Supplementary Material for "Adsorption Mechanism and Collapse Propensities of the Full Length, Monomeric $A\beta_{1-42}$ on Surface of a Single-Walled Carbon Nanotube: A Molecular Dynamics Simulation Study"

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System	Simulation box dimensions (Å)	Number of water molecules
Control	95.0 × 62.2 × 50.0	9412
NT1	102.4 × 62.2 × 46.1	9342
NT2	102.4 × 72.0 × 40.5	9497
NT3	102.4 × 60.0 × 48.5	9473
NT4	102.4 × 62.9 × 44.5	9119
NT5	102.4 × 69.3 × 44.1	9960

Table S1. Dimensions of the orthorhombic simulation box in the six systems, and the number of solvent water molecules used.

System	θ_1 (º)	θ_2 (º)	d_1 (Å)	d_2 (Å)	CA (Å^2)
NT1	0.0	53.0	8.5	9.5	517.3
NT2	62.7	0.0	24.7	8.5	181.4
NT3	16.7	45.0	12.8	8.5	256.4
NT4	32.8	30.0	17.2	8.5	227. 8
NT5	45.0	86.6	8.5	19.3	245.6

Table S2. Details of the five peptide-SWCNT configurations used in the study. The angles (in degrees) made by the helices 1 and 2 with the SWCNT axis are θ_1 and θ_2, respectively. The center of mass distance (in Å) between helix 1 and the SWCNT is d_1; the center of mass distance (in Å) between helix 2 and the SWCNT is d_2. The initial contact area (in Å^2) between the peptide and SWCNT is denoted as CA.

Residue	NT1	NT2	NT3	NT4	NT5
SER 8	7.5	35.1	15.6	19.5	8.4
GLY 9	9.9	34.6	16.1	16.9	10.0
TYR 10	11.8	34.1	18.1	18.9	11.4
GLU 11	9.1	31.5	16.0	19.2	8.8
VAL 12	6.6	29.5	12.4	16.0	5.6
HSD 13	9.6	28.8	13.7	14.1	7.6
HSD 14	10.8	28.9	16.0	16.8	9.7
GLN 15	7.5	26.7	14.1	18.0	7.3
LYS 16	6.8	23.9	11.0	14.5	5.4
LEU 17	10.4	24.4	13.3	13.0	8.6
VAL 18	9.9	23.8	14.8	15.7	10.3
PHE 19	6.5	20.7	11.4	15.0	7.5
PHE 20	8.3	19.6	10.0	11.1	6.9
ALA 21	10.5	19.2	12.4	11.2	10.6
GLU 22	7.8	16.2	10.6	13.0	10.9
ASP 23	5.4	15.3	7.2	12.2	7.3
VAL 24	8.3	14.4	7.4	8.7	8.1
GLY 25	8.8	13.3	9.0	10.3	11.9

Table S3. Radial distance (in Å) of residues 8 to 25 from the single walled carbon nanotube, in the initial setups.

Residue	NT1	NT2	NT3	NT4	NT5
SER 26	6.5	12.0	8.9	13.7	13.4
ASN 27	3.2	13.0	7.7	15.6	10.4
LYS 28	4.6	11.3	4.2	13.6	10.3
GLY 29	6.0	10.1	3.8	10.2	14.0
ALA 30	9.4	9.0	5.2	9.3	15.7
ILE 31	9.0	8.0	5.5	13.0	18.5
ILE 32	8.7	5.4	5.6	13.3	19.5
GLY 33	12.3	6.7	6.5	9.5	20.0
LEU 34	13.6	9.9	9.6	10.3	22.0
MET 35	12.7	8.9	10.5	13.6	24.2
VAL 36	13.0	6.0	9.8	12.1	24.5
GLY 37	13.2	6.9	13.1	13.4	27.7
GLY 38	15.5	10.6	15.5	14.2	30.2

Table S4. Radial distance (in Å) of residues 26 to 38 from the single walled carbon nanotube, in the initial setups.

	0-2 ns	18-22 ns	40-48 ns	58-62 ns	76-80 ns
Full Peptide					
NT1	624.6 (223.0)	938.0 (42.1)	799.3 (33.5)	972.01 (29.9)	924.1 (33.5)
	391.5 (126.0)	942.7 (81.3)	1029.2 (38.2)	1075.0 (25.3)	1030.5 (37.9)
	505.6 (102.0)	876.4 (33.3)	938.6 (25.7)	911.3 (28.7)	938.4 (42.5)
NT2	345.9 (68.9)	392.1 (21.8)	454.3 (57.8)	586.6 (48.3)	920.1 (22.5)
	276.4 (41.7)	516.4 (30.0)	897.0 (50.6)	945.1 (51.5)	956.4 (24.4)
	373.1 (55.7)	1026.0 (45.0)	885.0 (32.4)	860.4 (27.1)	902.7 (42.0)
N-term. seg.					
NT1	257.4 (106.2)	416.0 2.3)	294.0 (26.1)	414.2 (19.9)	379.0 (17.1)
	146.0 (98.4)	445.1 (52.8)	490.6 (27.6)	515.7 (16.0)	433.0 (28.5)
	256.8 (36.3)	350.8 (28.8)	440.7 (20.0)	405.3 (20.4)	434.3 (42.2)
NT2	0.0 (0.0)	0.0 (0.0)	0.1 (1.0)	18.7 (17.9)	391.2 (17.3)
	0.0 (0.0)	0.0 (0.0)	259.1 (33.3)	322.1 (39.5)	304.5 (12.2)
	0.0 (0.0)	406.0 (20.8)	443.5 (21.4)	405.4 (14.2)	413.5 (15.2)
HP1					
NT1	93.3 (25.2)	146.9 (13.1)	182.9 (15.7)	196.8 (13.6)	197.9 (10.2)
	47.7 (26.7)	77.4 (60.0)	152.6 (9.8)	172.4 (8.7)	172.3 (11.5)
	72.7 (16.5)	118.0 (28.6)	131.0 (22.5)	137.5 (24.7)	123.5 (26.5)
NT2	0.0 (0.0)	0.0 (0.0)	53.3 (60.9)	193.9 (10.3)	186.3 (9.8)
	0.0 (0.0)	2.2 (4.7)	180.2 (16.3)	165.2 (19.1)	205.1 (9.7)
	0.0 (0.0)	189.0 (11.7)	169.1 (9.1)	163.0 (7.0)	179.3 (8.6)
HP2					
NT1	73.7 (59.7)	159.0 (13.7)	189.0 (12.6)	186.7 (10.5)	182.4 (12.7)
	72.3 (49.7)	139.7 (8.5)	122.2 (8.4)	138.6 (7.5)	130.2 (11.7)
	18.0 (23.5)	202.7 (10.3)	194.8 (9.7)	195.7 (7.7)	196.1 (8.0)
NT2	153.2 (15.7)	144.1 (8.0)	144.4 (13.8)	162.7 (9.8)	182.5 (9.5)
	140.8 (18.7)	210.7 (21.3)	229.8 (12.6)	225.3 (12.0)	251.0 (16.1)
	156.1 (23.6)	228.1 (28.4)	181.3 (20.2)	167.6 (14.0)	157.1 (18.2)

Table S5. The contact area of the SWCNT (in $Å^2$) with the entire peptide, with the N-terminal segment (residues 1 to 16), HP1 (residues 17 to 21) and HP2 (residues 30 to 35), averaged over selected parts, for the three trajectories generated with the NT1 and NT2 setups. Standard deviations are specified within braces.

	0-2 ns	18-22 ns	40-48 ns	58-62 ns	76-80 ns
Full Peptide					
NT3	550.0 (197.6)	728.0 (34.5)	886.2 (23.1)	920.0 (22.7)	896.2 (35.0)
NT4	407.3 (100.0)	884.0 (24.3)	959.1 (28.6)	911.6 (30.1)	949.7 (29.6)
NT5	457.0 (118.7)	938.0 (27.7)	941.6 (49.7)	962.1 (31.5)	972.1 (25.6)
N-term. seg.					
NT3	128.0 (105.7)	390.6 (27.8)	389.7 (16.2)	430.1 (17.6)	416.0 (29.4)
NT4	0.0 (0.0)	352.3 (21.1)	455.0 (21.9)	432.2 (17.6)	432.3 (23.7)
NT5	269.4 (55.2)	413.3 (19.3)	406.5 (50.0)	453.3 (18.5)	471.5 (16.0)
HP1					
NT3	81.0 (41.4)	96.6 (6.8)	140.7 (12.5)	149.4 (12.2)	131.2 (12.9)
NT4	44.3 (29.9)	192.9 (6.0)	202.6 (10.5)	202.0 (7.0)	210.2 (8.0)
NT5	154.4 (46.1)	194.2 (6.8)	192.6 (8.6)	187.1 (7.7)	186.0 (7.3)
HP2					
NT3	165.3 (26.1)	158.5 (8.0)	160.0 (13.2)	155.1 (6.3)	166.2 (10.6)
NT4	153.0 (20.2)	129.2 (6.8)	151.2 (11.4)	149.3 (13.2)	159.8 (17.8)
NT5	5.0 (20.7)	118.5 (9.8)	142.3 (10.7)	133.5 (14.7)	123.5 (12.4)

Table S6. The contact area of the SWCNT (in $Å^2$) with the entire peptide, with the N-terminal segment (residues 1 to 16), HP1 (residues 17 to 21) and HP2 (residues 30 to 35), averaged over selected parts of the trajectories with NT3, NT4 and NT5 setups. Standard deviations are specified within braces.

Peptide Localization on SWCNT

The distance moved by the center of mass of the peptide relative to its position at the setup configuration (time = 0 ns) has been calculated as,

$$\Delta d = \left|\vec{r}_{c.o.m}(t) - \vec{r}_{c.o.m}(0)\right| \quad (1)$$

where $\boldsymbol{r}_{c.o.m}(0)$ and $\boldsymbol{r}_{c.o.m}(t)$ denote the position of the center of mass at the beginning of the simulation, and at time *t*. In Figure S1, we show the temporal evolution of the values averaged for the NT1 and NT2 trajectories, along with the values for the 'control' simulation of the free peptide. The free peptide moves to more than 47 Å from the original position within the first 20 nanoseconds, while the corresponding average values in the NT1 and NT2 simulations are ~20 Å and ~22 Å, respectively. On the average, the peptide's overall diffusion in the NT2 simulation slightly exceeds that in the NT1 simulation. The final values of Δd for the NT1, NT2, NT3, NT4, NT5 and 'control' simulations are 19.4 Å, 27.6 Å, 10.7 Å, 23.6Å, 12.0 Å and 44.5 Å, respectively. This data shows that overall diffusion of the peptide is restricted when in the proximity of a SWCNT.

In Figure S2, we show the evolution of the 'contact angles' between the SWCNT axis (unit vector $\boldsymbol{u}_{SWCNT}$) and the line joining the C_a atoms of the end residues of the two helical domains (unit vector $\boldsymbol{u}_{ca}$), averaged over the independent NT1 and NT2 simulation trajectories. q_1 and q_2 are, respectively, the acute angles made by the SWCNT with the first and second helix, and are calculated as,

$$\theta = \cos^{-1}[\hat{u}_{ca}(t).\hat{u}_{SWCNT}] \quad (2)$$

The values of q_1 and q_2 at the setup are provided in Table S2. It is seen that irrespective of the initial values, all trajectories attain a low (~15º) value of q_1 within a few tens of nanoseconds. On the other hand, for most trajectories, q_2 remains high and shows large fluctuations. For NT1 and NT2, the final (q_1, q_2) values are (15.0º, 27.3º) and (14.7º, 37.3º), while they are (11.0º, 45.0º), (14.3º, 65.2º) and (17.0º, 23.0º), respectively, for NT3, NT4 and NT5. The stronger preference of the first helical domain to align with the SWCNT indicates an overall greater favorability in their interactions compared with the interactions due to the second helical domain.

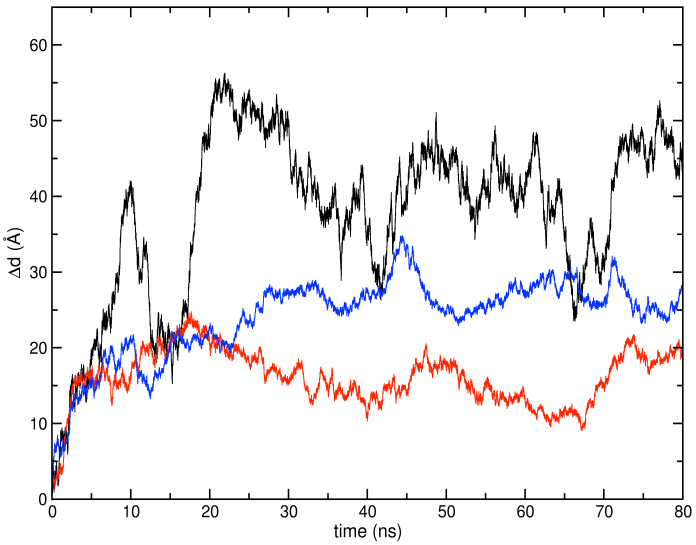


Figure S1. Average time evolution of the center of mass movement of the peptide, in the control simulation (*black)* and the NT1 (*red*) and NT2 (*blue*) simulations.

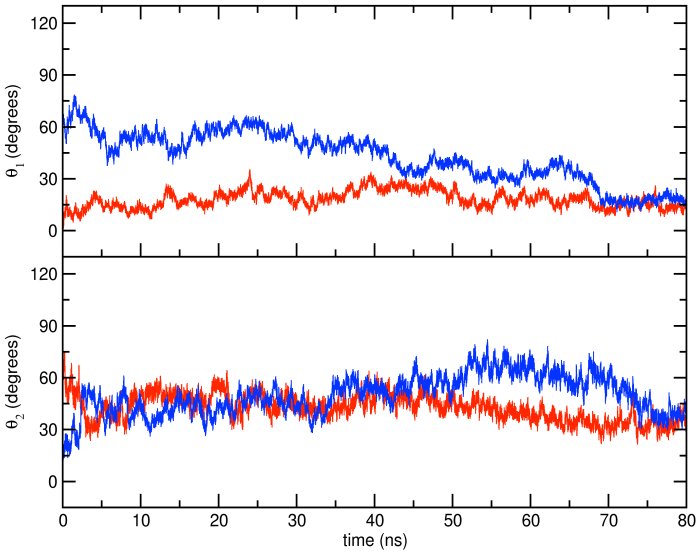
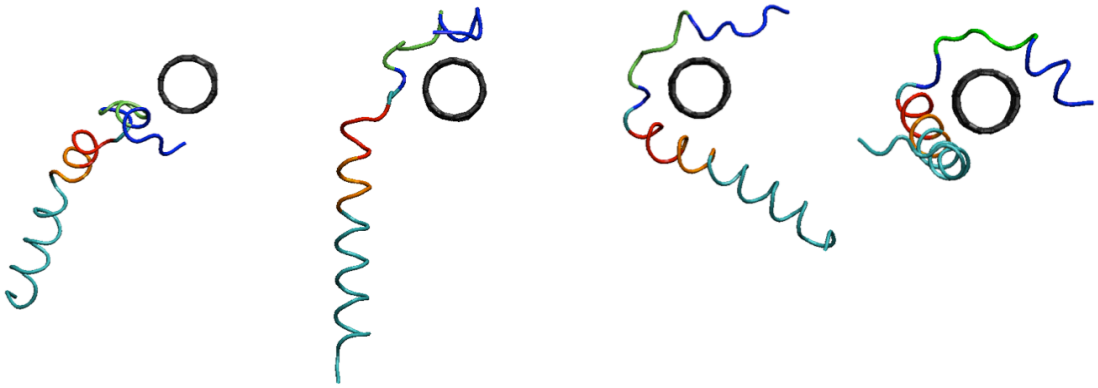


Figure S2. Average time evolution of the angles θ_1 and θ_2 for the NT1 (*red*) and the NT2 (*blue*) simulations.

a)

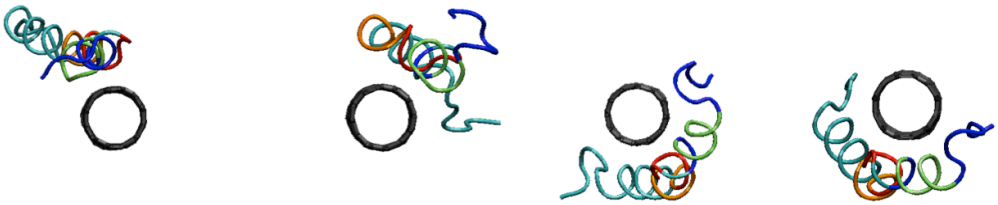
1 ns 20 ns 60 ns 80ns

b)



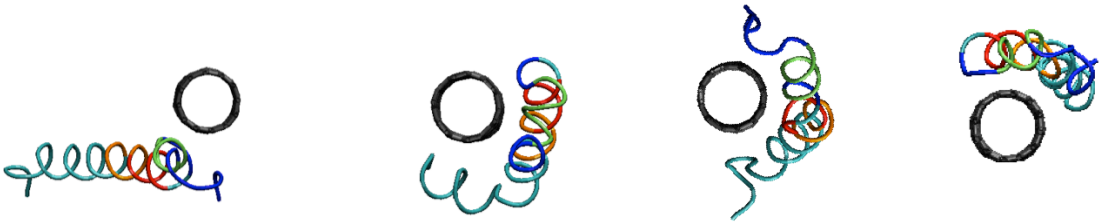
1 ns 20 ns 60 ns 80ns

c)



1 ns 20 ns 60 ns 80ns

d)



1 ns 20 ns 60 ns 80ns

e)

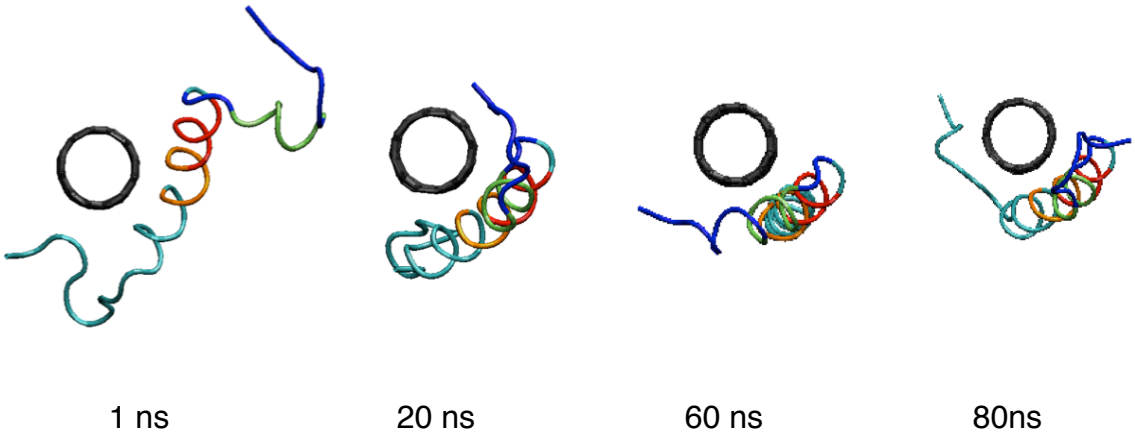


Figure S3. Snapshots of the peptide-SWCNT complex as observed perpendicular to the SWCNT axis, at different points along the a) NT1, b) NT2, c) NT3, d) NT4 and e) NT5 trajectories. Color specifications are the same as in Figure 1 of main text.

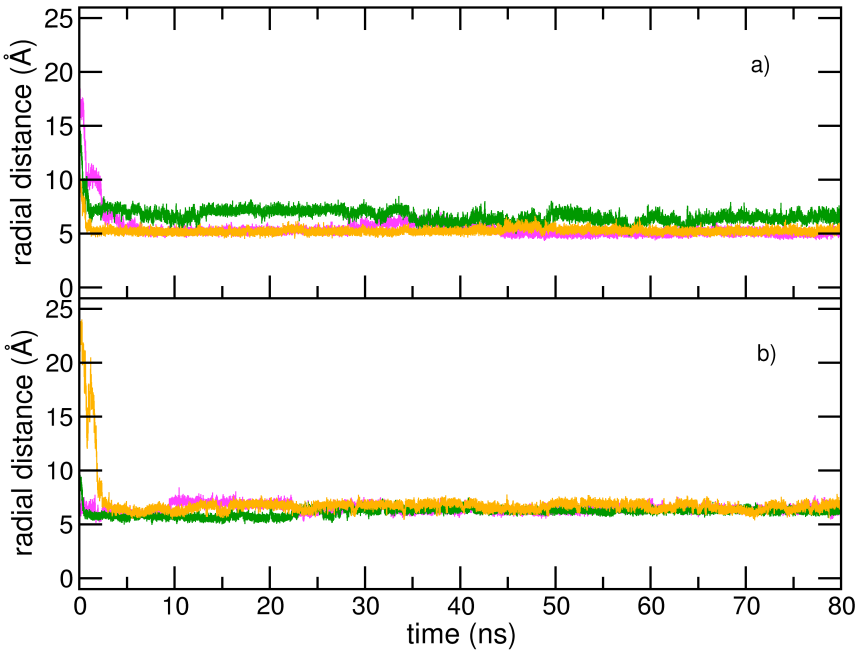


Figure S4. Radial distance of *a)* segment HP1 and, *b)* segment HP2, from the SWCNT surface, for the NT3 (*green*), NT4 (*magenta*) and NT5 (*orange*) simulation trajectories.

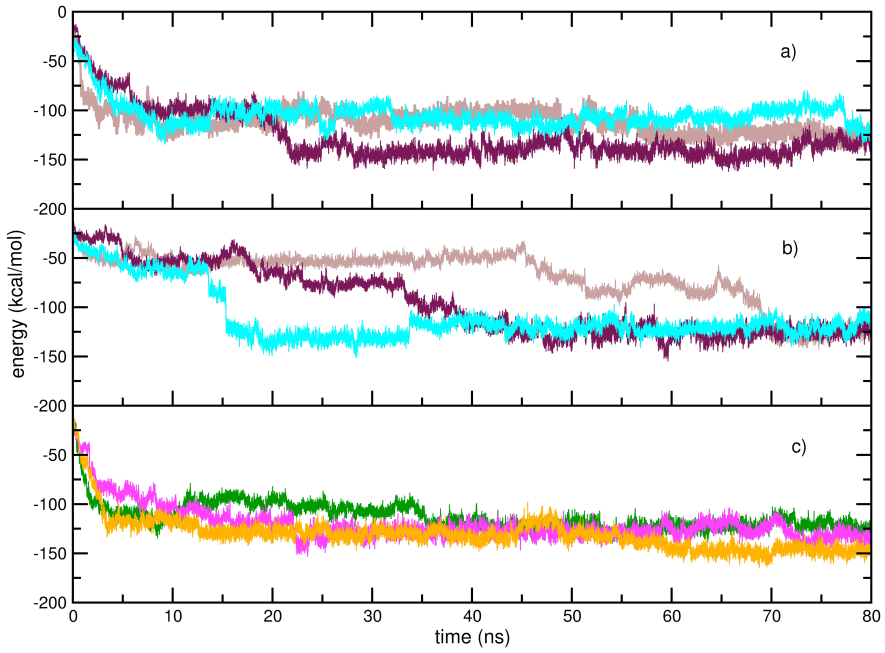


Figure S5. Total peptide-SWCNT interaction energy for, *a)* the three independent NT1 trajectories, *b)* the three independent NT2 trajectories, *c)* NT3 (*green*), NT4 (*magenta*) and NT5 (*orange*) trajectories. (Snapshots shown in Figure S3 correspond to data plotted in brown color).

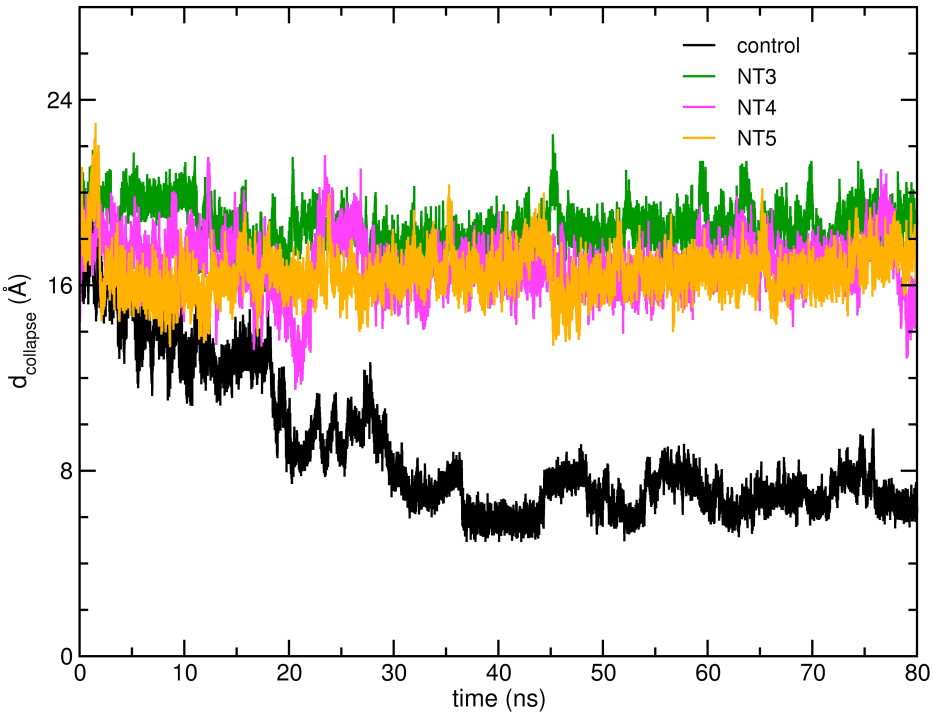


Figure S6. Time evolution of $d_{collapse}$ for the control, NT3, NT4 and NT5 trajectories.