

Supplementary Material

Curvature Induced Structural Changes of Chicken Villin Headpiece Subdomain by Single Walled Carbon Nanotube

Srijita Paul and Parbati Biswas*

Department of Chemistry, University of Delhi, Delhi-110007, India.

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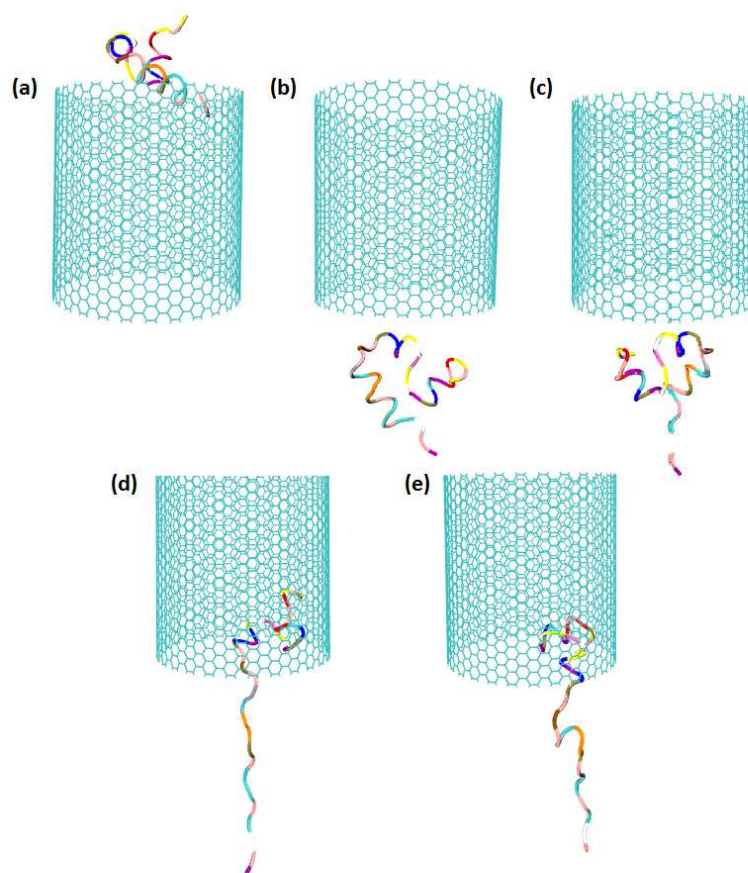


FIG. S1: This figure represents the snapshots of selected SMD simulations. Figure (a) depicts the initial position of all the SMD simulations, (b), (c), (d) and (e) are the final snapshots of the SMD simulations with velocity 5 \AA/ns , 4 \AA/ns , 3 \AA/ns , and 0.5 \AA/ns .

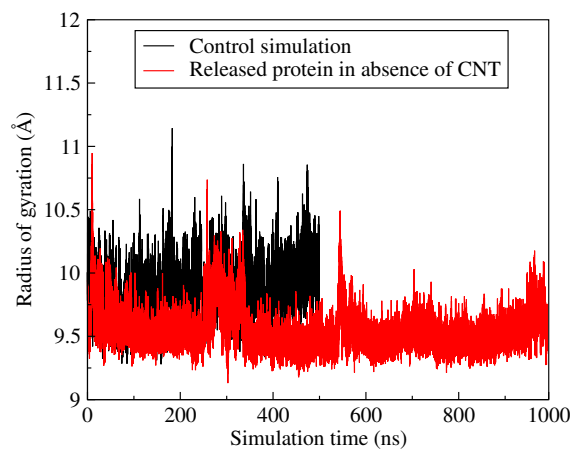


FIG. S2: Radius of gyration plot of the protein backbone for the control simulation (protein in pure water) and for the released protein in absence of CNT with simulation time.

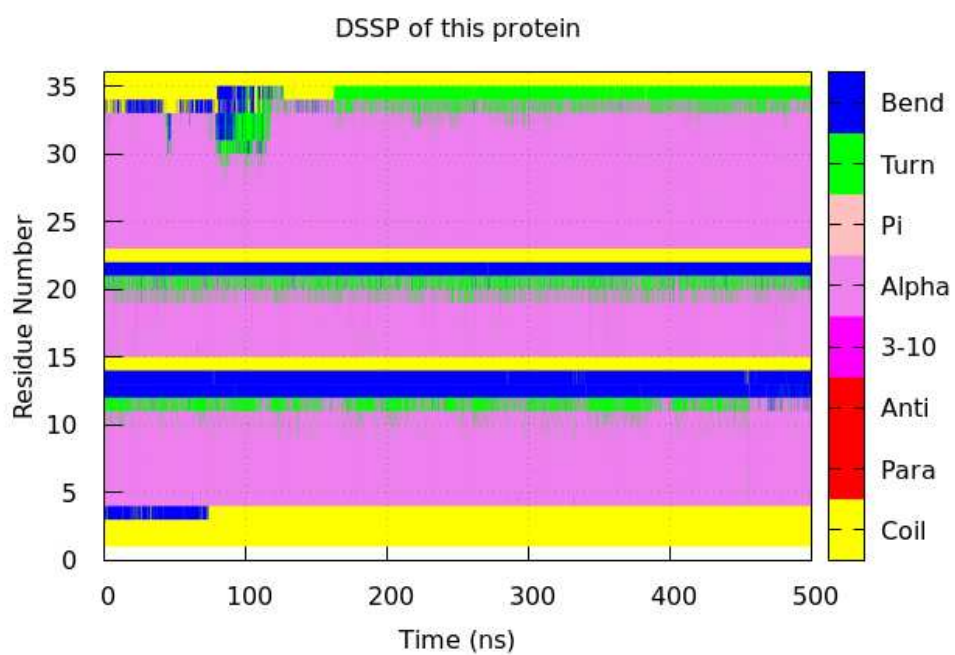


FIG. S3: Secondary structure vs simulation time plot for the released protein after removing the CNT from the system.

* Electronic address: pbiswas@chemistry.du.ac.in