

Figure S1: Plots of the number of residues forming secondary structure elements of the nanofibers over the simulation time.

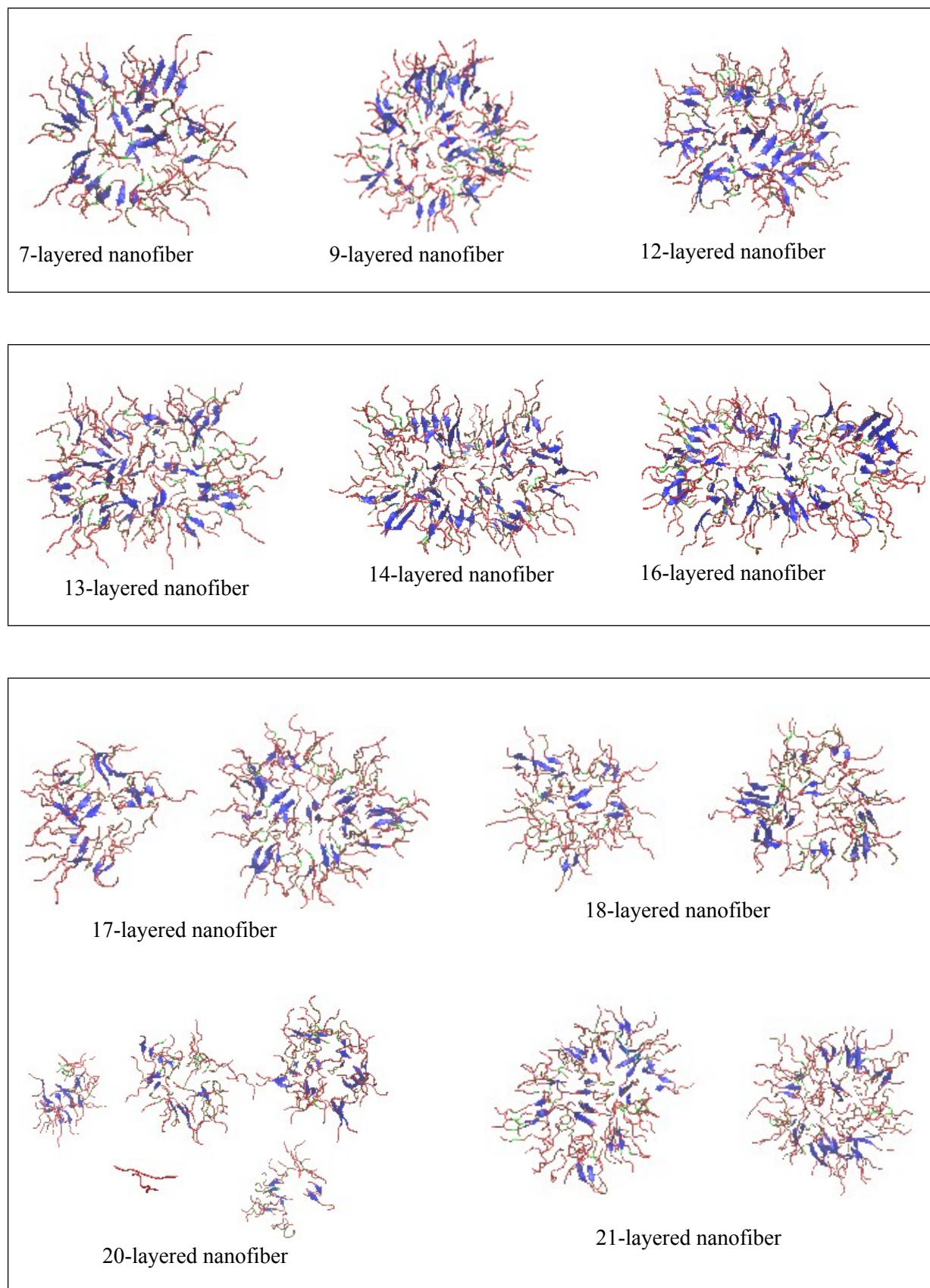
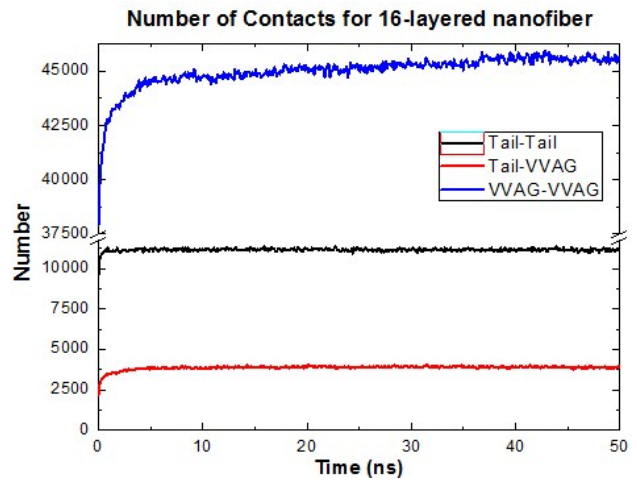
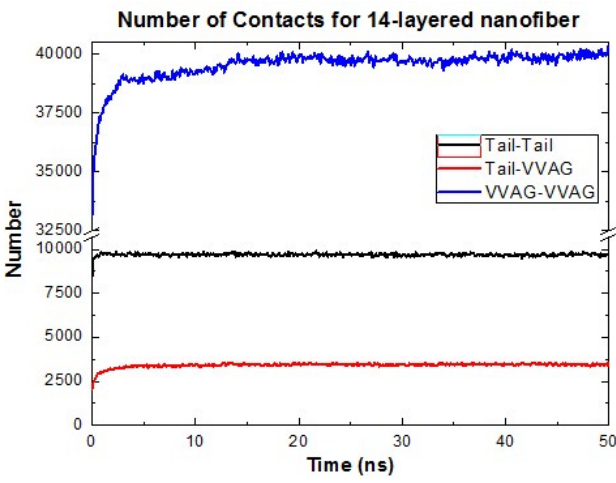
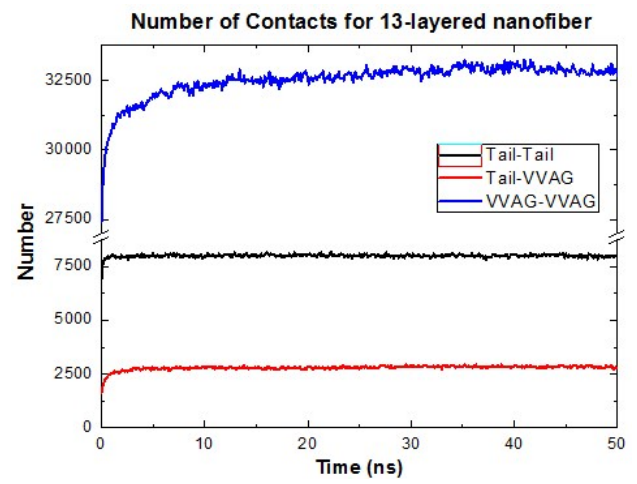
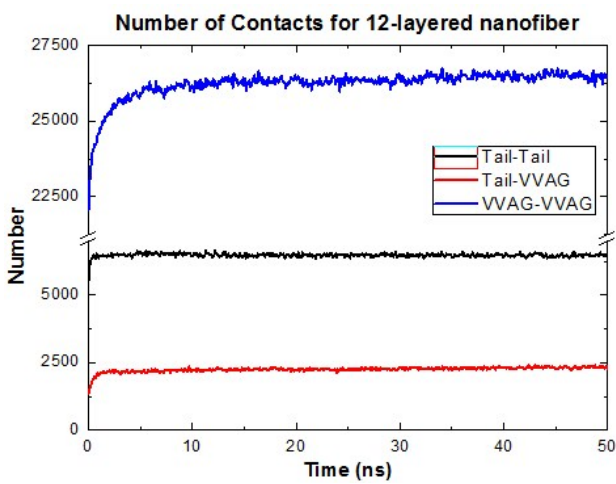
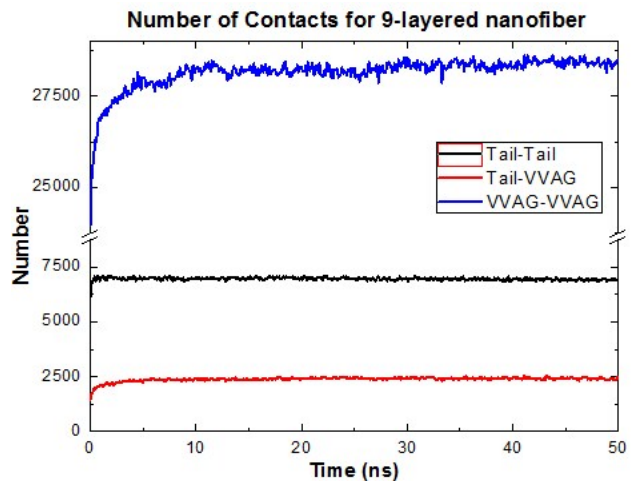
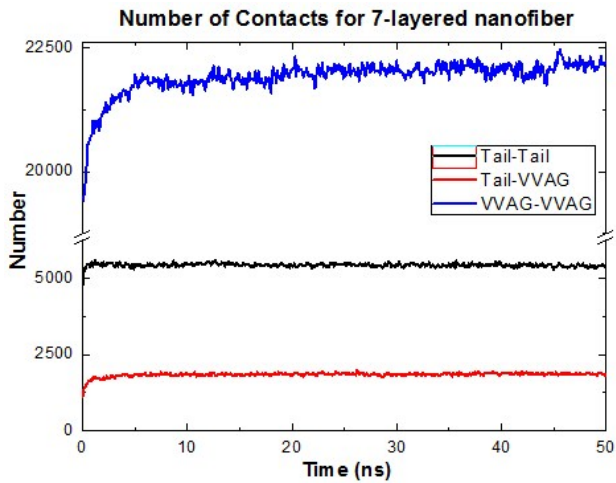


Figure S2: β -sheets in the self-assembled nanofibers at 50th ns.



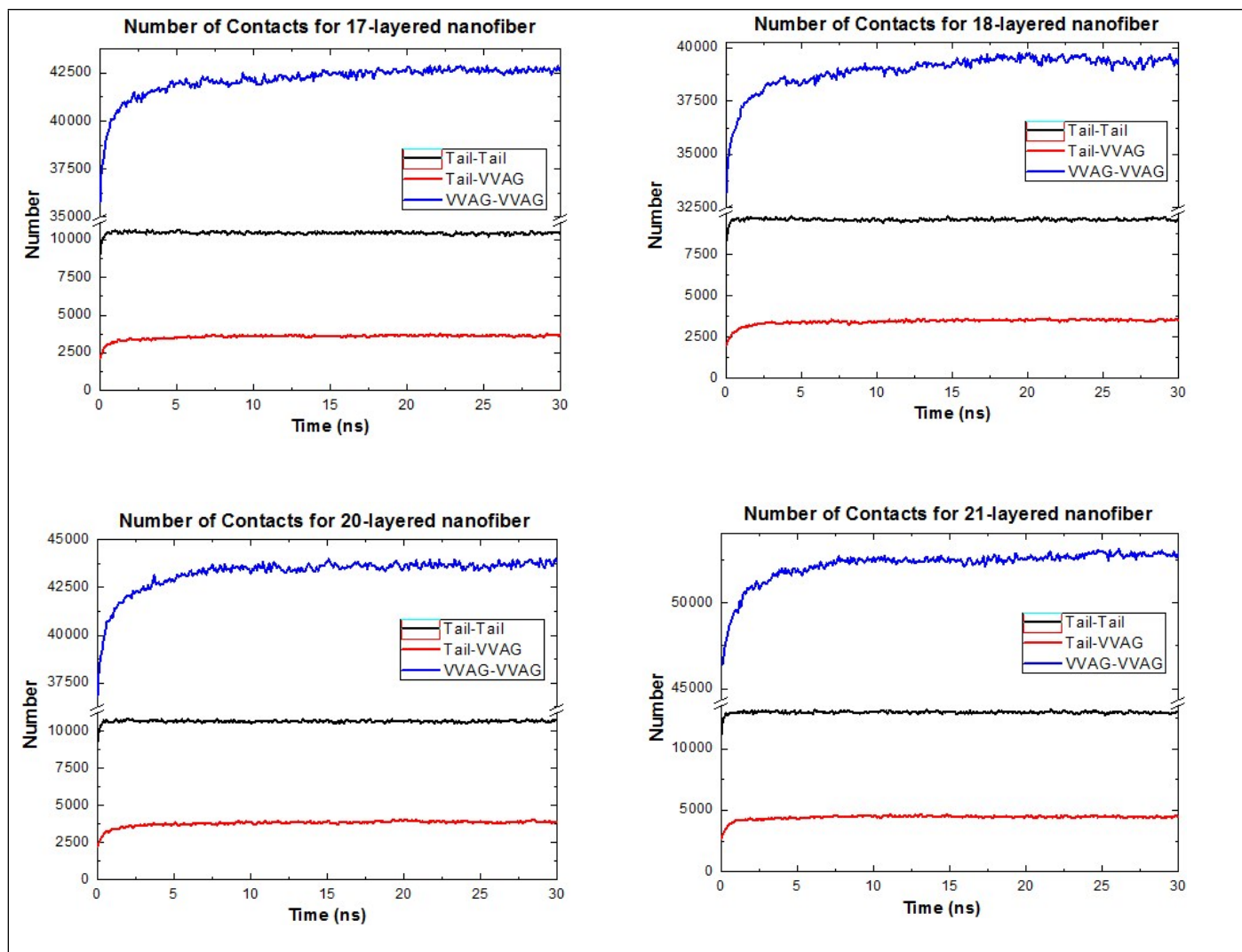
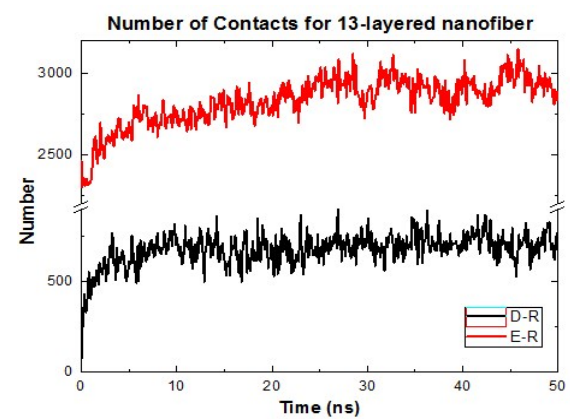
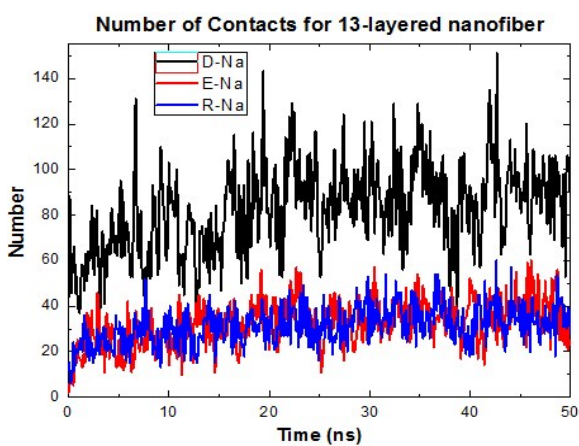
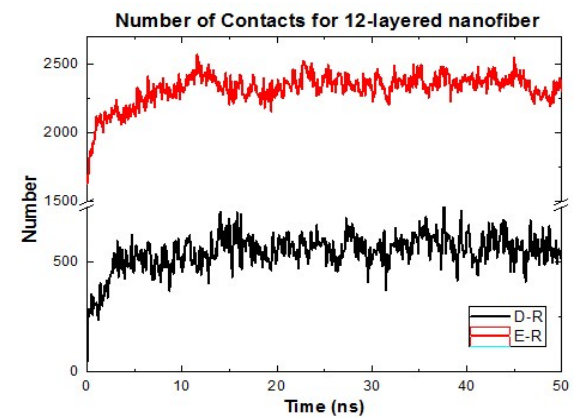
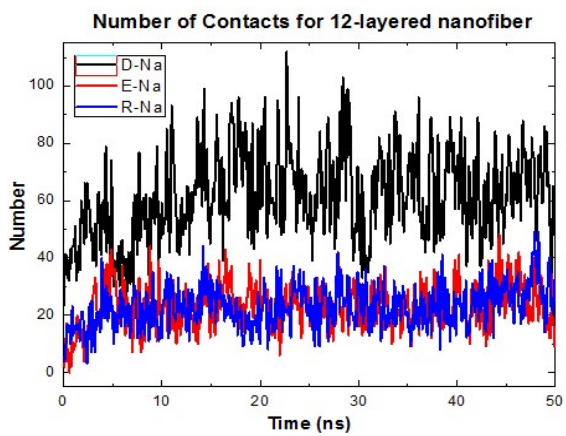
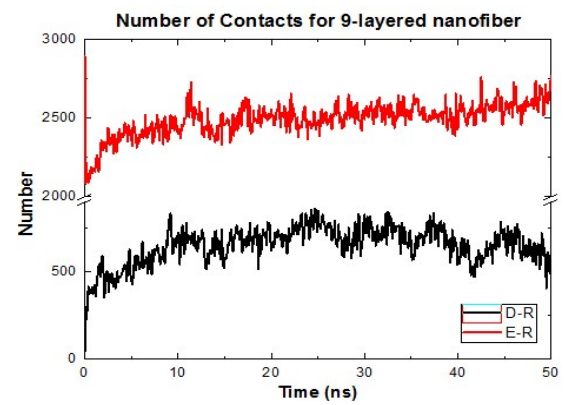
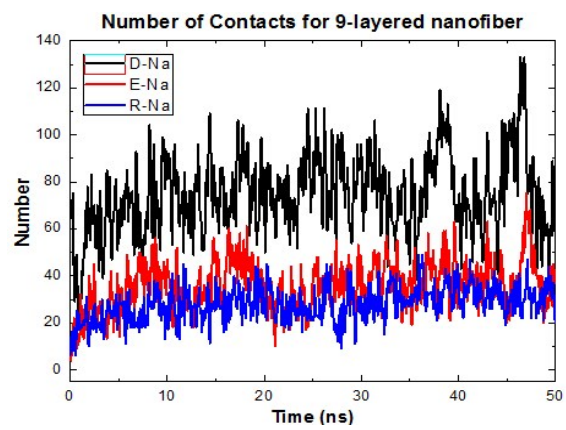
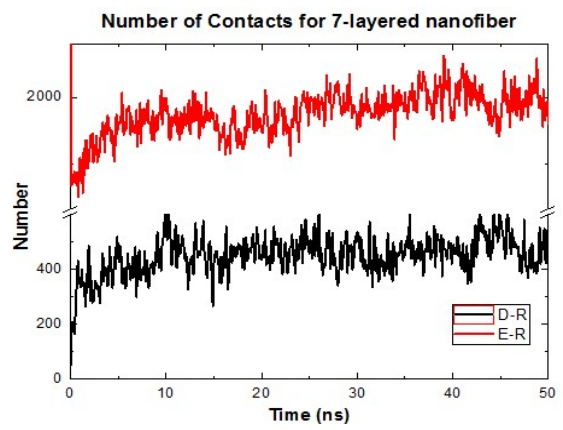
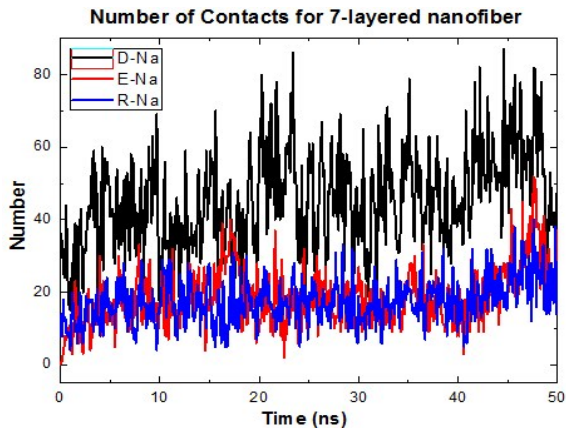
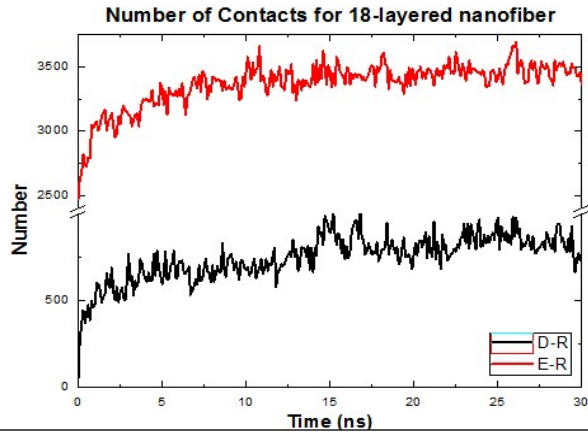
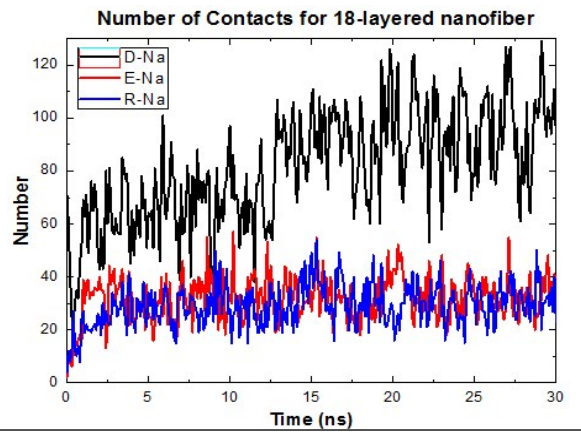
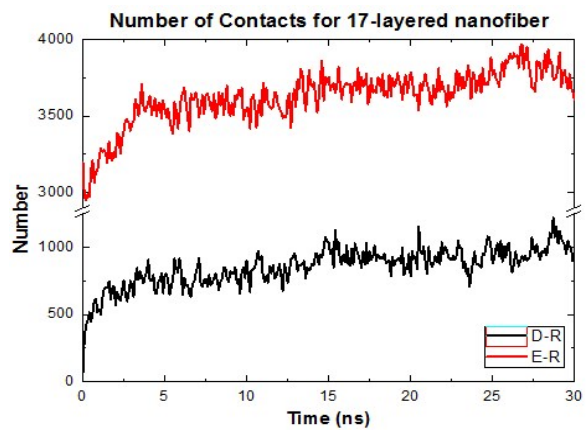
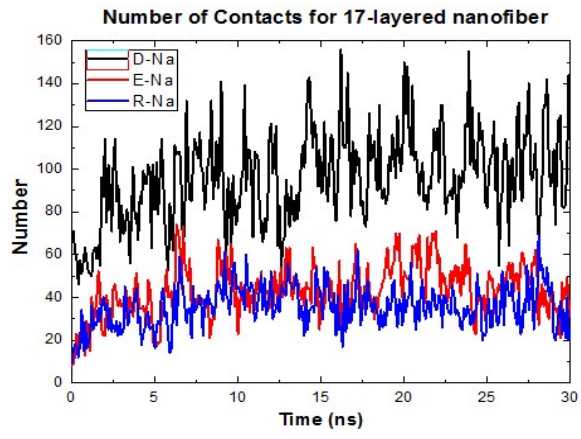
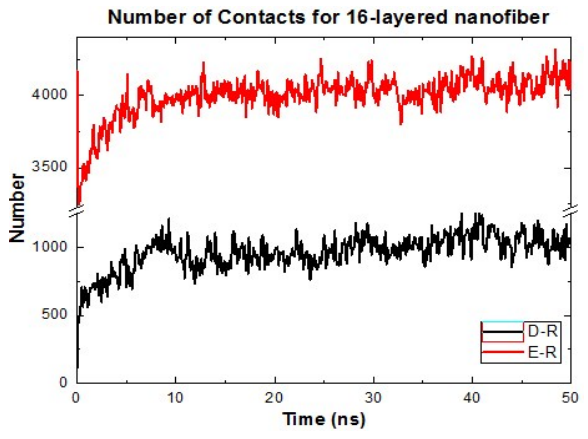
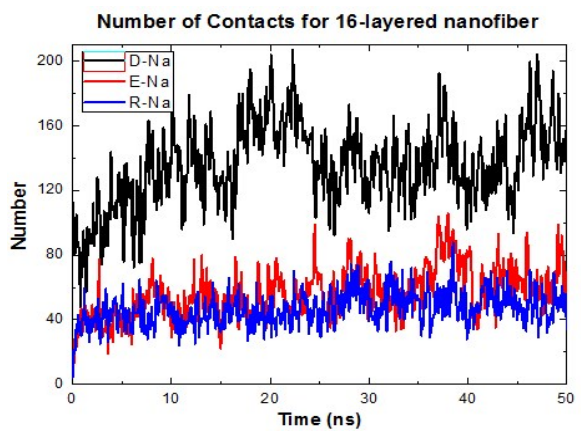
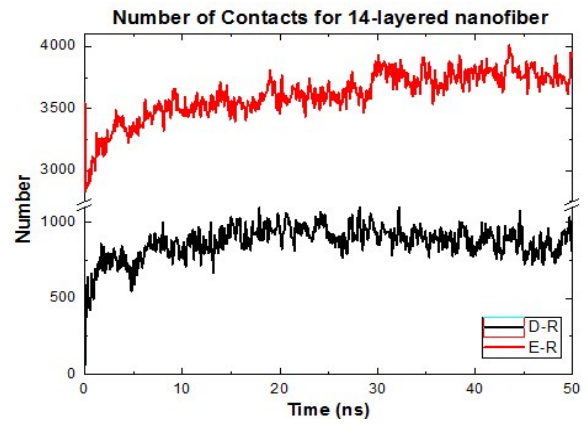
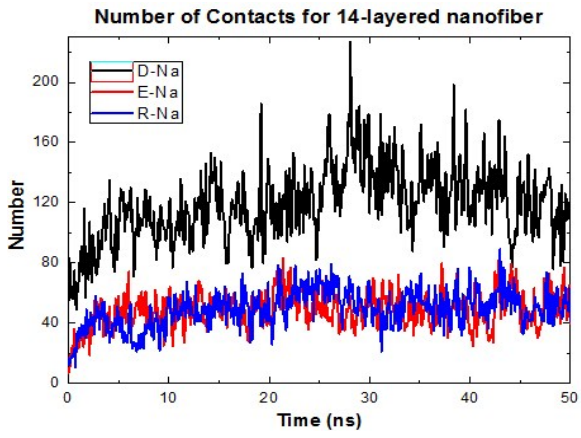


Figure S3: Hydrophobic interactions (number of contacts $< 0.4 \text{ nm}$) of the nanofibers over the simulation time.





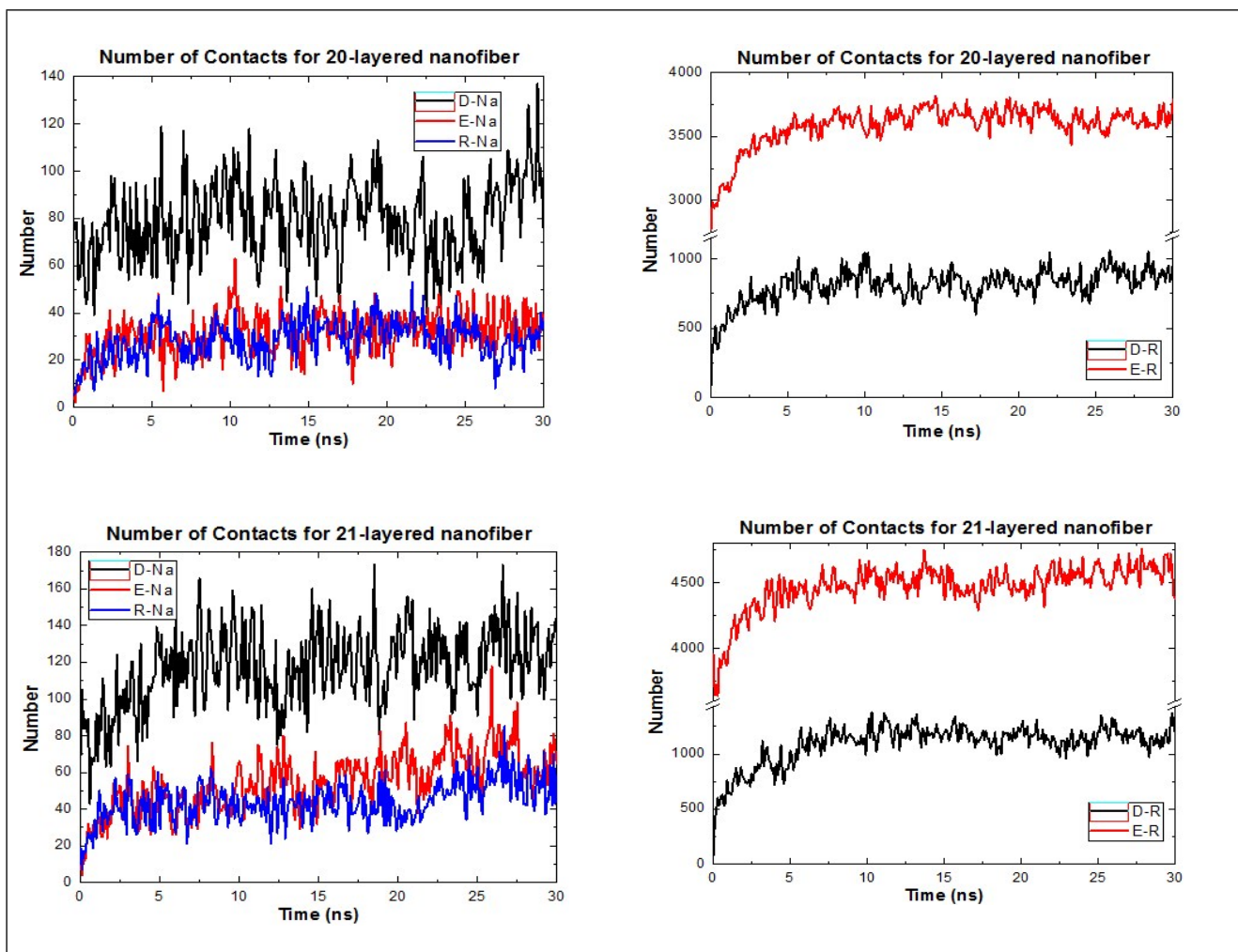


Figure S4: Electrostatic interactions (number of contacts $< 0.4 \text{ nm}$) of the nanofibers over the simulation time.

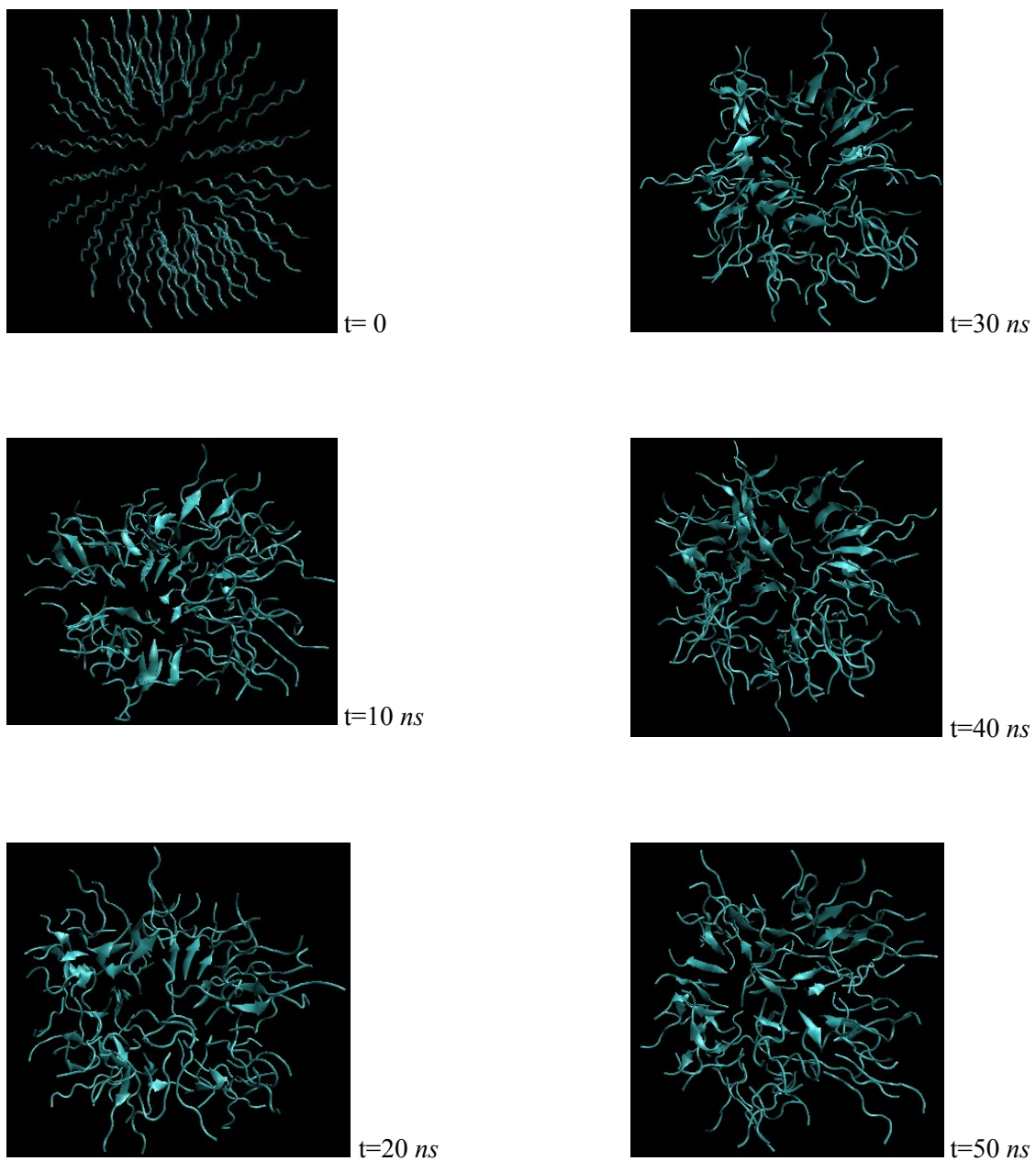


Figure S5. Snapshots of self-assembled 7-layered nanofiber for each 10 ns of 50 ns simulation.

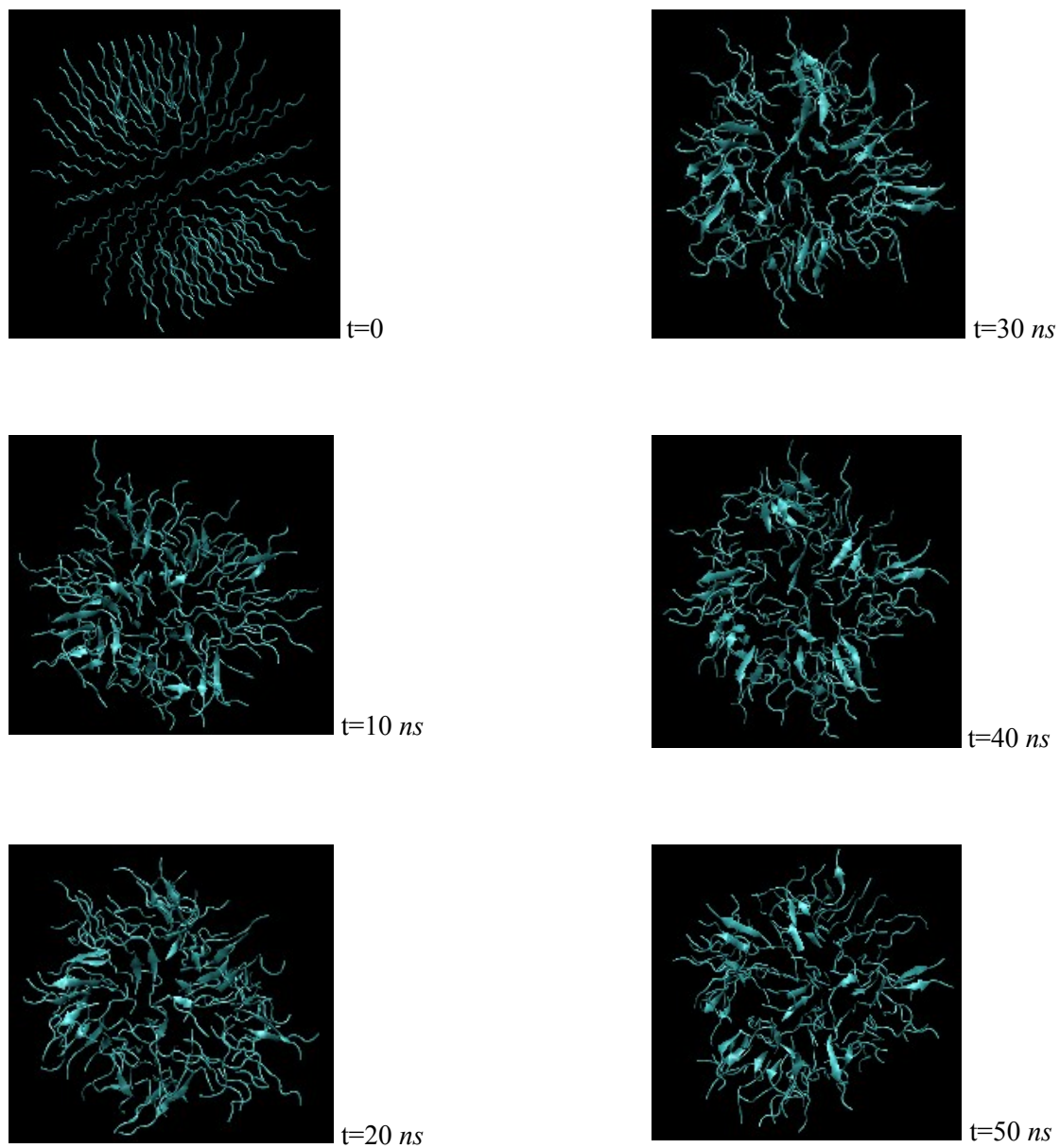


Figure S6. Snapshots of self-assembled 9-layered nanofiber for each 10 *ns* of 50 *ns* simulation.

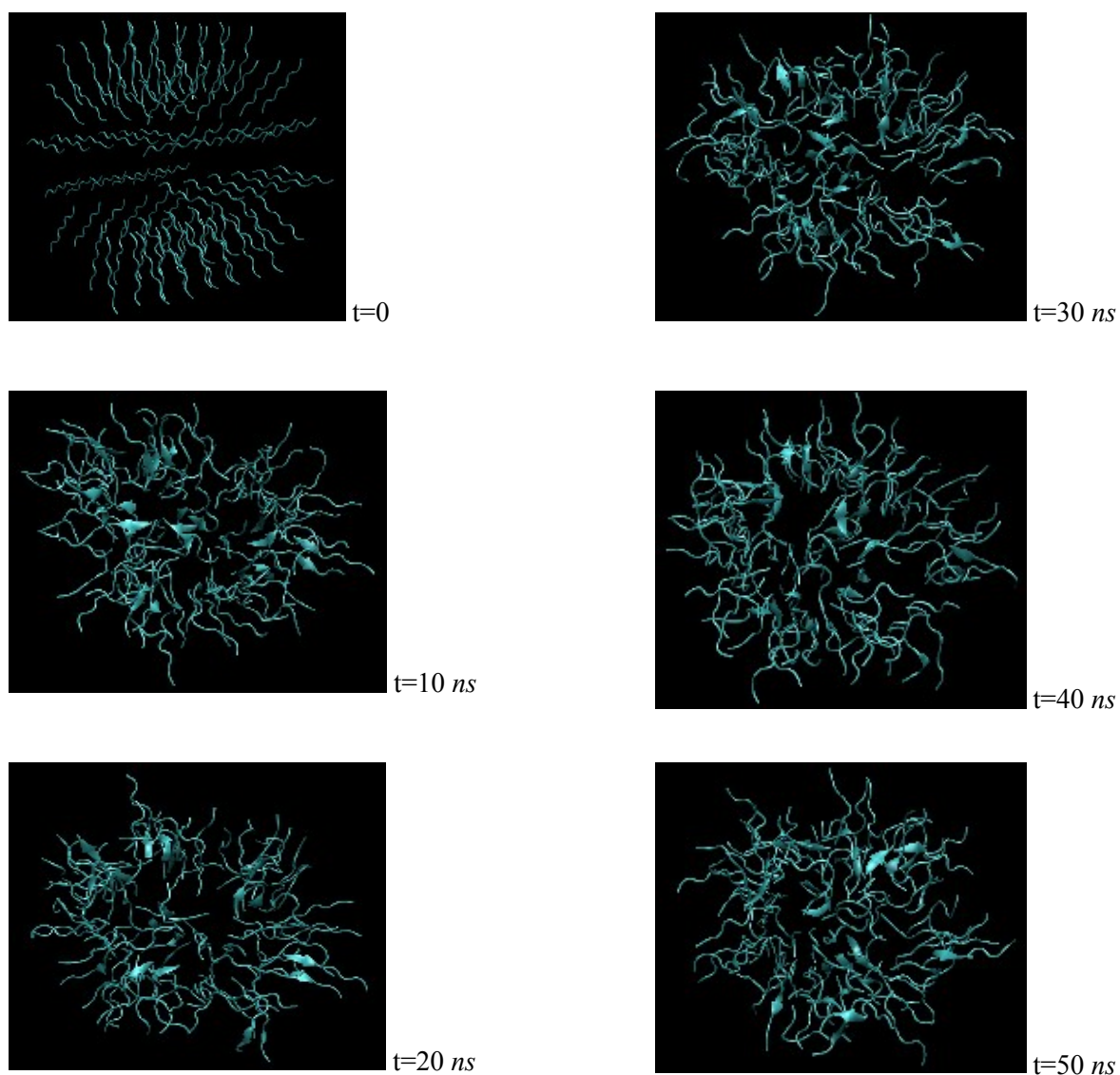


Figure S7. Snapshots of self-assembled 12-layered nanofiber for each 10 *ns* of 50 *ns* simulation.

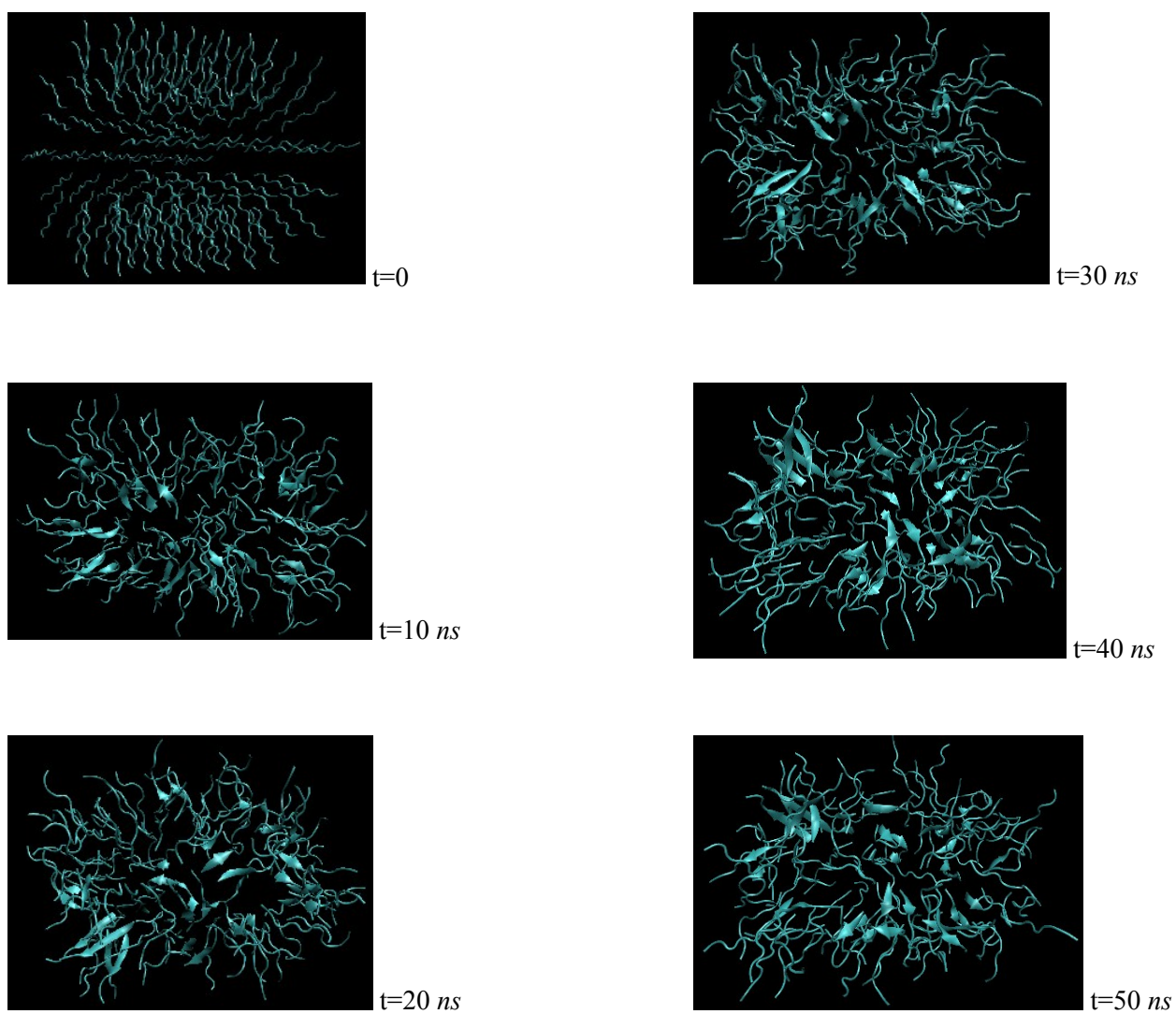


Figure S8. Snapshots of self-assembled 13-layered nanofiber for each 10 *ns* of 50 *ns* simulation.

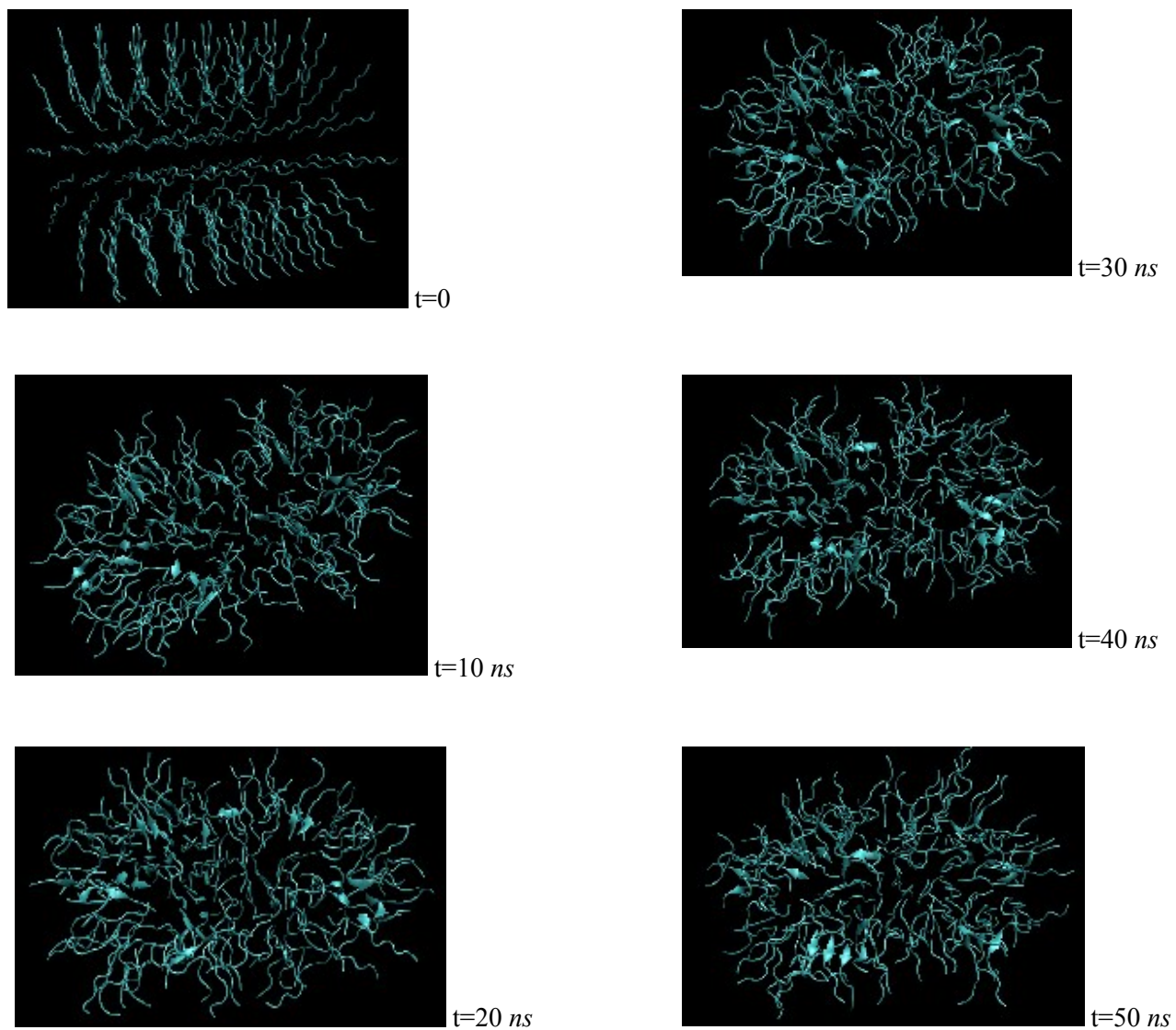


Figure S9. Snapshots of self-assembled 14-layered nanofiber for each 10 *ns* of 50 *ns* simulation.

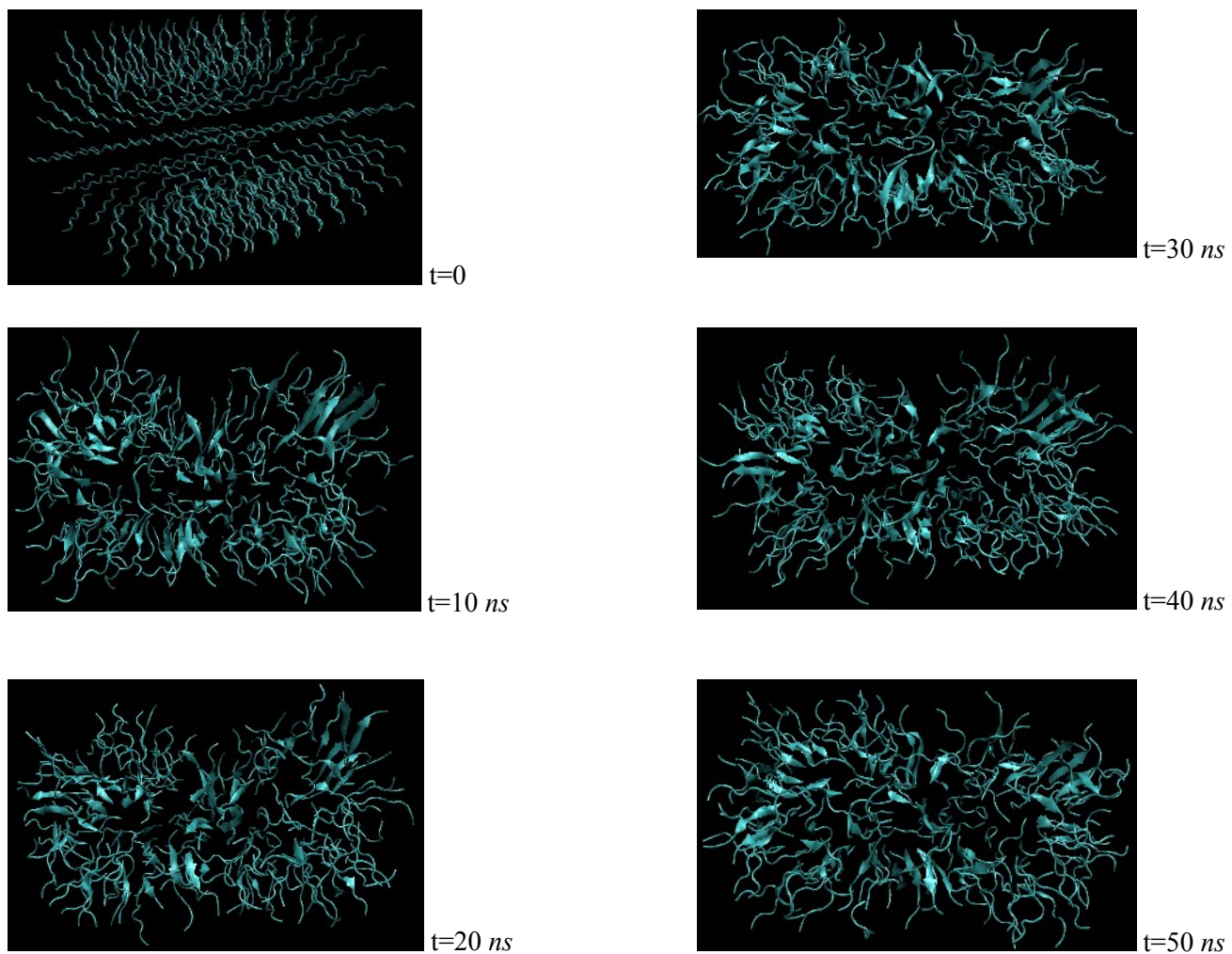


Figure S10. Snapshots of self-assembled 16-layered nanofiber for each 10 *ns* of 50 *ns* simulation.

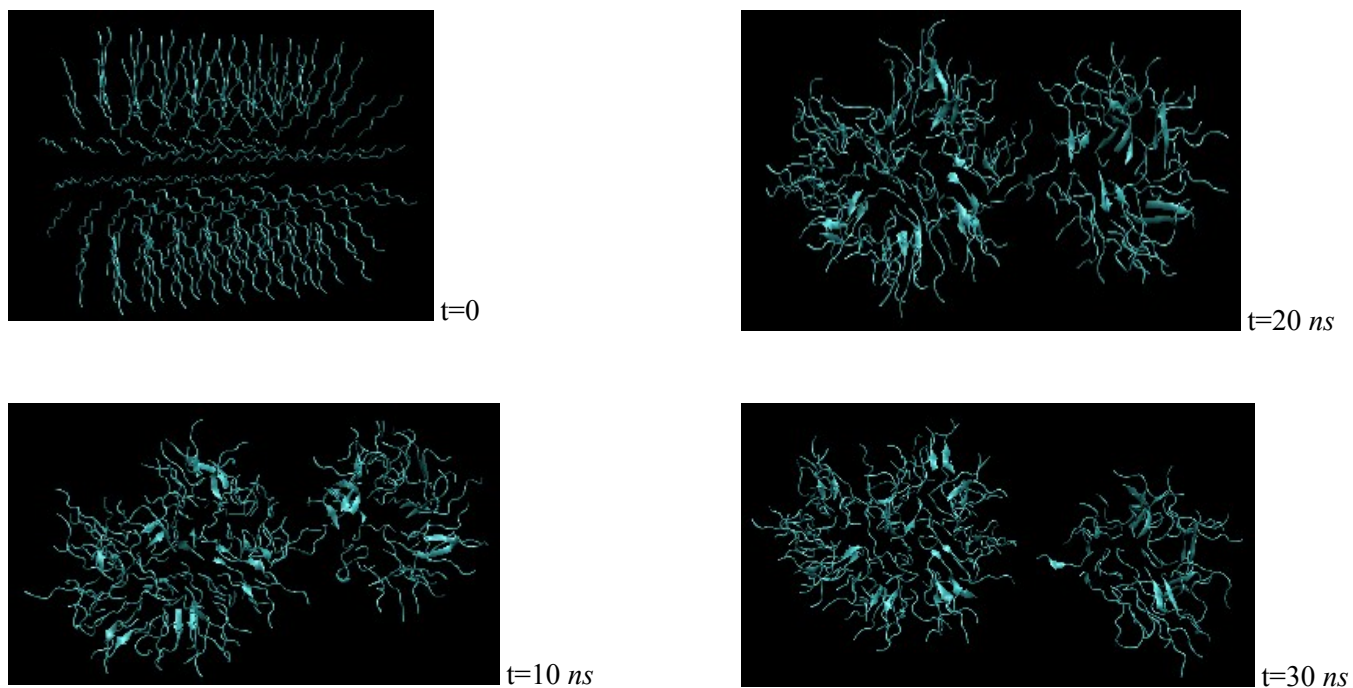


Figure S11. Snapshots of self-assembled 17-layered nanofiber for each 10 *ns* of 30 *ns* simulation.

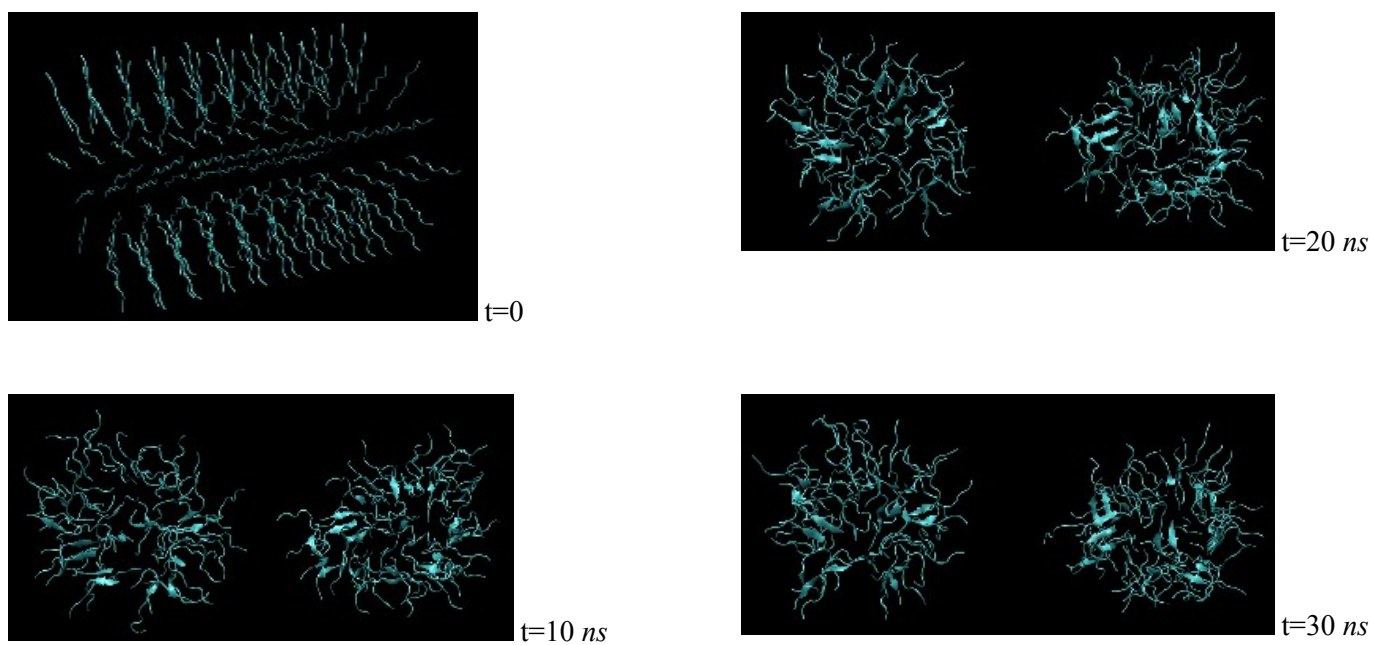


Figure S12. Snapshots of self-assembled 18-layered nanofiber for each 10 *ns* of 30 *ns* simulation.

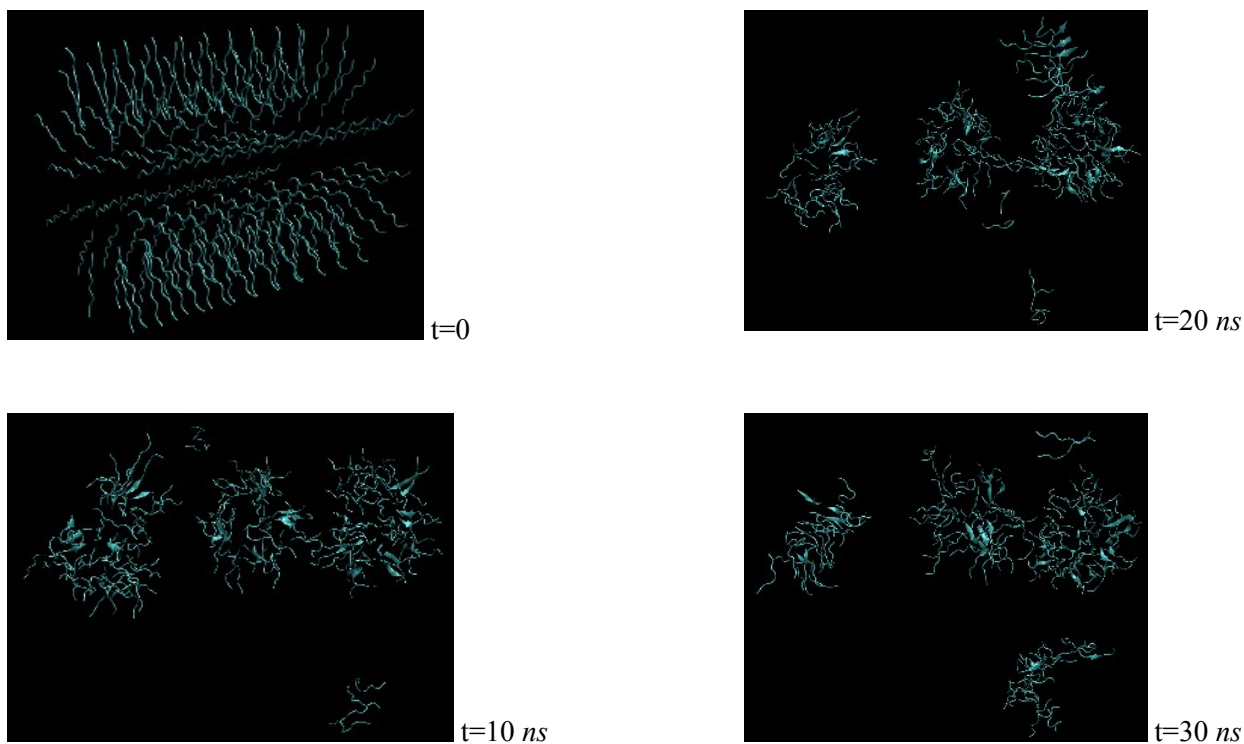


Figure S13. Snapshots of self-assembled 20-layered nanofiber for each 10 *ns* of 30 *ns* simulation.

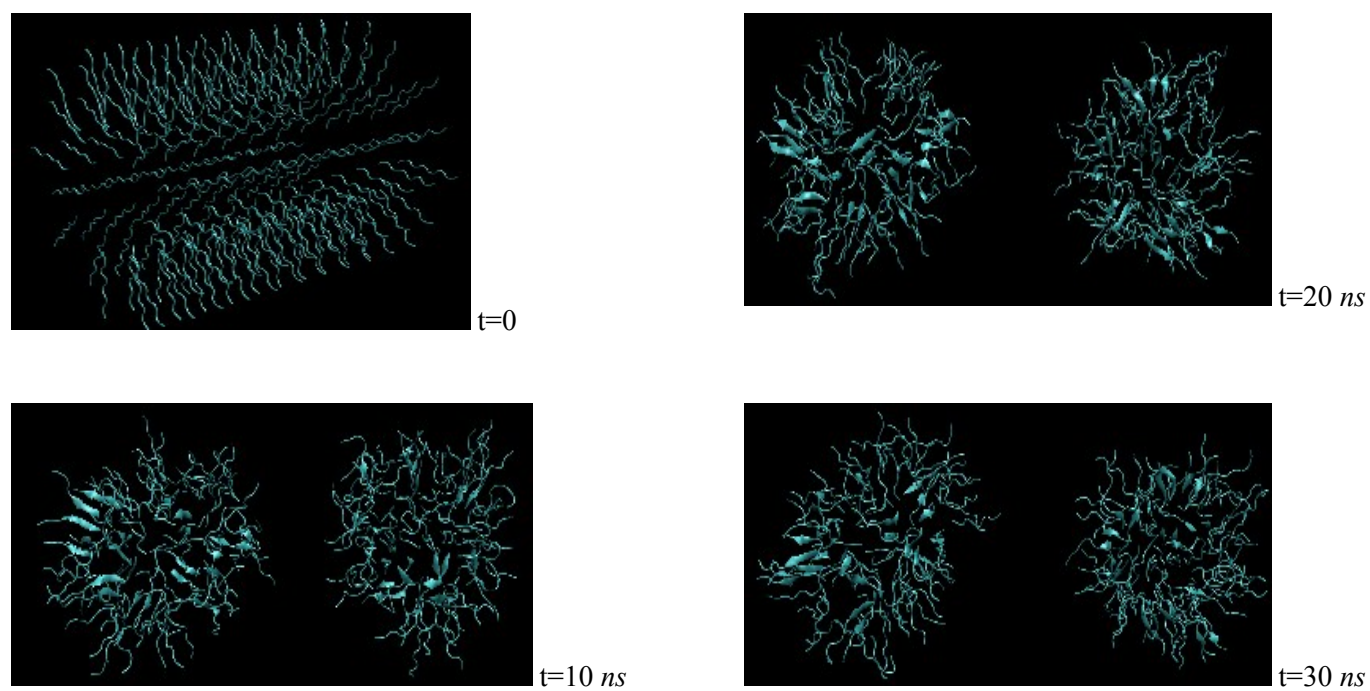


Figure S14. Snapshots of self-assembled 21-layered nanofiber for each 10 *ns* of 30 *ns* simulation.