Supporting Information

Turning the structure of $A\beta_{42}$ peptide by different functionalized carbon nanotubes: a molecular dynamics simulations study

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1. Initial configuration of $A\beta_{42}$ peptide with different CNTs.

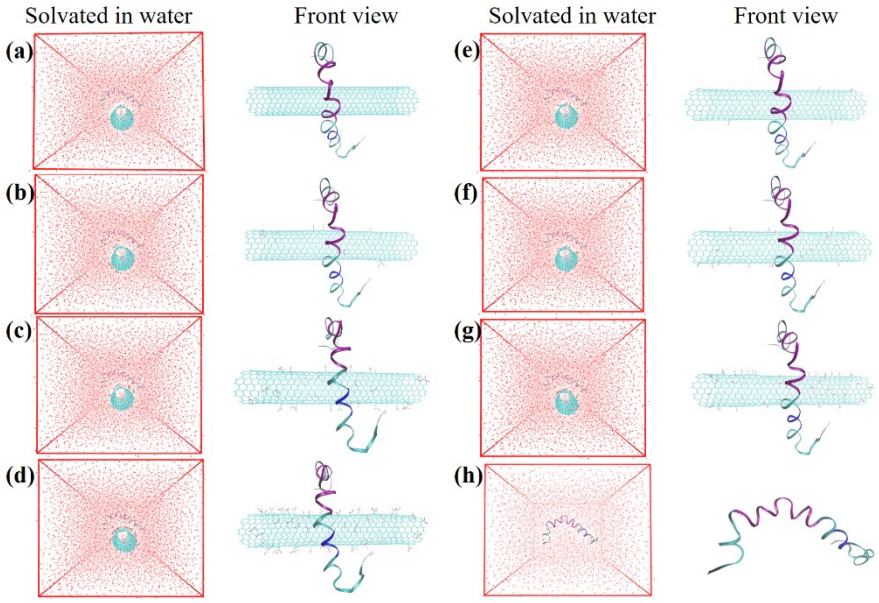

Fig. S1 Initial configuration of $A\beta_{42}$ peptide with CNTs: (a) CNT, (b) $CNT(COOH)_{12}$, (c) $CNT(COOH)_{36}$, (d) $CNT(COOH)_{72}$, (e) $CNT(OH)_{12}$, (f) $CNT(OH)_{36}$, (g) $CNT(OH)_{72}$, (h) without CNT.

2. Setups of different MD simulations systems.

Table S1 The detailed information for different MD simulation systems.

Simulation systems	Box size (nm^3)	Number of water molecules	Total atom number
CNT-$A\beta_{42}$ peptide	7.7x6.2x9.8	15123	47219
$CNT(COOH)_{12}$-$A\beta_{42}$ peptide	7.7x6.4x9.8	15618	48752
$CNT(COOH)_{36}$-$A\beta_{42}$ peptide	7.7x6.4x9.7	15583	48743
$CNT(COOH)_{72}$-$A\beta_{42}$ peptide	7.7x6.4x9.7	15449	48485
$CNT(OH)_{12}$- $A\beta_{42}$ peptide	7.7x6.4x9.8	15642	48800

$CNT(OH)_{36}$- $A\beta_{42}$ peptide	7.7x6.4x9.8	15833	49421
$CNT(OH)_{72}$- $A\beta_{42}$ peptide	7.7x6.4x9.8	15762	49280
$A\beta_{42}$ peptide without CNT	7.7x5.2x5.2	6803	21039

3. Representative snapshots for other MD simulations systems.

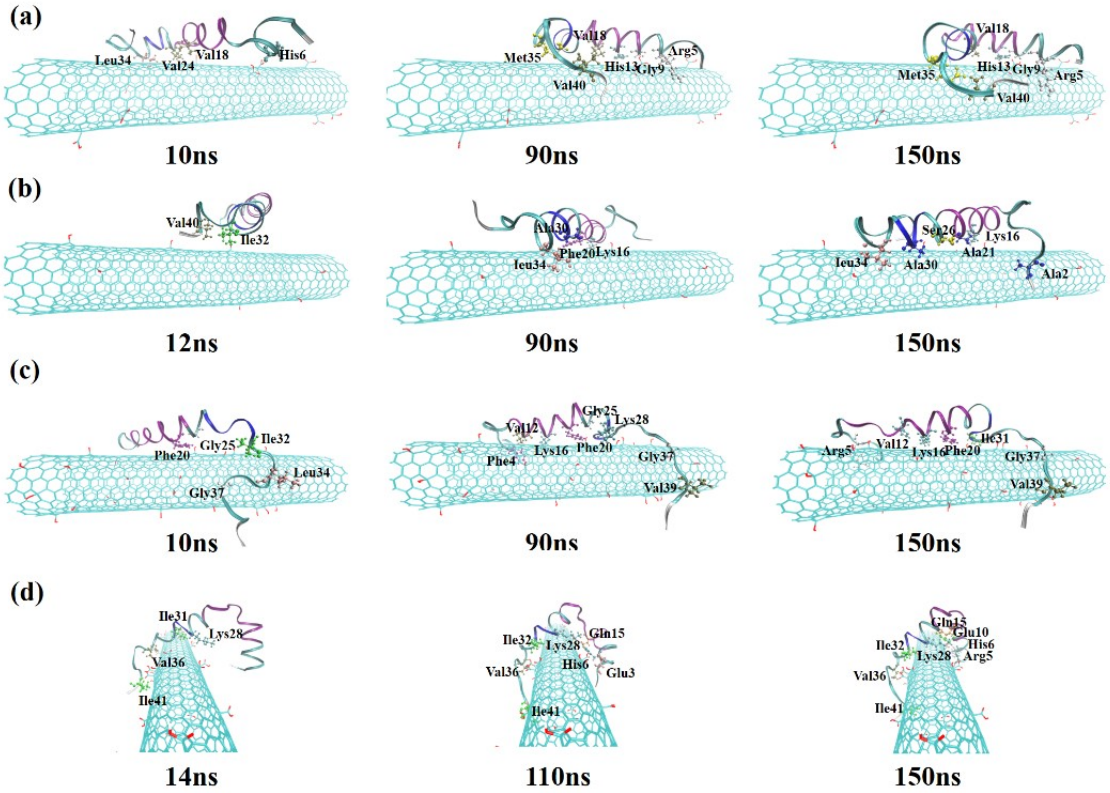

Fig. S2 Representative snapshots during the binding process between $A\beta_{42}$ peptide and (a) $CNT(COOH)_{12}$, (b) $CNT(COOH)_{36}$, (c) $CNT(OH)_{12}$, (d) $CNT(OH)_{36}$.

4. Other independent simulations trajectory snapshots of the three systems: $A\beta_{42}$ peptide and CNT, $CNT(COOH)_{72}$, $CNT(OH)_{72}$.

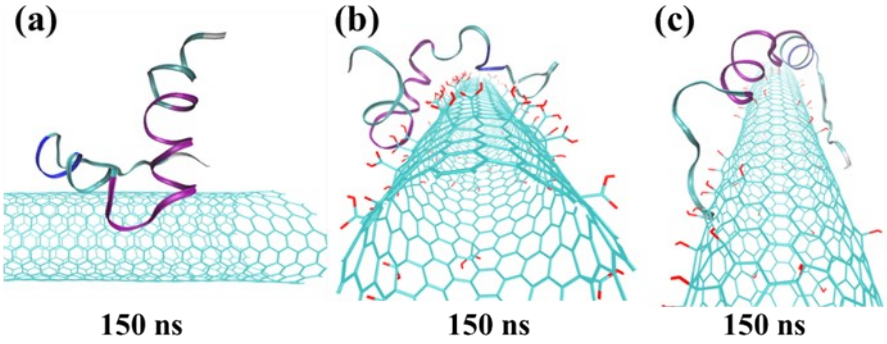

Fig. S3 Snapshot trajectory of $A\beta_{42}$ peptide - (a) CNT, (b) $CNT(COOH)_{72}$, (c) $CNT(OH)_{72}$ at the end of simulation time.

5. The RMSD of other independent simulations for each system.

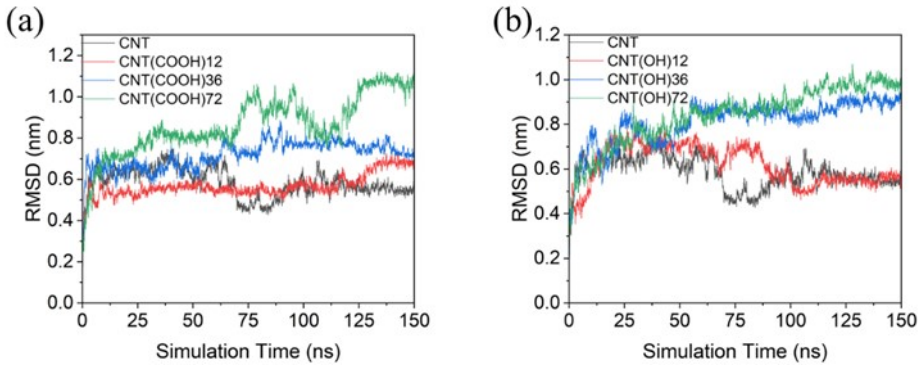

Fig. S4 (a, b) The RMSD of other independent simulations for each system.

6. The time evolution of H-bonds (a, b) within $A\beta_{42}$ peptide, and (c, d) between $A\beta_{42}$ peptide and water molecules.

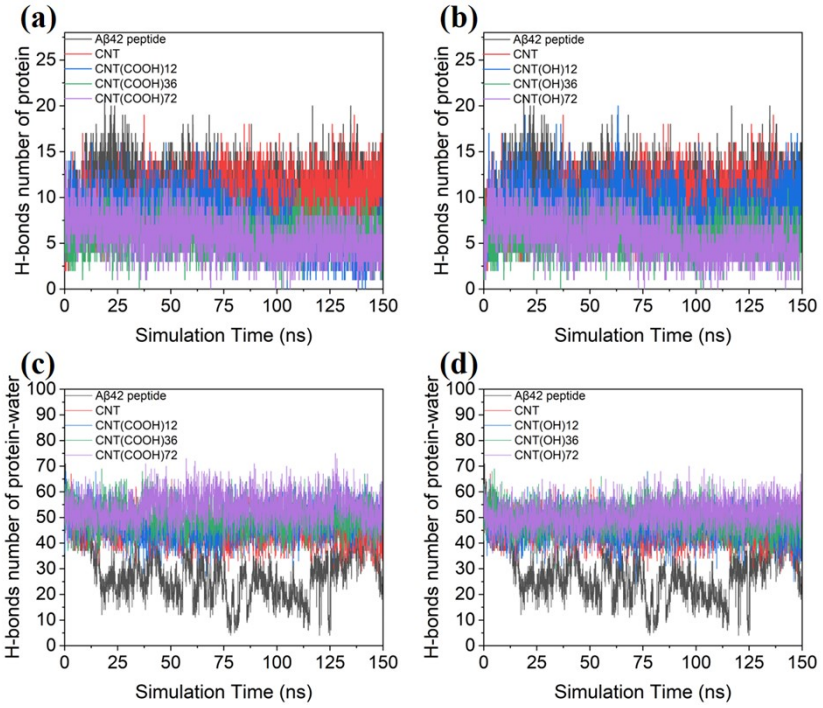

Fig. S5 The time evolution of H-bonds (a, b) within $A\beta_{42}$ peptide, and (c, d) between $A\beta_{42}$ peptide and water molecules.

7. The H-bonds between the $A\beta_{42}$ peptide and $CNT(COOH)_{72}/CNT(OH)_{72}$.

Table S2 The kinds of H-bonds between the $A\beta_{42}$ peptide and $CNT(COOH)_{72}/CNT(OH)_{72}$.

$A\beta_{42}$ peptide -$CNT(COOH)_{72}$		$A\beta_{42}$ peptide -$CNT(OH)_{72}$	
Donor	Acceptor	Donor	Acceptor
Ala42-Main	CNT1192-Main	Val40-Main	CNT1303-Main
Ile41-Main	CNT1260-Main	Ile41-Main	CNT1303-Main
Ala42-Main	CNT1260-Main	Leu34-Main	CNT1275-Main
His13-Side	CNT1424-Main	Met35-Main	CNT1275-Main
His6-Side	CNT1400-Main	Leu34-Main	CNT1269-Main

Arg5-Side	CNT1404-Main	Ala30-Main	CNT1261-Main
Ser8-Side	CNT1424-Main	Lys28-Side	CNT1251-Main
His13-Side	CNT1208-Main	His6-Side	CNT1349-Main
His6-Side	CNT1434-Main	His6-Side	CNT1363-Main
HIS13-Side	CNT1204-Main	Ser8-Side	CNT1355-Main
His13-Side	CNT1202-Main	Arg5-Side	CNT1349-Main
His13-Side	CNT1200-Main	Asn27-Side	CNT1251-Main
Ser26-Side	CNT1238-Main	Arg5-Main	CNT1225-Main
His13-Side	CNT1212-Main		
His13-Side	CNT1206-Main		
His6-Side	CNT1402-Main		
His6-Side	CNT1378-Main		
Val36-Main	CNT1260-Main		
Gly37-Main	CNT1260-Main		
Gly38-Main	CNT1194-Main		
Glu3-Main	CNT1464-Main		

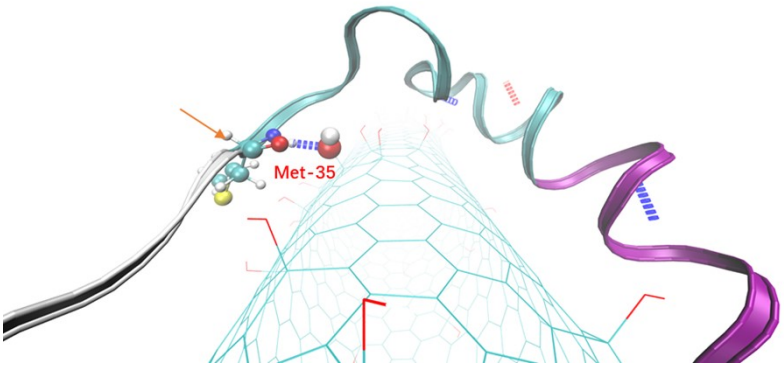

Fig. S6 Met35 forms H-bonds with the surface of CNTs, which destroys the original secondary structure (β-turn) and forms random coils.

8. Interaction energy analyses (kcal/mol)

Table S3 The binding energy (ΔG_{bind}) between $A\beta_{42}$ peptide and different CNTs

CNTs	$\Delta G_{complex}$	$\Delta G_{protein}$	ΔG_{CNT}	$\Delta G_{interaction}$
CNT	+3778.14±64.67	-674.75±61.32	+4464.03±28.61	-109.39±6.90
$CNT(COOH)_{12}$	+4441.05±29.12	-486.19±55.74	+3818.85±63.14	-136.01±7.02
$CNT(COOH)_{36}$	+3719.62±59.14	-539.00±56.73	+4406.50±30.35	-147.88±9.82
$CNT(COOH)_{72}$	+3738.43±66.26	-468.39±56.45	+4362.59±31.68	-155.77±10.27
$CNT(OH)_{12}$	+3682.10±67.09	-669.95±59.65	+4465.20±28.89	-113.15±7.61
$CNT(OH)_{36}$	+3778.71±68.14	-518.51±44.10	+4470.35±28.73	-173.45±7.41
$CNT(OH)_{72}$	+3854.30±43.27	-416.78±28.75	+4456.81±30.71	-185.56±7.92

9. The interaction energy between amino acids and CNT, $CNT(OH)_{72}$, $CNT(COOH)_{72}$

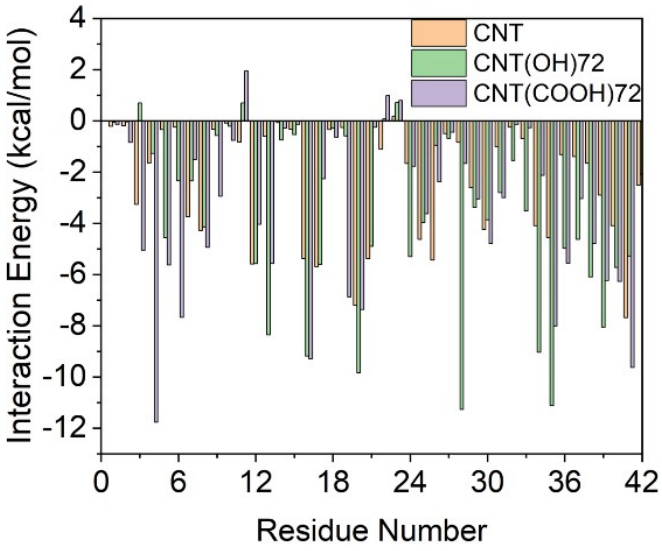

Fig. S7 The interaction energy between amino acids of $A\beta_{42}$ peptide and CNT, $CNT(OH)_{72}$, $CNT(COOH)_{72}$.

10. Time evolution of the number of water molecules

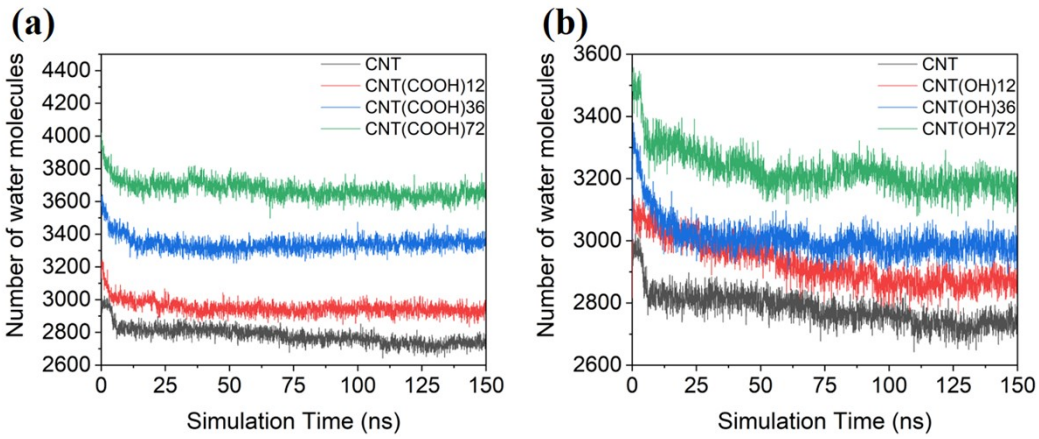

Fig. S8 (a, b) Time evolution of the number of water molecules (within 6 Å of CNTs).

11. Relative conformation test

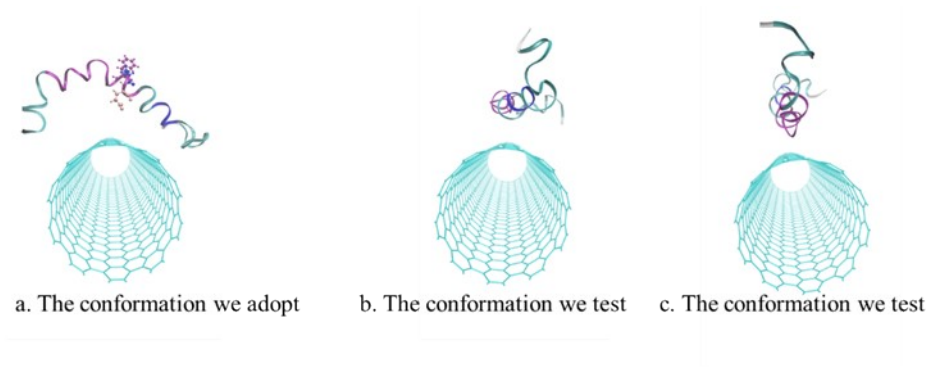

Fig. S9 Different conformations we test.