Supplemental Material:

Membrane partitioning of peptide aggregates – coarse grained molecular dynamics simulations.

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Supplemental Tables

Suppl. Tab. 1: Details of the simulated systems. Number of atoms and molecules used in the systems. In the CG simulations the number of peptides in each simulation is 36.

UA systems	Protein atoms (amino acids)	Water atoms (molecules)	Lipid atoms (molecules)	Counter ions (ion type)	Total number of atoms
^{u}B-*H*-*T*-*H*	391 (42)	71451 (23817)	-	-	71842
^{u}B-*T*	192 (23)	46461 (15487)	-	-	46653
^{u}B-*T*/2	93 (12)	22644 (7548)	-	-	22737
^{u}B-*H*-*T*/2	186 (20)	34614 (11538)	-	-	34800
^{u}B-R9-*T*/2	246 (21)	51006 (17002)	-	9 (Cl-ion)	51261
^{u}R9-*P*	339 (28)	64161 (21387)	-	8 (Cl-ion)	64509

CG systems	Protein beads (molecules)	Water beads (molecules)	Lipid beads (molecules)	Counter ions (ion type)	Total number of beads
B-*H*-*T*-*H*	3060 (36)	49491 (16497)	14352 (1104)	-	66903
B-*T*	1548 (36)	50847 (16949)	14352 (1104)	-	66747
B-*T*/2	720 (36)	51471 (17157)	14352 (1104)	-	66543
B-*H*-*T*/2	1440 (36)	50838 (16946)	14352 (1104)	-	66630
B-R9-*T*/2	1692 (36)	50703 (16901)	14352 (1104)	9 (Cl-ion)	66756
R9-*P*	2412 (36)	50139 (16713)	14352 (1104)	8 (Cl-ion)	66912
^{uc}B-*H*-*T*/2	1440 (36)	63588 (21196)	-	-	65028
^{uc}B-R9-*T*/2	1692 (36)	63045 (21015)	-	9 (Cl-ion)	65061

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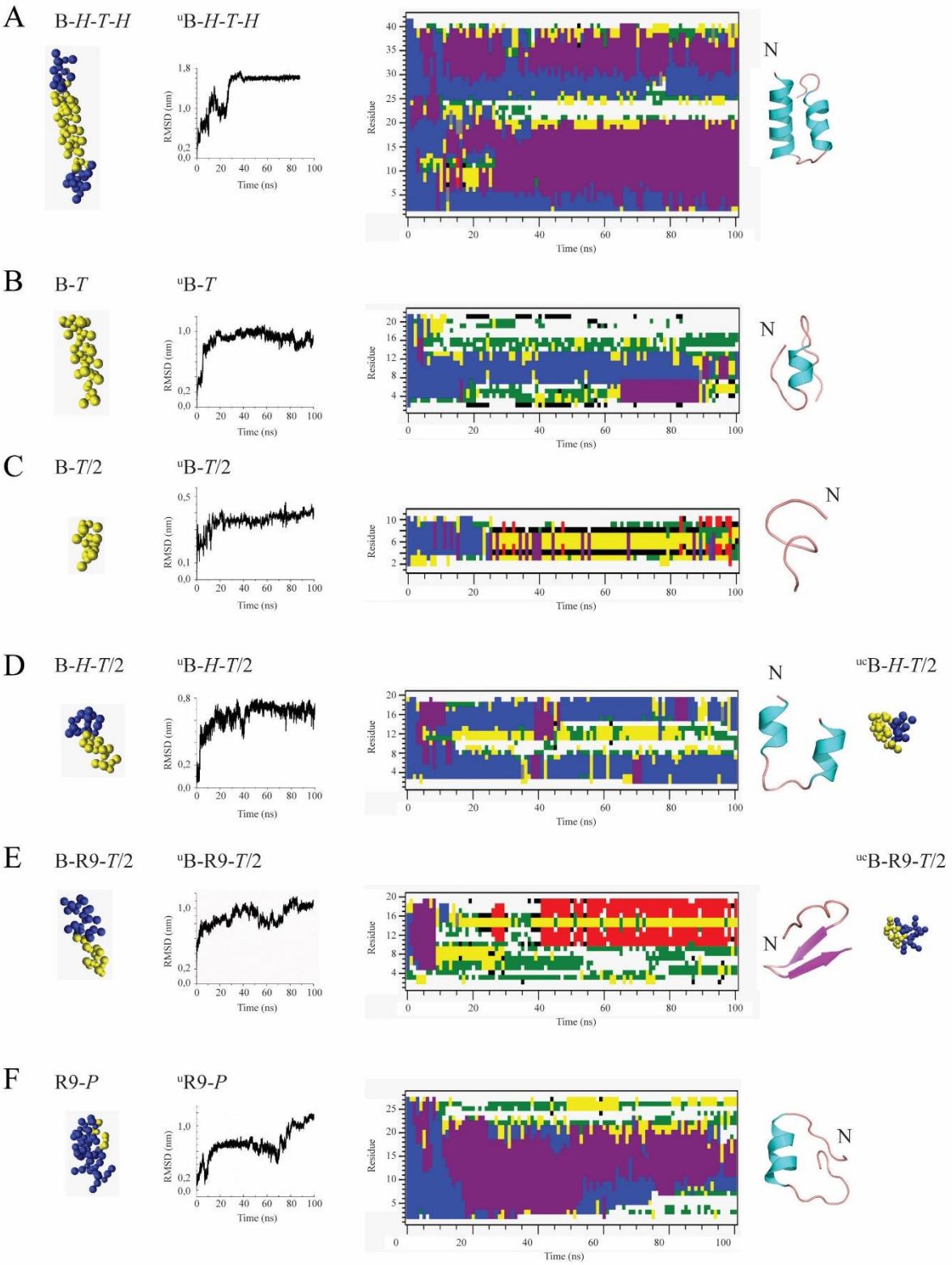
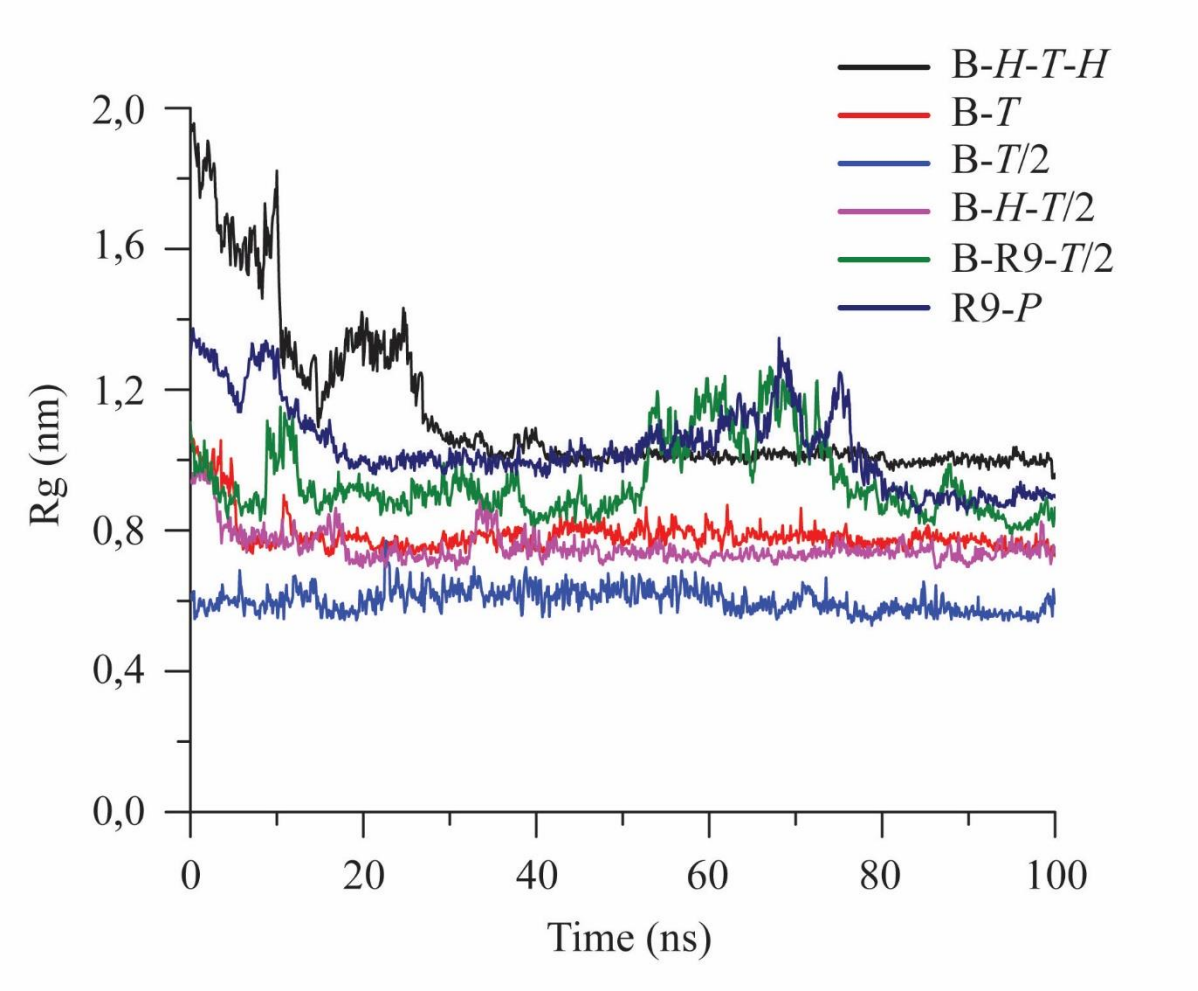
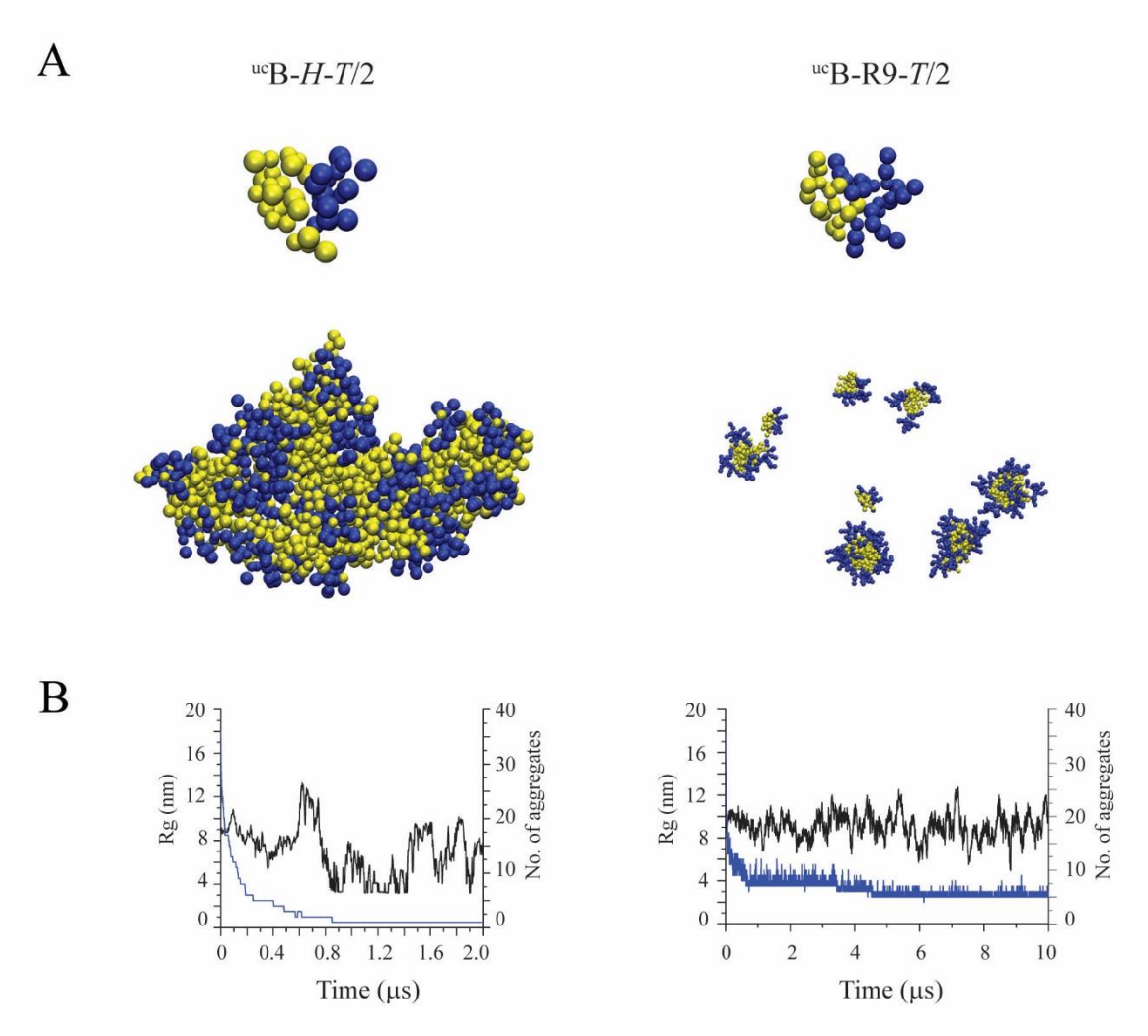


Suppl. Figure 1: (see next page)

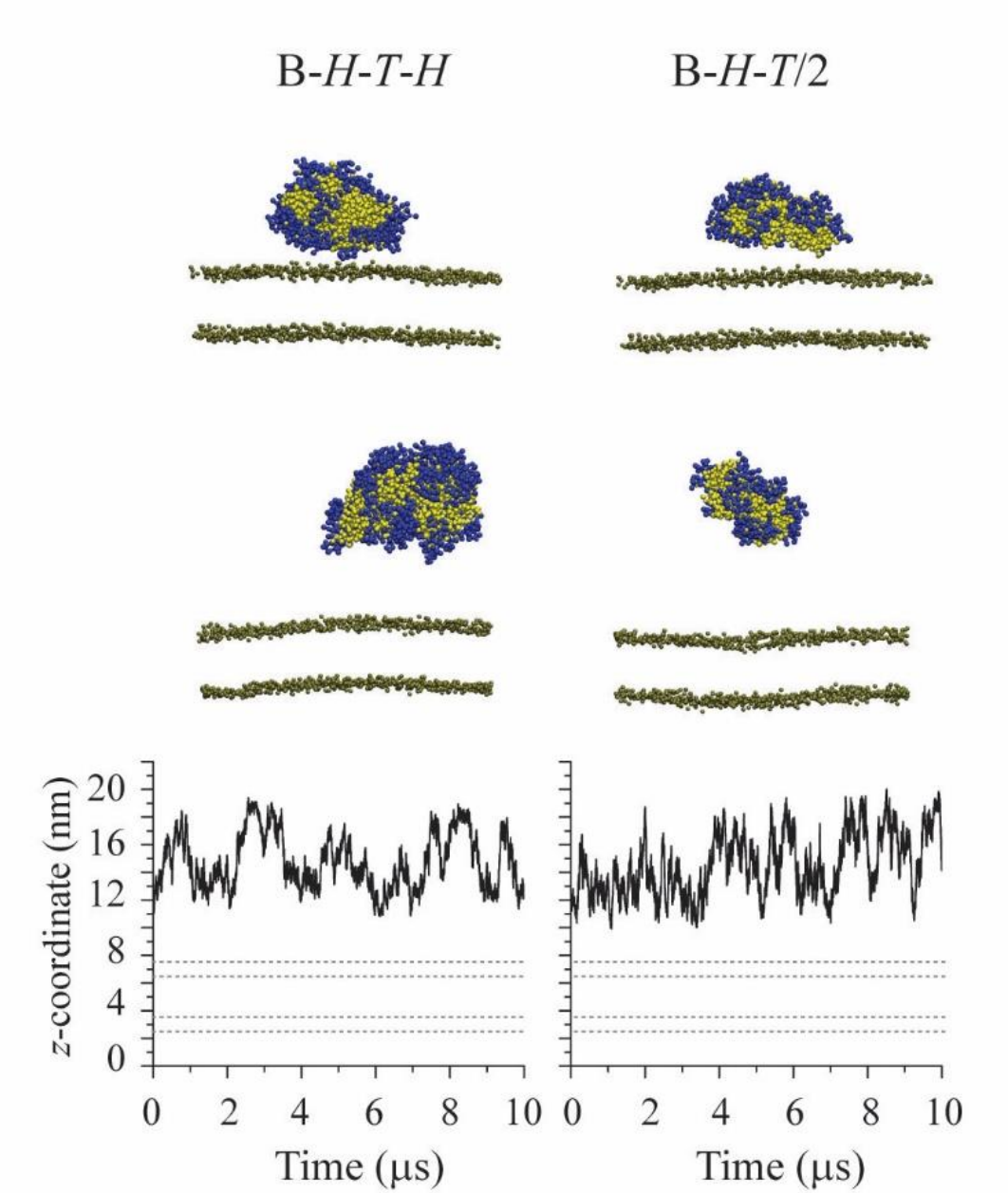
Suppl. Fig. 1: Analysis of the UA MD simulations of the peptides. (A) ^{u}B-*H*-*T*-*H*, (B) ^{u}B-*T*, (C) ^{u}B-*T*/2, (D) ^{u}B-*H*-*T*/2, (E) ^{u}B-R9-*T*/2, and (F) ^{u}R9-*P*. From left to right is shown (i) the coarse grained representations of the respective ideal helical models (based on ϕ = -65 °, ψ = -39 °, from left to right: B-*H*-*T*-*H*, B-*T*, B-*T*/2, B-*H*-*T*/2, B-R9-*T*/2, and R9-*P*), (iii) the *Define* Secondary Structure of *Proteins* (DSSP) plot, (iv) the structure of the peptides taken at 100 ns with the helical motifs shown as blue ribbons, β-sheet motifs as grey arrows and random coil motifs as lines, and (v) the respective CG models of the structures ^{u}B-*H*-*T*/2 (D) and ^{u}B-R9-*T*/2 (E) as ^{uc}B-*H*-*T*/2, and ^{ug}B-R9-*T*/2, respectively. The hydrophobic and hydrophilic amino acids of the CG models are highlighted in yellow and blue spheres, respectively. u = from **u**nited atom simulations; uc = referring to a '**u**nited atom to **c**oarse grained' model.



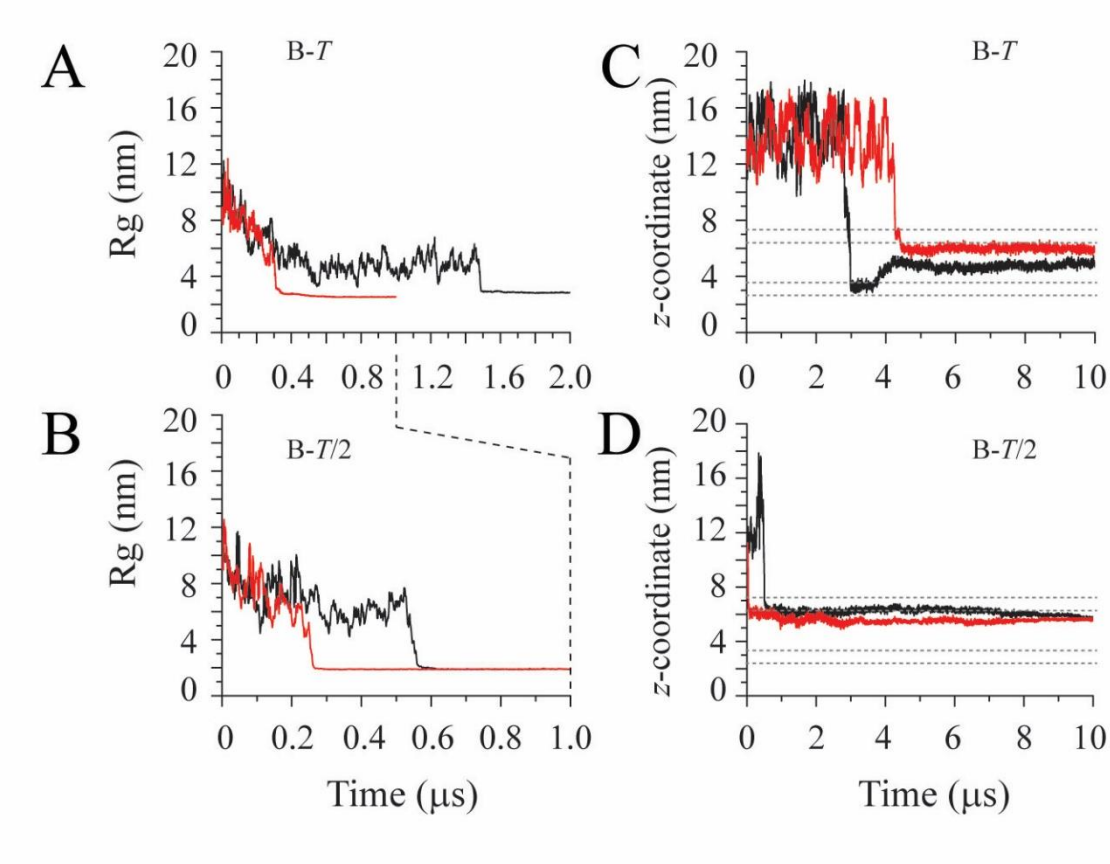
Suppl. Fig. 2: Time resolved calculation of the radius of gyration (Rg) of the UA atom model peptides. The peptides started as ideal helices (based on ϕ = -65 °, ψ = -39 °): ^{u}B-*H*-*T*-*H* (black), ^{u}B-*T* (red), ^{u}B-*T*/2 (blue), ^{u}B-*H*-*T*/2 (pink), ^{u}B-R9-*T*/2 (green), and ^{u}R9-*P* (dark blue).



Suppl. Fig. 3: Aggregation of non-helical peptides. (A) Coarse grained model of ^{uc}B-*H*-*T*/2 (see also Suppl. Figure 1B) as a monomer (upper panel left) as well as ^{uc}B-R9-*T*/2 (upper panel right) and as 36 copies aggregated after a 10 μs MD simulation (lower panel left and right, respectively). (B) Dynamics of peptide aggregation monitored by calculating the radius of gyration (Rg) (black lines) and the number of aggregates (blue lines) for ^{uc}B-*H*-*T*/2 (left) and ^{uc}B-R9-*T*/2 (right).



Suppl. Fig. 4: Membrane insertion of peptide aggregates. Dynamics of the aggregates of the amphipathic peptides B-*H*-*T* (left panel) and B-*H*-*T*/2 (right panel) are shown with structures of the system at 10 μs (upper part). The dynamics are followed monitoring the *z*-coordinate of the center of mass of the peptide aggregates. The boundaries of the lipid head group regions are outlined as dashed lines. The spheres of the peptides are shown in yellow for the hydrophobic residues and in blue for the hydrophilic residues, those of the lipids in green and the head groups as brown spheres.



Suppl. Fig. 5: Dynamics of aggregation of selected peptides. Dynamics of assembling peptides B-*T* (A,C) and B-*T*/2 (B,D) monitored by calculating (A,B) the radius of gyration (Rg) of the all the peptides as a single unit and (C,D) when inserting into lipid membrane followed by monitoring the *z*-coordinate of the center of mass of the peptide aggregates. The peptides are simulated with their N and C termini either in their charged (black curves) or uncharged (red curves) form.