Electronic Supplementary Material (ESI) for RSC Advances.

In silico design of peptides with binding to the receptor binding domain (RBD) of the SARS-CoV2 and their utility in Bio-sensor Development for SARS-CoV2 Detection

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SUPPORTING INFORMATION

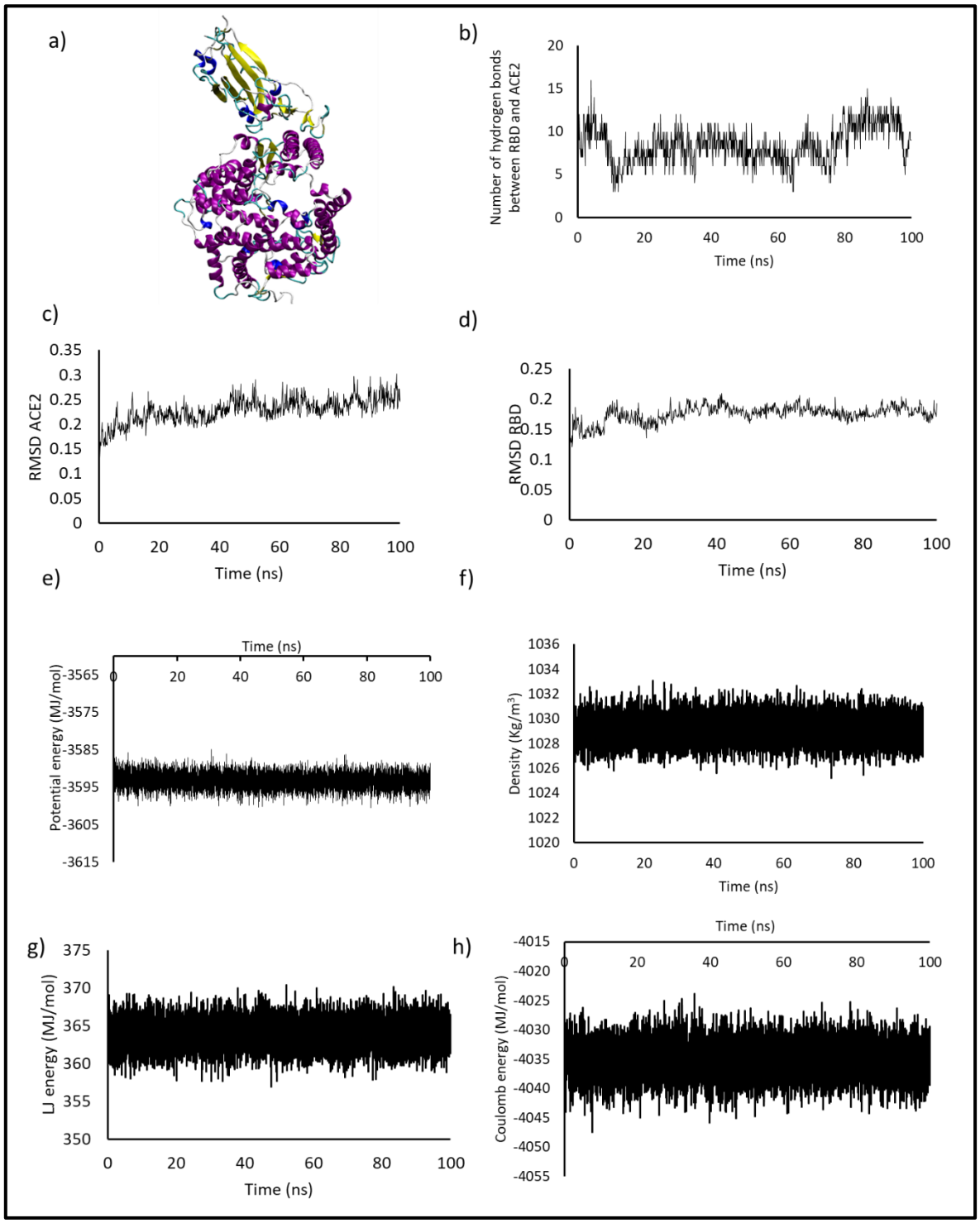

Figure S1. MD simulation of RBD-ACE2 complex. a) The snapshot of complex simulated, alpha-helix, extended beta sheet, 3 to 10-helix, turn and coil are colored purple, yellow, blue, cyan and white respectively. Evolution of quantities as function of time for simulated system: b) The number of hydrogen bonds (8.47 ± 2.15) between RBD and ACE2. The cutoff distance and angle for hydrogen bond are taken as 0.35 nm and 30 degree respectively. c) RMSD of RBD (0.18 ± 0.01). d) RMSD of ACE2 (0.23 ± 0.03). e) The evolution of potential energy. f) density of system. g) Lennard-Jones potential energy. h) Coulombic interaction energy for system.

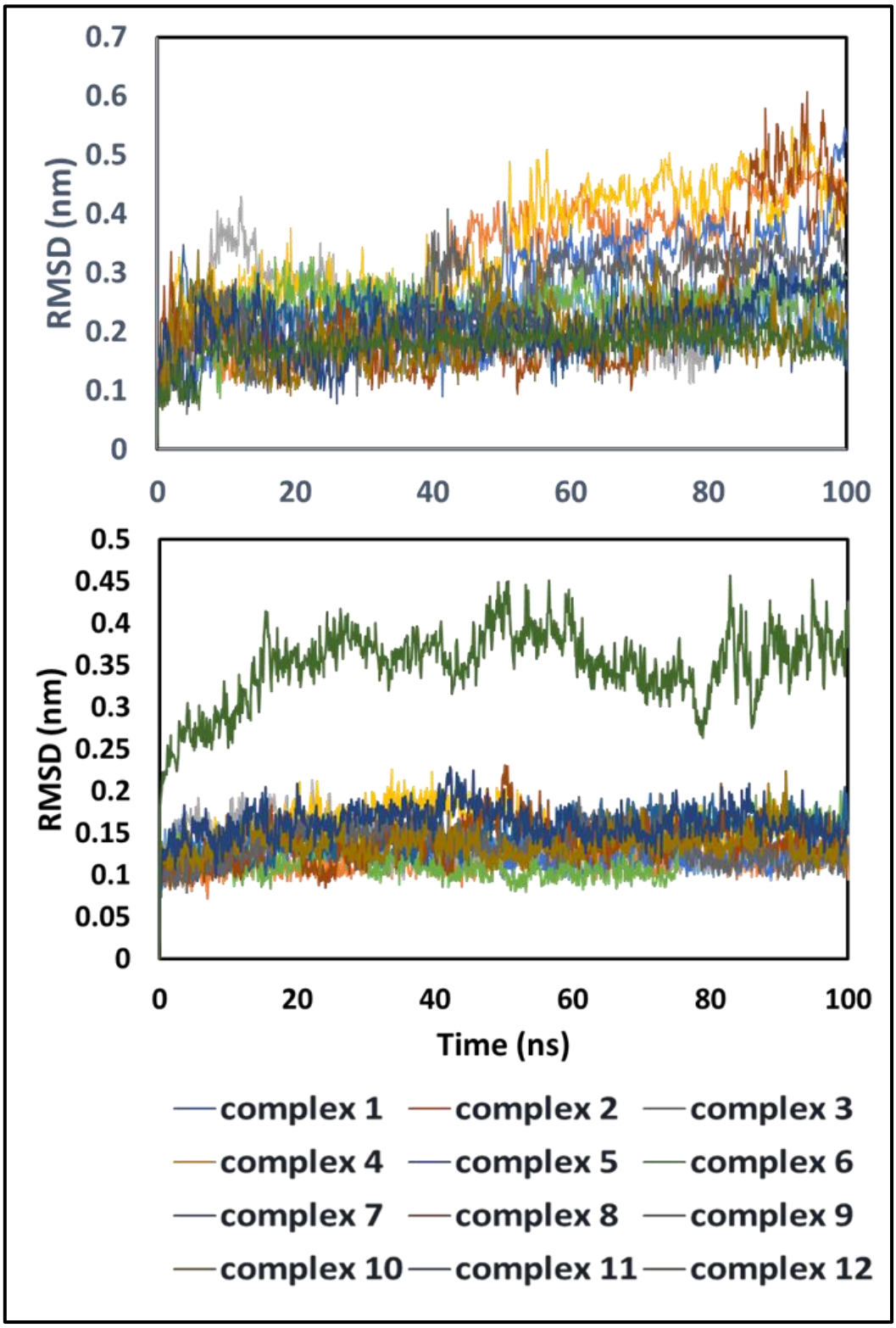

Figure S2. RMSD of each peptide (*top*) and RBD (*bottom*) calculated in RBD-peptide complex simulations.

Figure S3. RMSD (average value) of amino acid residues in each peptide computed in RBD-PD complex system. *In peptide 12, ILE_21, GLN_42 and SER_43 have very large value of 1.59, 2.57 and 3.88 respectively.

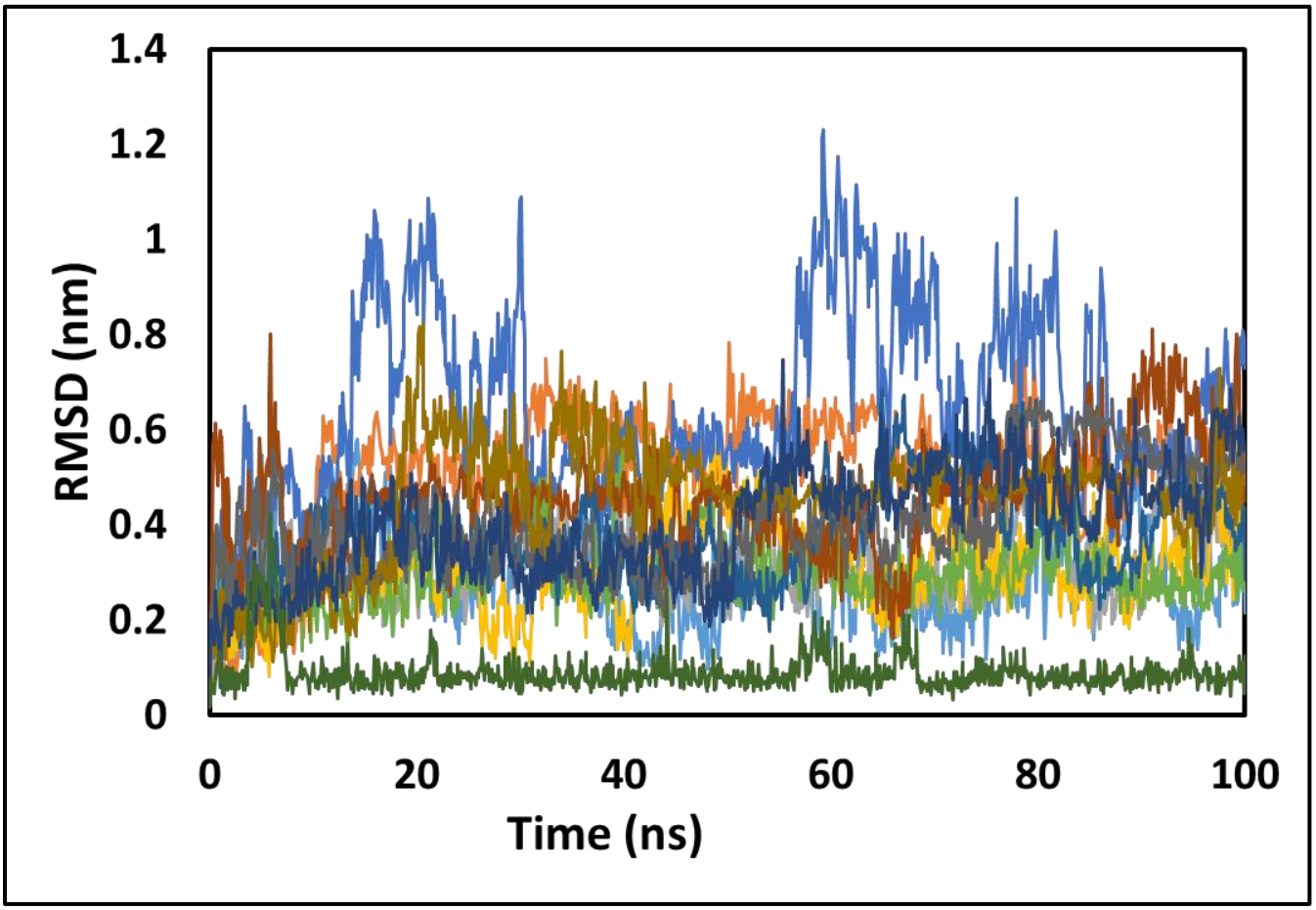

Figure S4. RMSD of each peptide in aqueous condition calculated during 100 ns NPT run. The minimized structures used as a reference for generating the RMSD graph.

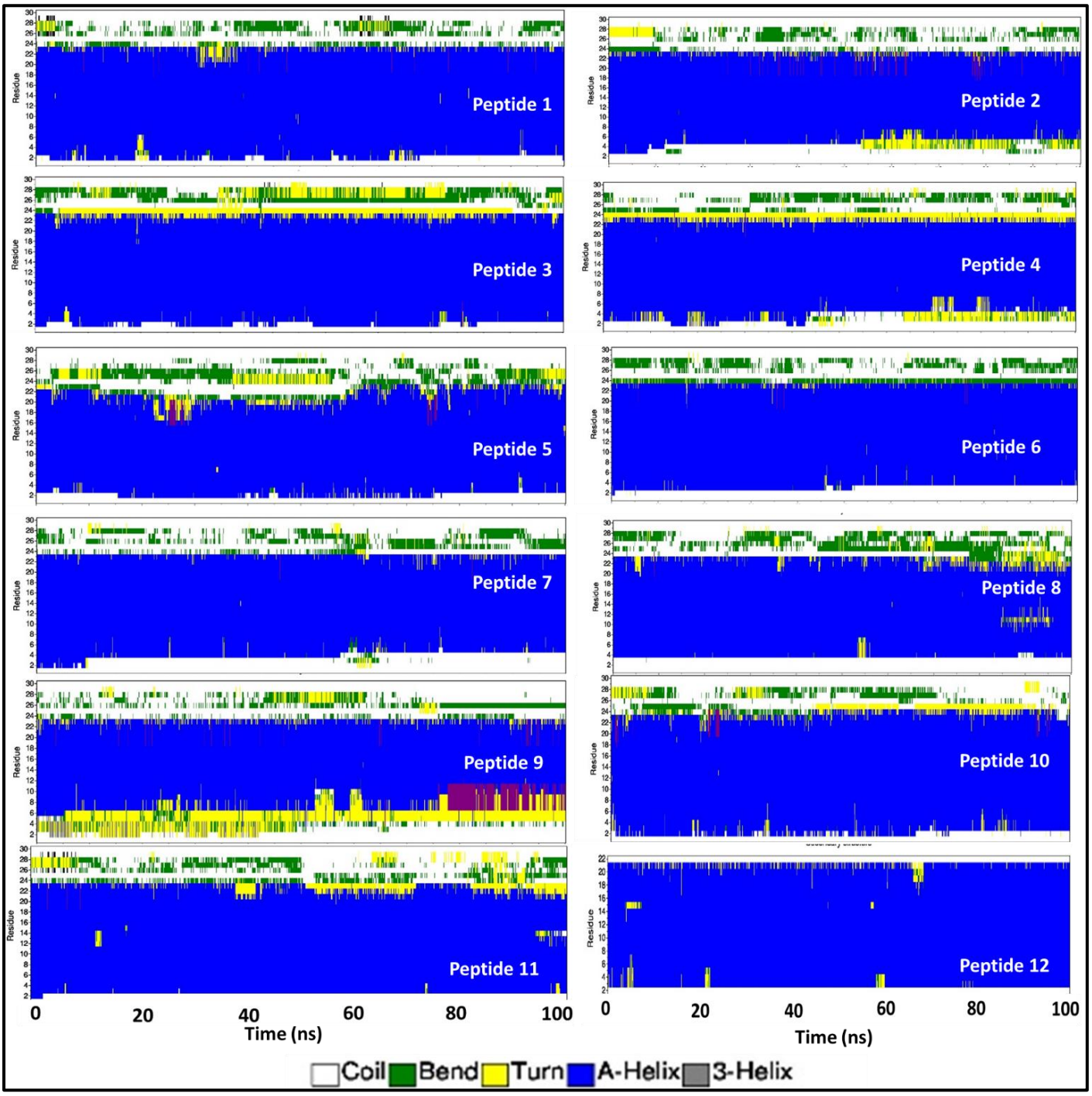

Figure S5. Evolution of secondary structure of amino acid residue in each peptide calculated using DSSP program.

Figure S6. RMSD (average value) of amino acid residues in each peptide calculated in aqueous peptide system. *Few amino acids have very large RMSD, in peptide 7, GLN_51 and PRO_52 have RMSD of 2.66 and 2.78 respectively, in peptide 8, ARG_26, LYS_33, GLU_37 and GLU_40 have RMSD of 3.94, 2.82, 2.59 and 2.59 respectively.

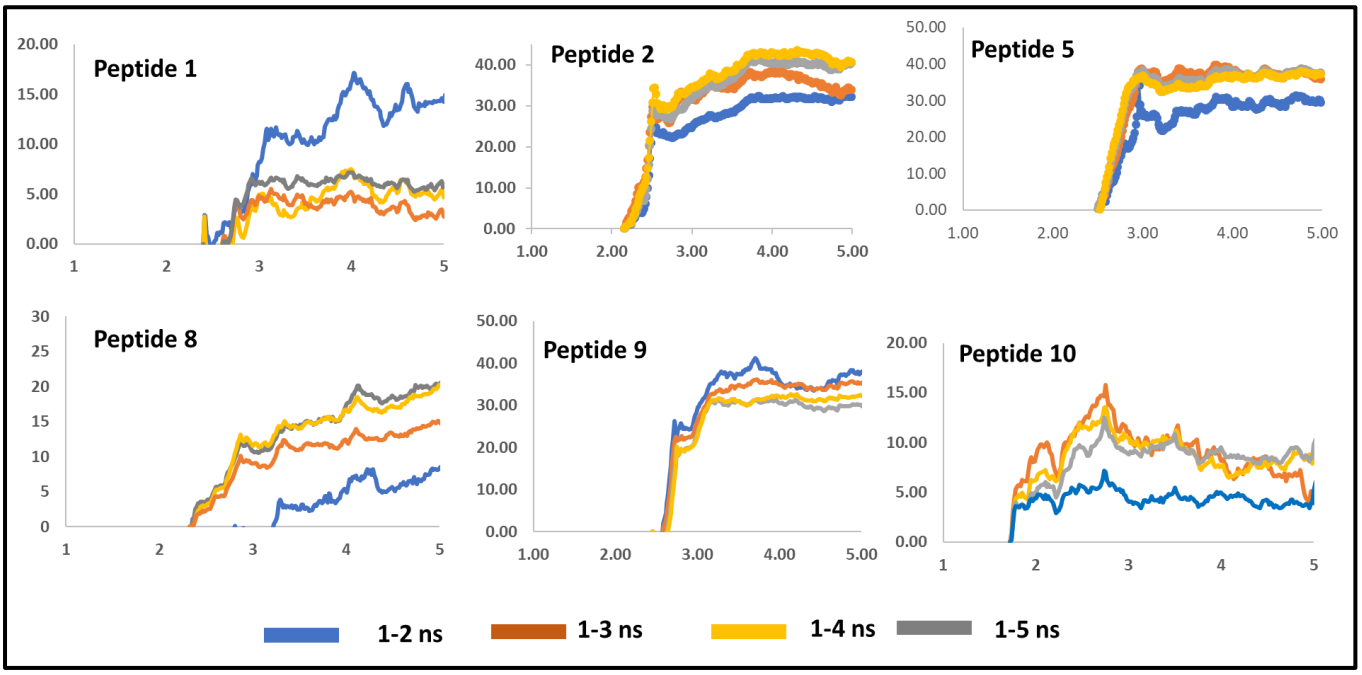

Figure S7 Convergence of the PMF profile in umbrella sampling simulation.

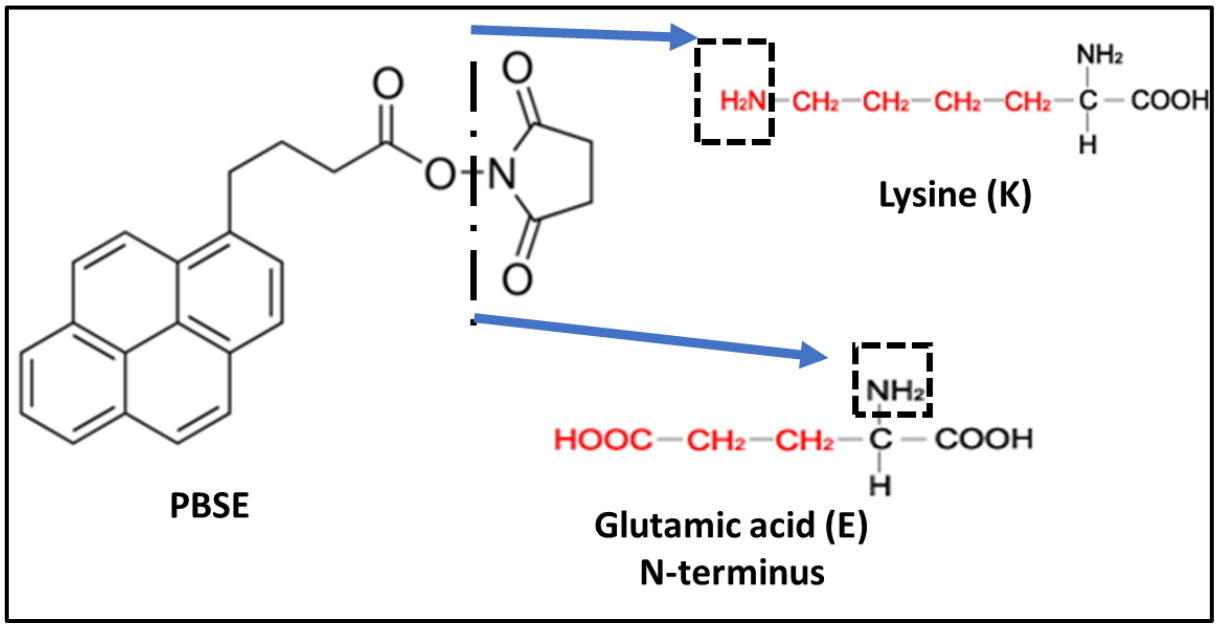

Figure S8. Structure of PBSE linker. The oxygen atom of carboxylic group is attached with the nitrogen atom of the either Lysine (K), or Glutamic acid (E). The O-N bond is broken during synthesis to make PBSE active, to make bond with the amino acids.

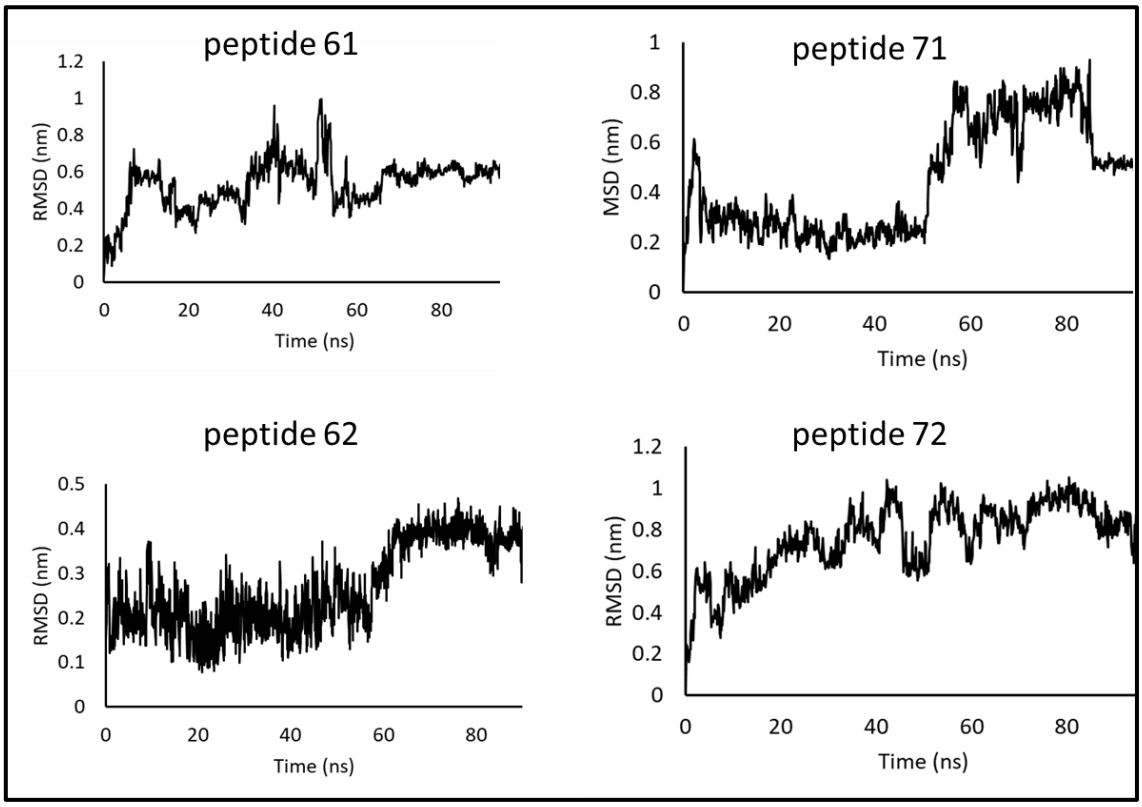

Figure S9. RMSD for peptide interacting with CNT. The Peptide 62 showed least variation in the RMSD as compared to the other systems.

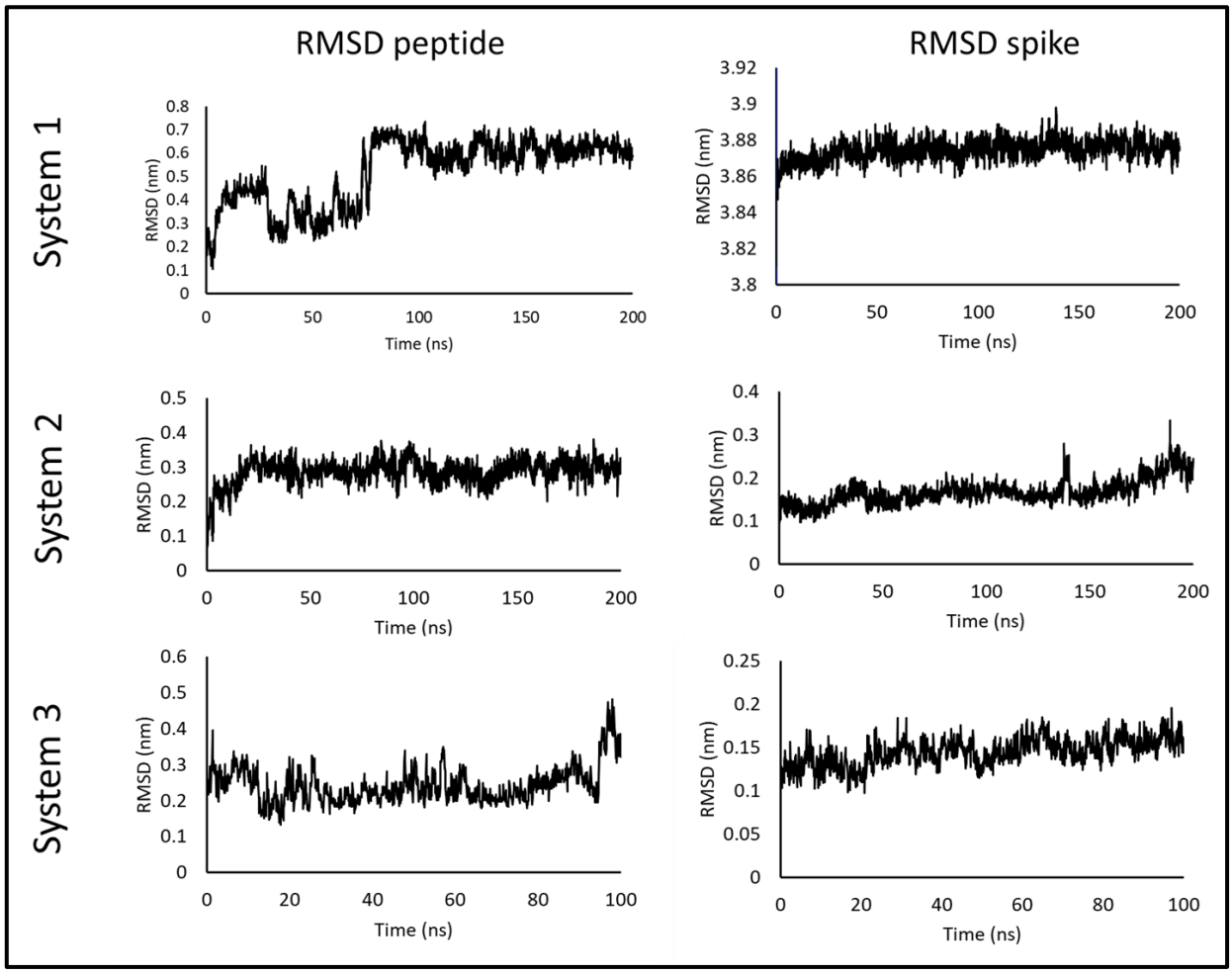

Figure S10. The variation in RMSD for peptide 72 in system 1, 2 and 3. In the system 1, the peptide 72 and spike moved freely, lead to increased RMSD in the peptide and spike. In case of spike, it found to be strongly interacting with the graphene sheet, resulting in significant increase in RMSD. In system 2 and 3, the RMSD remained well within the bounds, below 0.4 nm. Here strong interaction between peptide and spike resulted in less deviation in the RMSD.

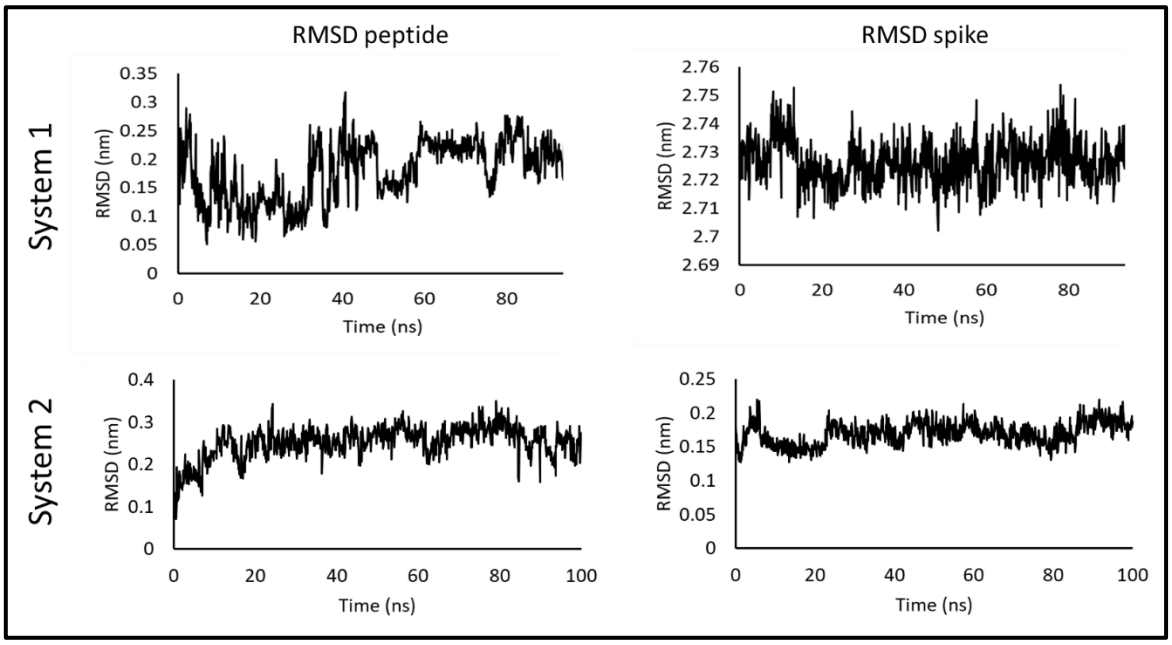

Figure S11. The variation in RMSD for peptide 62 in system 1 and 2. For system 1, where peptide 62 and spike moved freely, increase in RMSD observed. The spike lost its secondary structure significantly. The peptide interacting with CNT, showed less deviation. In system 2, the peptide 62 and spike complex remained stable, which led to lesser deviation in the secondary structure.

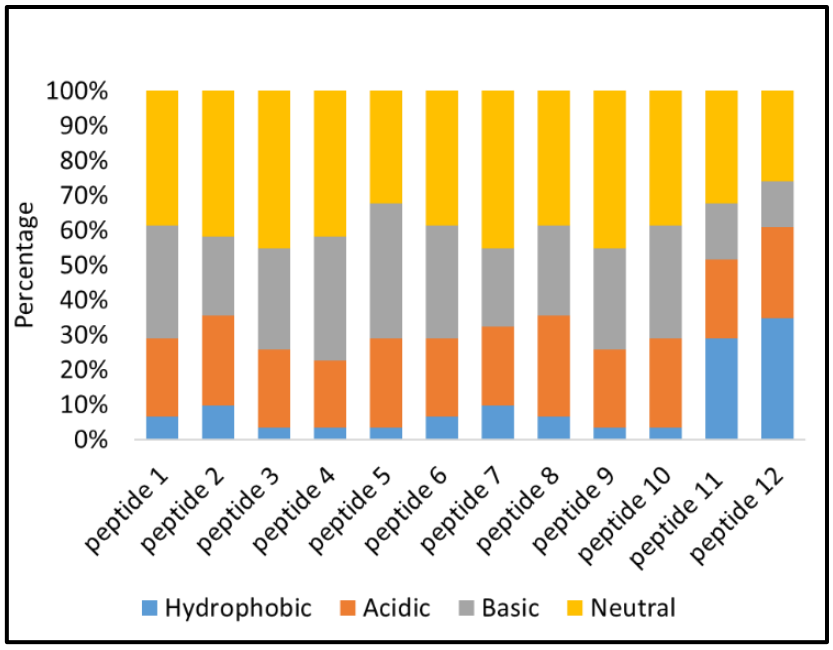

Figure S12. The percentage of polar and nonpolar amino acid residues in each of the peptide.

Table S1: Secondary structure for peptide in water.

Peptide name	Residue 1 to 4	Residue 5 to 23	Residue 24 to 31
Peptide 1	Coil, bent, turn, A-helix	A-helix, turn	Coil, bent, turn, B-bridge
Peptide 2	Coil, bent, turn, A-helix	A-helix, turn, 5-helix, bend	Coil, bent, turn
Peptide 3	Coil, bent, turn, A-helix	A-helix, turn	Coil, bent, turn
Peptide 4	Coil, bent, turn, A-helix	A-helix, turn, 3-helix	Coil, bent, turn
Peptide 5	Coil, A-helix	A-helix, turn, bent, 5-helix	Coil, bent, turn
Peptide 6	Coil, A-helix	A-helix	Coil, bent
Peptide 7	Coil, A-helix	A-helix	Coil, bent, turn
Peptide 8	Coil, A-helix	A-helix, turn	Coil, bent, turn
Peptide 9	Coil, bent, turn, 3-helix	A-helix, turn, 5-helix	Coil, bent, turn
Peptide 10	Coil, A-helix	A-helix, turn, 5-helix	Coil, bent, turn, 5-helix
Peptide 11	Coil, A-helix	A-helix, turn	Coil, bent, turn
Peptide 12	Coil, A-helix	A-helix, turn	-

Table S2: Key amino acids participating in the hydrogen bonding from peptide and RBD side. The amino acids are listed in the descending order based on their occupancy. For each peptide, the top amino acid showed highest occupancy, and the bottom showed the lowest occupancy. Please refer Fig. S9 for atom nomenclature

	peptide	RBD		peptide	RBD
peptide1	LYS48 -main-O	GLY502 -main-N	**peptide7**	LYS48 -main-O	GLY502 -main-N
	ASP30 -side-OD1	LYS417 -side-NZ		ASP30 -side-OD2	LYS417 -side-NZ
	TYR41 -side-OH	GLN498-side-OE1		TYR41 -side-OH	GLN498 -side-OE1
	GLU37 -side-OE2	TYR505 -side-OH		GLN28 -side-OE1	TYR489 -side-OH
	GLU37 -side-OE1	TYR505 -side-OH		HIS50 -main-O	VAL503 -main-N
peptide2	ASP30 -side-OD2	LYS417 -side-NZ	**peptide8**	LYS48 -main-O	GLY502 -main-N
	GLN28 -side-OE1	TYR489 -side-OH		GLN28 -side-OE1	TYR489 -side-OH
	LYS48 -main-O	GLY502 -main-N		TYR41 -side-OH	ASN501-side-OD1
	HIS50 -side-NE2	THR500 -side-OG1		ASP30 -side-OD2	LYS417 -side-NZ
	ARG46 -side-NH1	VAL445 -main-O		GLN51 -main-N	THR500 -main-O
peptide3	LYS48 -side-NZ	ASP405-side-OD1	**peptide9**	LYS48 -main-O	GLY502 -main-N
	ASP30 -side-OD2	LYS417 -side-NZ		ASP30 -side-OD2	LYS417 -side-NZ
	GLN24 -side-OE1	TYR489 -side-OH		ASP30 -side-OD1	LYS417 -side-NZ
	ASP30 -side-CG	LYS417 -side-NZ		ASP30 -side-CG	LYS417 -side-NZ
	GLN24 -side-OE1	TYR473 -side-OH		GLU37 -side-OE1	TYR505 -side-OH
peptide4	CYS48 -main-O	GLY502 -main-N	**peptide10**	GLY49 -main-O	GLY504 -main-N
	GLU24 -side-OE1	TYR473 -side-OH		ASP30 -side-OD2	LYS417 -side-NZ
	GLU24 -side-OE2	TYR473 -side-OH		ASP30 -side-OD1	LYS417 -side-NZ
	GLU24 -side-OE2	LYS458 -side-NZ		LYS48 -main-O	GLY502 -main-N
	GLU24 -side-OE1	LYS458 -side-NZ		GLN23 -main-N	TYR473 -side-OH
peptide5	ASP30 -side-OD2	LYS417 -side-NZ	**peptide11**	LYS48 -main-O	GLY502 -main-N
	CYS48 -main-O	GLY502 -main-N		ASP30 -side-OD1	LYS417 -side-NZ
	ASP30 -side-CG	LYS417 -side-NZ		GLU37 -side-OE1	TYR505 -side-OH
	ASP30 -side-OD1	LYS417 -side-NZ		GLU37 -side-OE2	TYR505 -side-OH
	GLY45 -main-O	GLY502 -main-N		ASP30 -side-OD2	LYS417 -side-NZ
peptide6	LYS48 -main-O	GLY502 -main-N	**peptide12**	GLN24 -side-OE1	ASN487 -side-ND2
	ASP30 -side-OD1	LYS417 -side-NZ		LYS31 -side-NZ	GLN493 -side-OE1
	GLU37 -side-OE2	TYR505 -side-OH		GLU23 -side-OE2	LYS417 -side-NZ
	ASP30 -side-OD2	LYS417 -side-NZ		GLU23 -side-OE1	LYS417 -side-NZ
	TYR41 -side-OH	GLN498-side-OE1		THR27 -side-OG1	TYR489 -side-OH