Electronic supplementary information

Polymorphism of amyloid β peptide in different environments: implications for membrane insertion and pore formation†

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Supplementary Figures

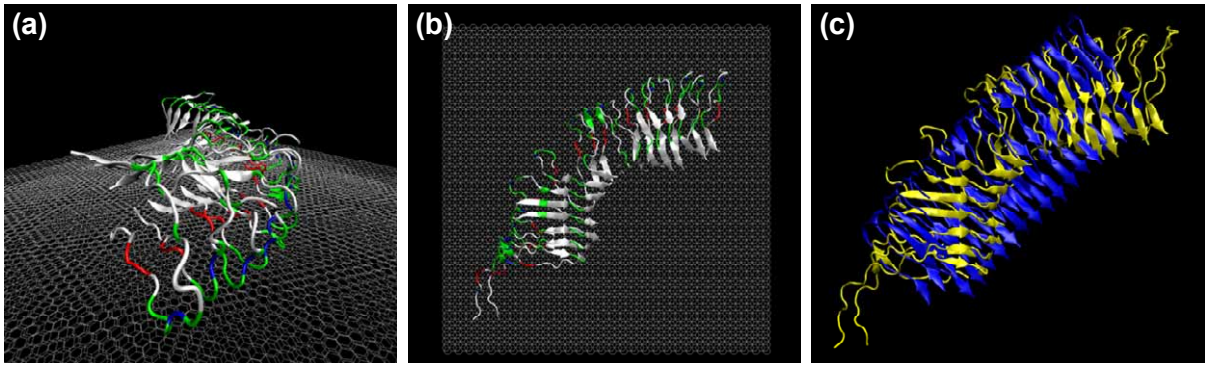

Figure S1. An additional simulation for the p3 fibril with the polar/hydrophilic N-terminal facing the graphite surface. Snapshots of the 16-mer p3 fibril on the surface of HOPG at the end of the 50 ns simulation in the (a) perspective and (b) top views. In the peptides, hydrophobic residues are shown in white, polar and Gly residues in green, negatively charged residues in red, and positively charged residues in blue. (c) Superposition of the p3 fibril conformations on the surface of HOPG from the starting points (blue) and the 50 ns simulation (yellow).

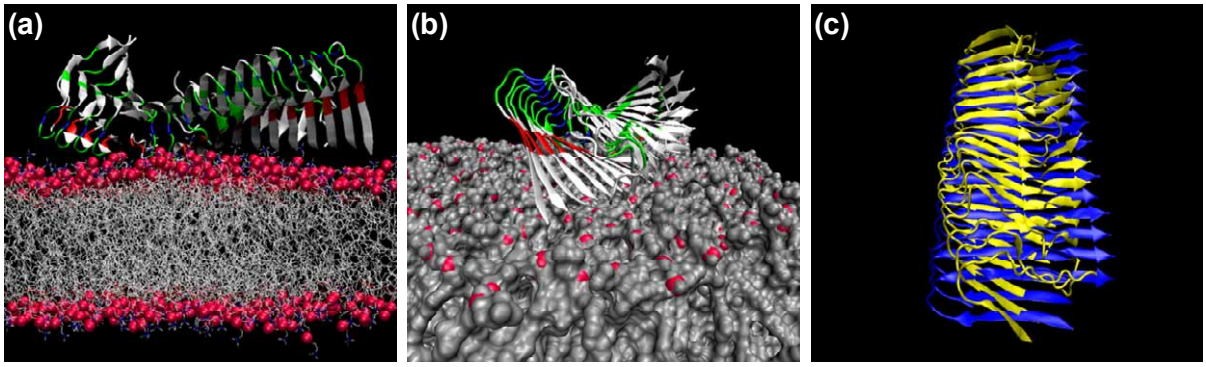

Figure S2. An additional simulation for the p3 fibril with the polar/hydrophilic N-terminal facing the DOPC bilayer surface. Snapshots of 16-mer p3 fibril on the surface of DOPC bilayer taken from the 50 ns simulation in the (a) lateral and (b) perspective views. In the peptides, hydrophobic residues are shown in white, polar and Gly residues are shown in green, negatively charged residues in red, and positively charged residues in blue. In the lipids in (a), nitrogen atoms are shown in red, carbon chains are represented as white threads, and phosphate atoms are shown as red spheres. In the perspective view, the gray surface represents the DOPC bilayer. (c) Superposition of the p3 fibril conformations on the surface of DOPC bilayer from the starting point (blue) and the 50 ns simulation (yellow).

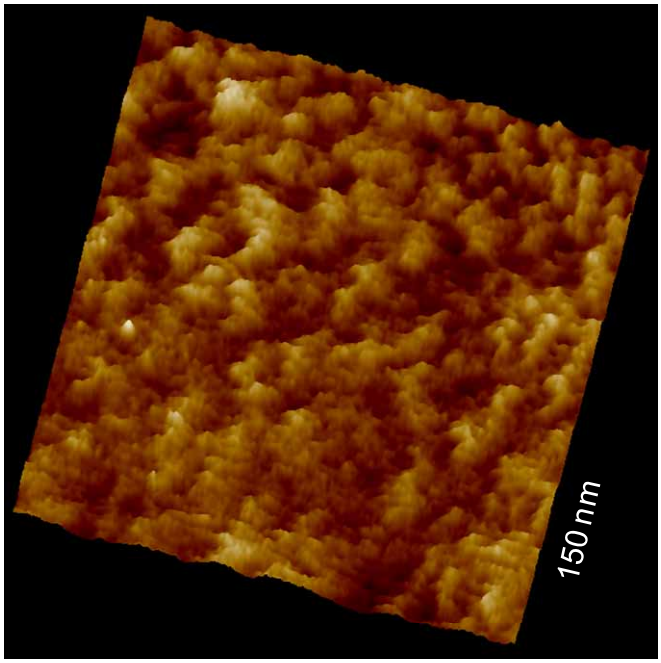

Figure S3. AFM image of globular p3 oligomers on the surface of DOPC bilayer.