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Supporting Material

Induced β-Barrel Formation of the Alzheimer's Aβ25–35 Oligomers on Carbon Nanotube Surfaces: Implication for Amyloid Fibril Inhibition

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Supporting Materials:

Figure S1: Analysis of a representative MD run (run 1) starting from a SWNT(3,3)–Aβ octamer system with parallel arrangement of β-strands. (A) States at t=0 (left) and 10 ns (right); (B) Secondary structure of each residue in the eight chains as a function of time calculated using DSSP program. [1]

Figure S2: MD-generated decamer at t=10 ns in a MD (run 86) without SWNT starting from mixed parallel-antiparallel β-sheets.

Figure S3: Analysis of the assembly process of two pentameric β-sheets into a 10-stranded β-barrel structure on a SWNT(4,4) surface observed in run 68. Time evolution of: (A) total Rg and Rg-HP of the decamer; (B) number of inter-sheet backbone H-bonds; (C) number of intra-sheet backbone H-bonds (the black curve is a smoothed line over 20 data points); (D) backbone RMSD of the decamer with respect to the β-barrel structure generated at 10 ns.

Figure S4: Dehydration process of SWNT–Aβ-decamer interface observed in Run 68. (A) Time evolution of number of water molecules within each cylinder along SWNT-axis. The cylinder is 1.0-nm thick from SWNT-axis and 0.5 nm high. (B) Four snapshots of SWNT(4,4)-water (view parallel to SWNT-axis) generated within the first 1 ns. To visualize the dehydration process clearly, the Aβ decamer is omitted, a radius of 1 nm from the SWNT is drawn in dotted line, and only the water molecules within 2 nm thick from the SWNT-axis are displayed.

Figure S5: MD run starting from a new orientation of the two β-sheets relative to SWNT-axis. Here the Cα-Cα distances of the two ends are 1.73 nm and 3.85 nm, respectively. (A): the initial state and the open β-barrel generated at t=20 ns. (B): the time evolution of inter-sheet H-bond1 (between strands *d* and *e*), H-bond2 (between strands *a* and *h*), and Cα-RMSD of the oligomer with respect to the open β-barrel formed at t=20 ns.

Figure S6: Time evolution of the Cα-RMSD of the oligomer with respect to the closed β-barrel generated at t=80 ns in run 10.

References:

1. Kabsch, W.; Sander, C. *Biopolymers* **1983,** 22, 2577-637.

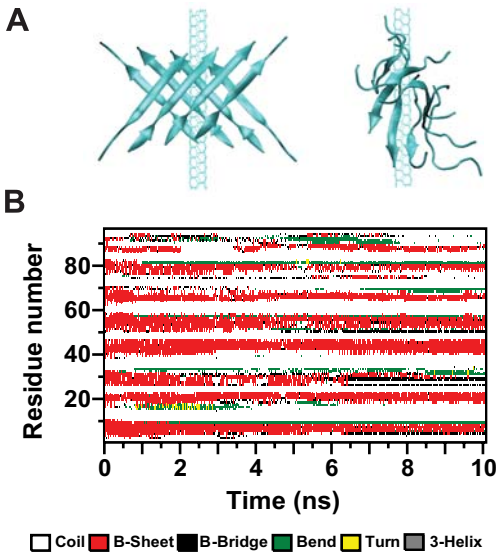
A
B
Residue number
80
60
40
20
0
2
4
6
8
10
Time (ns)
Coil
B-Sheet
B-Bridge
Bend
Turn
3-Helix

Figure S1

Top view Side view

Figure S2

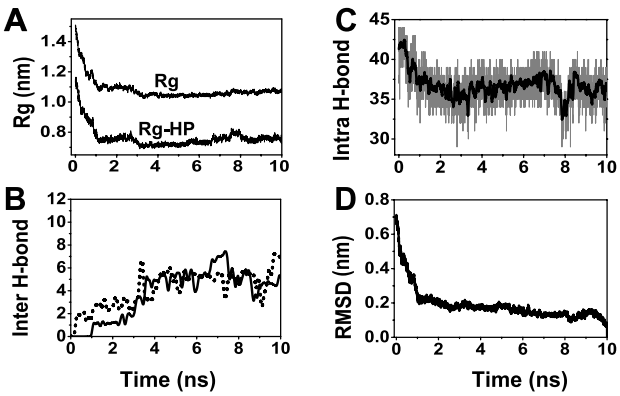
A
Rg (nm)
Rg
Rg-HP
B
Inter H-bond
Time (ns)
C
Intra H-bond
D
RMSD (nm)
Time (ns)

Figure S3

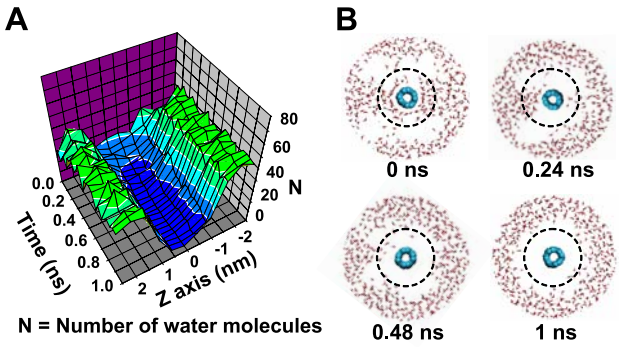
A
B
80
60
40
20
0
N
0.0
0.2
0.4
0.6
0.8
1.0
Time (ns)
2
1
0
-1
-2
Z axis (nm)
N = Number of water molecules
0 ns
0.24 ns
0.48 ns
1 ns

Figure S4

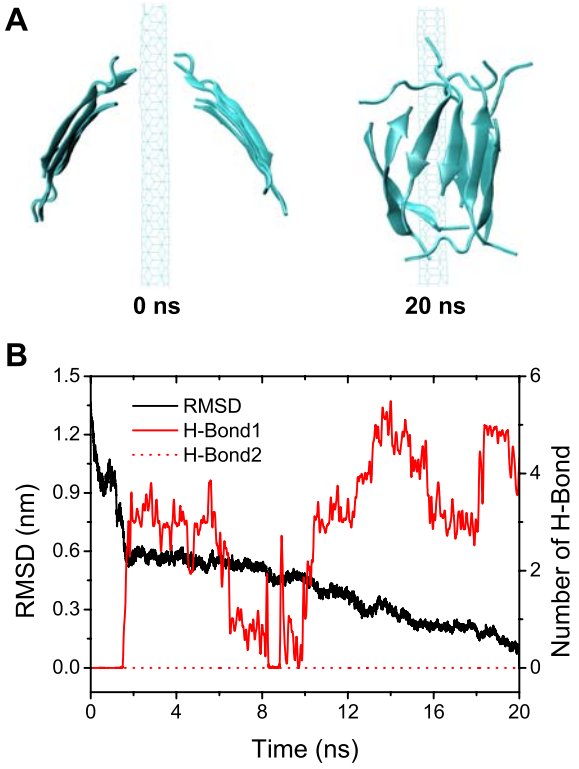
A
0 ns
20 ns
B
RMSD
H-Bond1
H-Bond2
RMSD (nm)
Number of H-Bond
Time (ns)
0.0
0.3
0.6
0.9
1.2
1.5
0
2
4
6
0
4
8
12
16
20

Figure S5

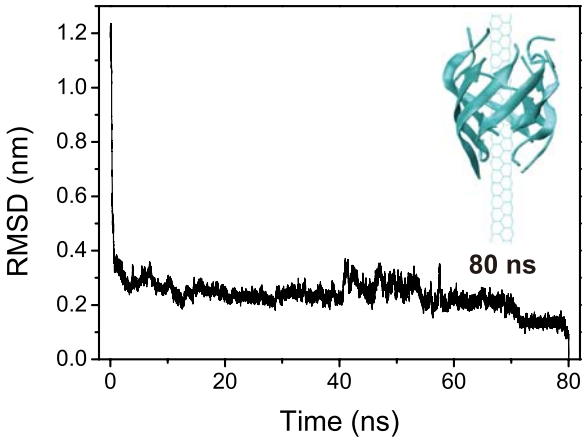

Figure S6