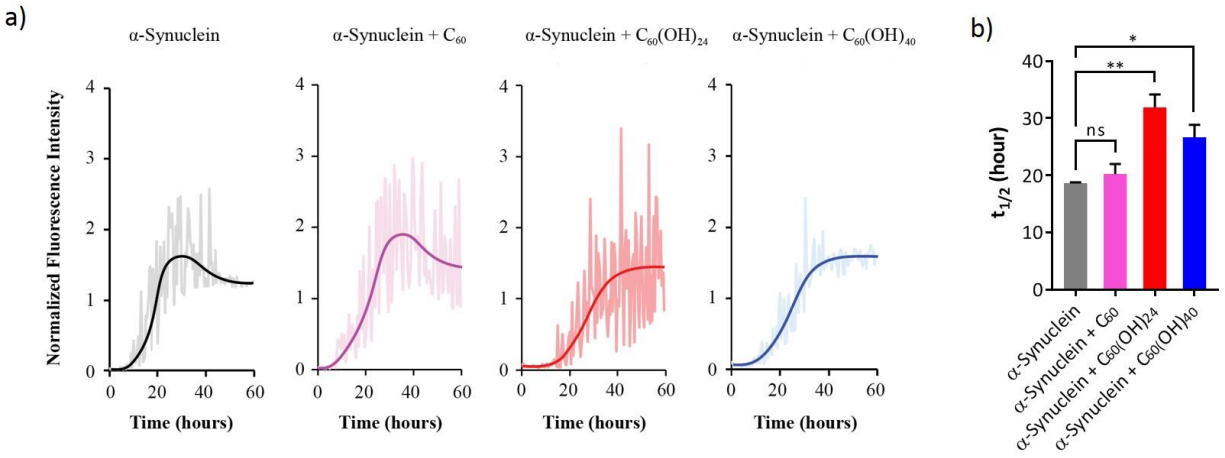

Figure S5. α-synuclein aggregation kinetics probed by the ThT assay. (a) Aggregation kinetics of 50 μM α-synuclein in the absence and presence of 50 μM fullerene/fullerenol (black, α synuclein only; magenta, C_{60}; red, $C_{60}(OH)_{24}$; blue, $C_{60}(OH)_{24}$). (b) Half-time ($t_{1/2}$) of α-synuclein aggregation derived from sigmoidal fitting. Error bars represent standard deviations of three independent measurements (ns : $P > 0.05$, *: $P \leqslant 0.05$, **: $P \leqslant 0.01$).