Supplementary Information to

Critical Roles of Key Domains in Complete Adsorption of Aβ Peptide on Single-Walled Carbon Nanotubes: Insights with Point Mutations and MD Simulations

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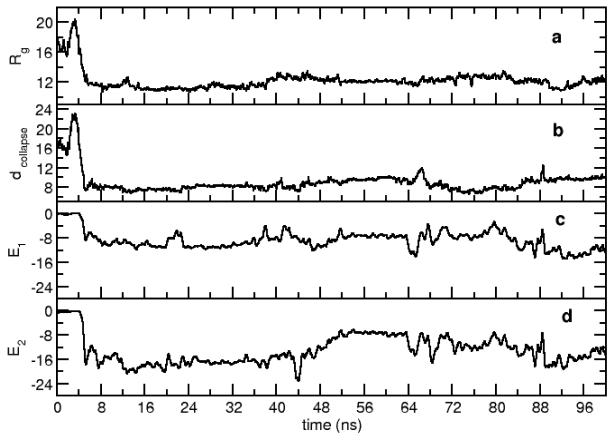

Figure I. Evolution of *a)* peptide radius of gyration, R_g (in Å); *b)* $d_{collapse}$ (in Å); *c)* interaction energy E_1 (in kcal mol^{-1}); *d)* interaction energy E_2 (kcal mol^{-1}), along an F19I trajectory.

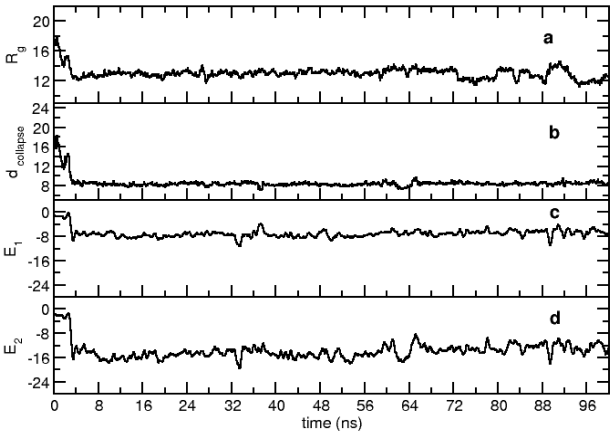

Figure II. Evolution of *a)* peptide radius of gyration, R_g (in Å); *b)* $d_{collapse}$ (in Å); *c)* interaction energy E_1 (in kcal mol^{-1}); *d)* interaction energy E_2 (kcal mol^{-1}), along a collapsing F19Y trajectory.

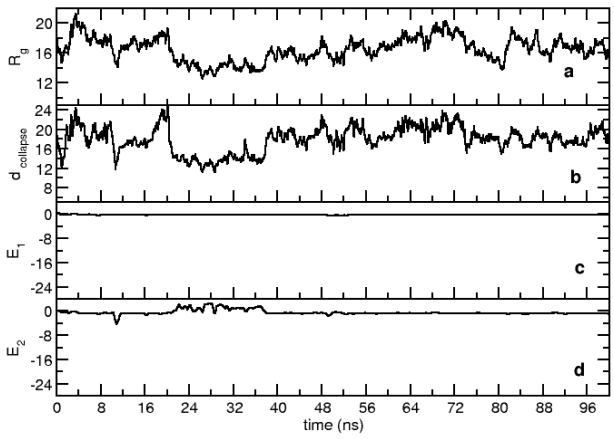

Figure III. Evolution of *a)* peptide radius of gyration, R_g (in Å); *b)* $d_{collapse}$ (in Å); *c)* interaction energy E_1 (in kcal mol^{-1}); *d)* interaction energy E_2 (kcal mol^{-1}), along a non-collapsing F19Y trajectory.

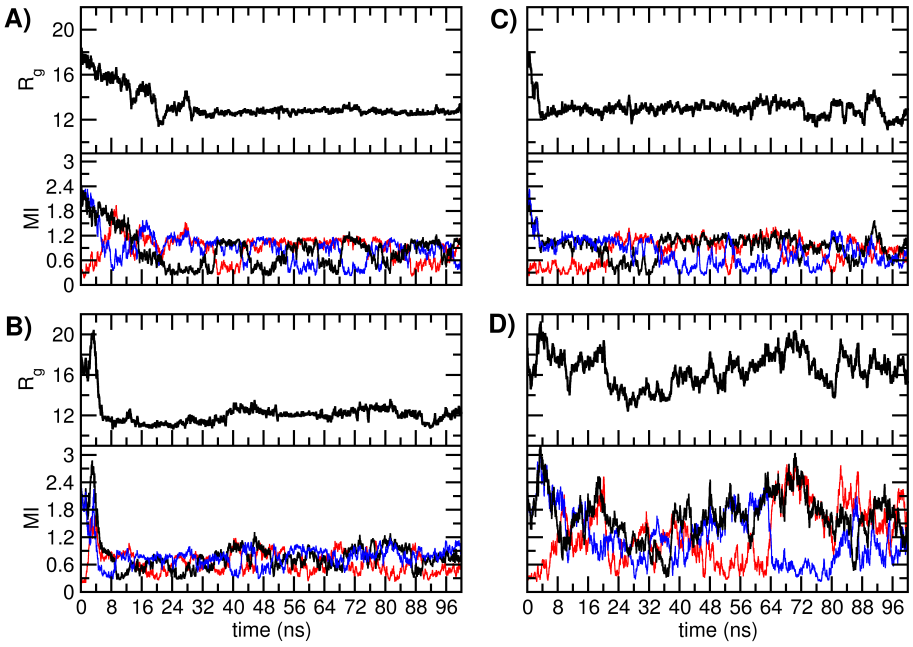

Figure IV. Comparisons of the evolution of the R_g (in Å) with the three principal moments of inertia, MI (in black, red and blue, in 10^{-34}•g cm^2), for the sample trajectories of *A)* F19, *B)* F19I, *C)* collapsing F19Y, *D)* non-collapsing F19Y. The moment of inertia tensor has been computed as per the method described in ref. 63 of the main text.

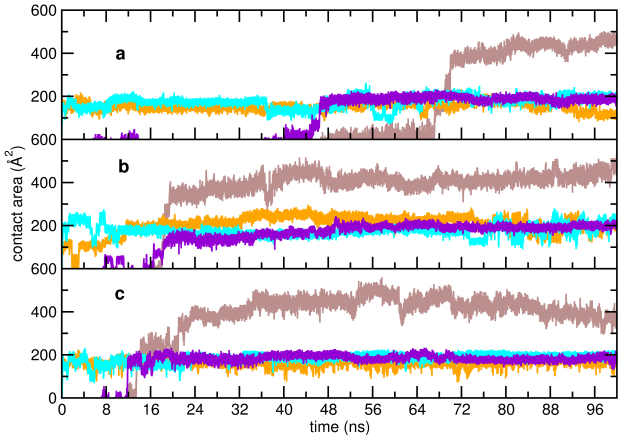

Figure V. Evolution of the contact area of key domains for representative fully adsorbing trajectories of *a)* NT2, *b)* NT2I, *c)* NT2Y. Contact area of HP1 is in purple; residues 1 to 16 in light brown; HP2 in orange; residues 36 to 41 in cyan.

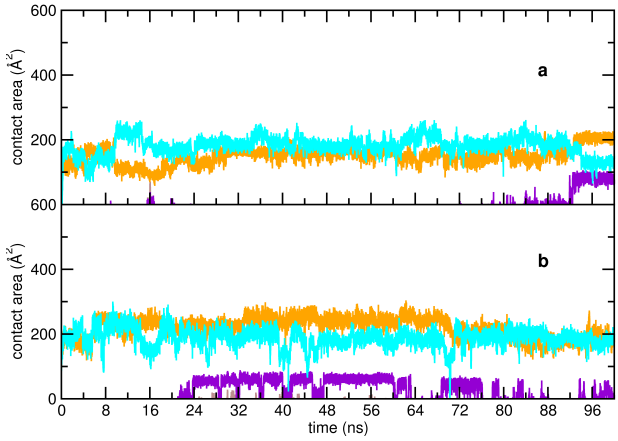

Figure VI. Evolution of the contact area of key domains for representative partially adsorbing trajectories of *a)* NT2I, *b)* NT2Y. Contact area of HP1 is in purple; residues 1 to 16 in light brown; HP2 in orange; residues 36 to 41 in cyan.

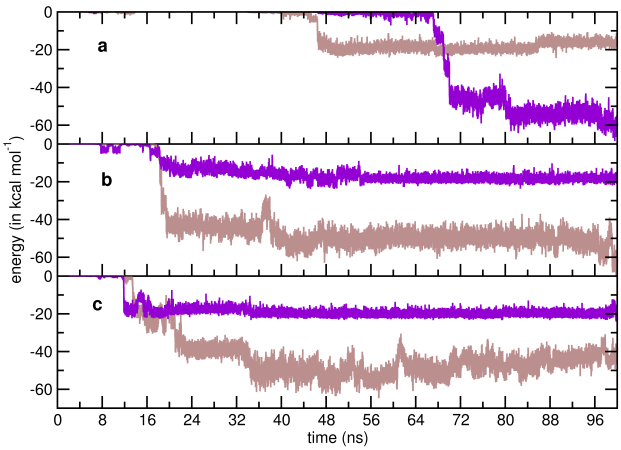

Figure VII. Evolution of the interaction energy with the SWCNT, of HP1 (in purple) and residues 1 to 16 (in light brown), for the representative fully adsorbing trajectories of *a)* NT2, *b)* NT2I, *c)* NT2Y.

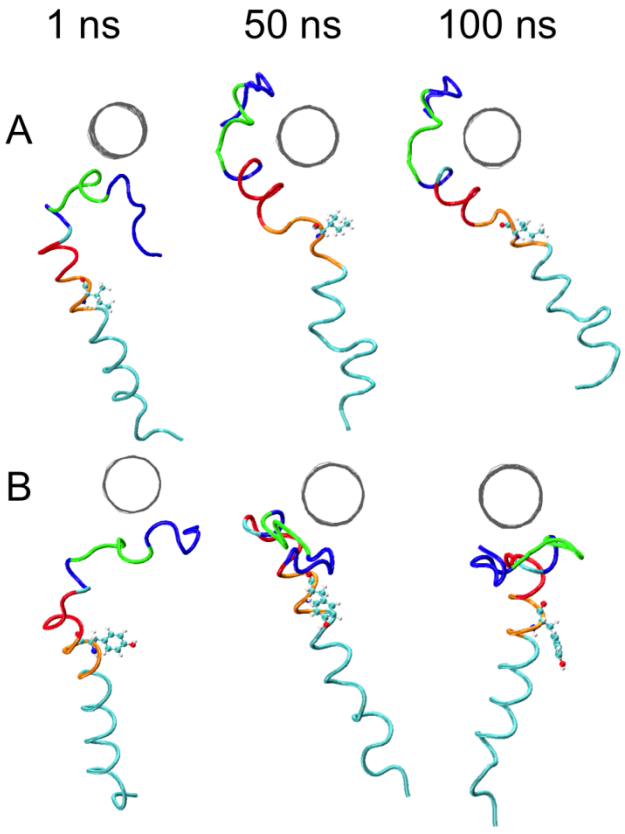

Figure VIII. Cross-sectional snapshots along the SWCNT axis of the partially adsorbing peptide, taken from sample *A)* NT2I and *B)* NT2Y trajectories.

System	Total	1-16	HP1	30-35	36-41
NT2	935.6 (52.7)	423.4 (66.9)	179.5 (18.5)	171.2 (50.4)	168.2 (29.3)
$NT2I_a$	963.6 (55.0)	405.5 (40.8)	159.0 (44.3)	219.1 (24.0)	165.4 (39.8)
$NT2Y_a$	936.4 (45.1)	379.5 (26.6)	184.9 (13.2)	178.9 (19.2)	218.6 (24.7)
$NT2I_{na}$	511.4 (26.3)	0.0 (0.0)	75.1 (28.7)	138.0 (59.1)	156.4 (24.6)
$NT2Y_{na}$	390.6 (116.4)	0.0 (0.0)	2.7 (8.9)	174.7 (18.8)	167.0 (24.0)

Table I. Mean values of the contact area with the SWCNT (in $Å^2$) of key domains, over the simulated adsorbing (NT2; $NT2I_a$; $NT2Y_a$) and the partially adsorbing ($NT2I_{na}$; $NT2Y_{na}$) trajectories.

System	E_2	E_3
$NT2I_a$	- 1.5 (1.3)	- 14.0 (4.9)
$NT2Y_a$	- 0.1 (0.2)	-19.0 (2.0)
$NT2I_{na}$	- 0.7 (0.2)	- 7.1 (2.8)
$NT2Y_{na}$	- 0.2 (0.3)	- 0.2 (0.5)

Table II. Mean values of the interactions E_2 and E_3 (in kcal mol^{-1}), averaged over the last 10 ns of the fully adsorbing ($NT2I_a$; $NT2Y_a$) and the partially adsorbing ($NT2I_{na}$; $NT2Y_{na}$) mutated peptide-nanotube complexes trajectories. Standard deviations are provided within braces.