Molecular Dynamics Simulation of Carbon Nanotube & Pulmonary Surfactant Protein – B Interactions

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Abstract

Absorption of proteins onto carbon nanotubes is important part of biomedical engineering because it is helpful to fabricate stable, compatible and sensitive scaffold, which is the basic step of fabricating biosensors. Many previous researches show that most of the proteins can be absorbed on surface of carbon nanotube. However, the mechanism of this absorption is not specific clear. In this lecture, mechanism of protein absorbed on nanotube will be explained by molecular dynamics(MD) using NAMD and VMD software package.

Introduction

Primarily protein interacts with many surfaces including nanostructures like carbon spores, carbon nanotubes, fullerenes, graphene, silica, etc. This protein nanostructure interaction is an important and very first step to develop bio-sensors and diagnostic tools . Most of the proteins get readily absorbed on surface of carbon nanotube, to make use of this property a comprehensive study has to be carried out to find out which groups/residues of protein are been absorbed on surface of carbon nanotube . This absorption of protein on the surface of carbon nanotube occurs due to driving forces, these thermodynamically stable structure after absorption. These driving forces consists of Van Der Waals interaction, hydrophobic-hydrophilic interaction, hydrophilic-hydrophilic interaction, electrostatic interaction . Protein absorption on the carbon nanotube is phenomenon which includes the protein folding and unfolding.

From the broad range of nanostructures available in present time carbon nanotube is selected for this study because of their reported applications which includes nanoelectronics, biosensors, specificity and affinity of binding to biological molecule.

Structure and Functions of Surfactant Proteins

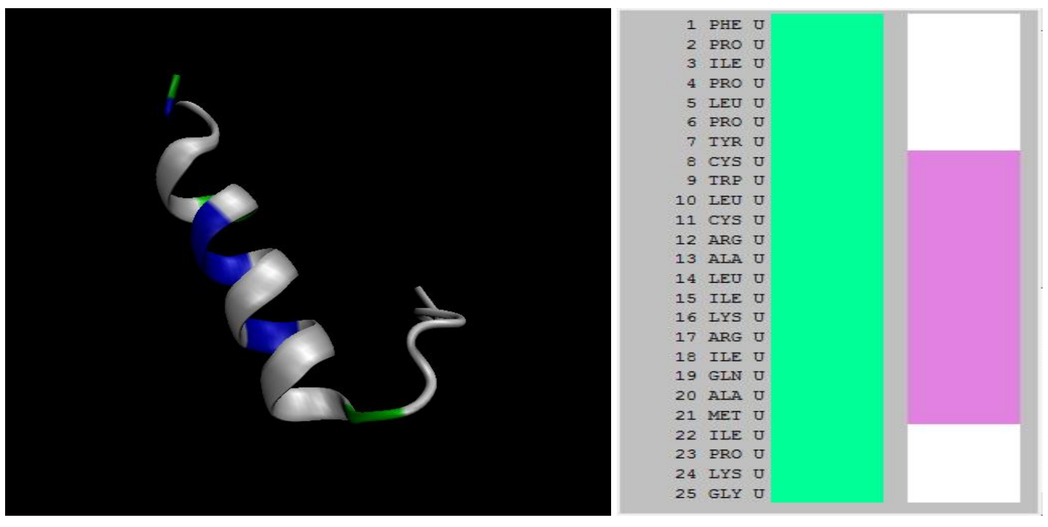

Figure 1: structures of Surfactant Proteins B(1-25)

Pulmonary surfactant is very complex mixture phospholipids (approximately 90%) and proteins (10%). There are four pulmonary surfactant associated proteins viz. SP-A, SP-B, SP-C and SP-D. Surfactant proteins SP-A and SP-D are responsible for pulmonary host defense and surfactant homeostasis. Remaining two surfactant proteins SP-B and SP-C are necessary to maintain optimal surface tension in alveolar air space for breathing. Pulmonary surfactant Proteins (PSP) SP-A and SP-D are large hydrophilic proteins and belong to family of proteins – collectins. Whereas, SP-B and SP-C are small hydrophobic proteins maintaining low surface tension at air liquid interface.

Human surfactant protein B is an important lung-associated protein because it can reduce the surface tension during the expiration process. Human surfactant protein B (amino acid residues 1–79; MW; 8700) is a small and hydrophobic protein in mammalian lung surfactant . In this study, SP-B (1-25) is used for simulation, sequence of SP-B (1-25) is shown in front.

Simulation methods

Four types of parameters file should be given during the simulation:

1. Pdb file : contains the coordinates of the atoms.
2. Psf file: contains the structure information.
3. Force field file : core of the simulation, which decides that how the system get force. In this study we use CHAEMM27 that widely be used for bio-system.
4. Configuration file : this file is for setting up parameters of simulation system.

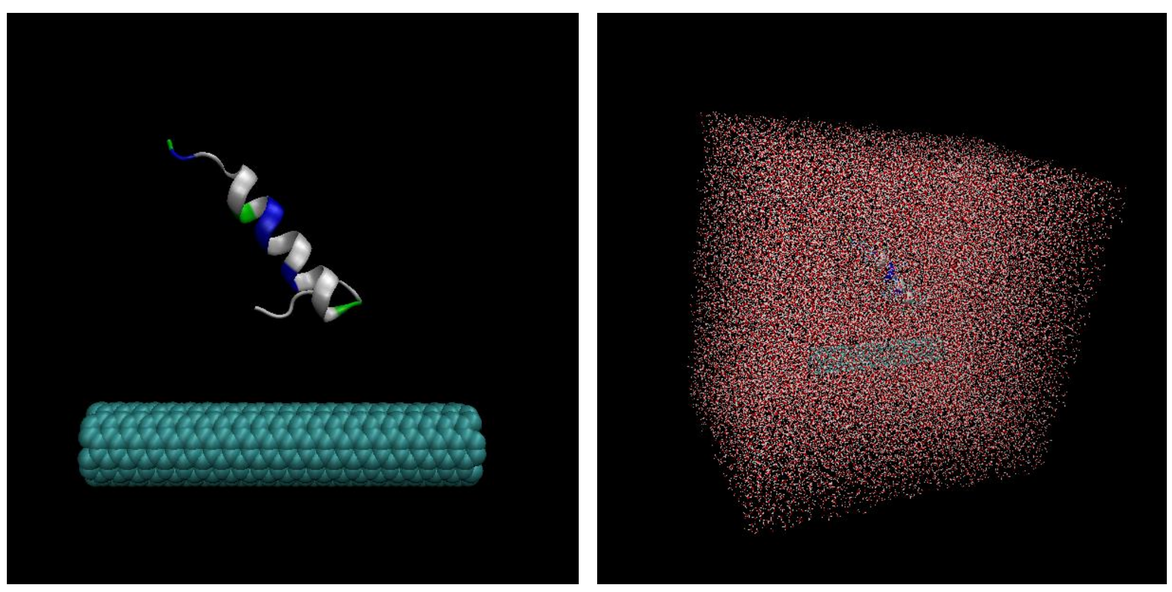

Figure 2: initial conditions between CNT and protein and the waterbox

The pdb file of SP-B is download from Protein Data Bank(ID: PD7988) We construct an armchair single-wall carbon nanotube with 5nm long and n=m=6.The initial distance between geometry center of protein and nanotube is 2.5nm. Make sure that the nearest distance between protein and nanotube is more than 0.6nm. The water box is set up by solvate plugin of VMD. The size of water box is 82 ^{x}106^{x} 111 A$^{3.}$

Results and Discussion

After 25ns, we give screenshot from trajectory . It shows that SP-B is absorbed on carbon nanotube . RMSD(root mean square deviation) is used to provide important reference that if the system is equilibrium. RMSD from figure 3 shows that the fluctuation Is getting stable. We calculated the absorbed residues and list them above

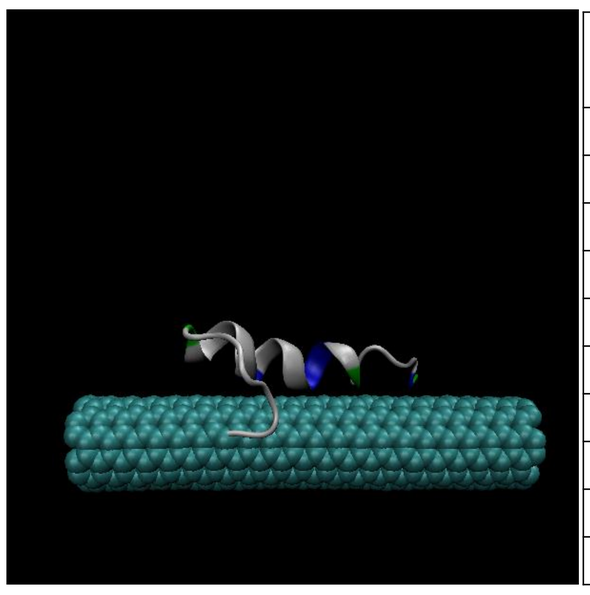

Figure 3: Final position of protein and CNT

Residue number	Residue Name	Polarity
1	PHE	Non-polar
4	PRO	Non-polar
6	PRO	Non-polar
8	CYS	Polar
11	CYS	Polar
12	ARG	Polar
15	ILE	Non-polar
16	LYS	Polar
19	GLN	Polar
20	ALA	Non-polar

Table 1: Absorbed residues

Absorption of protein on the surface of carbon nanotube also changes many surface and conformational properties of carbon nanotube. Out of 1 to 25 residues of SP-B 10 residues get absorbed on the surface of carbon nanotube half of them are polar and half are non-polar residues. This absorption of residues will change the electrical conductivity of carbon nanotube and further analysis is necessary. Table 1 lists the 10 residues name and number which are absorbed on the surface of carbon nanotube after 25 nsec. Figure 3 show the structure of SP-B in its residue types looking at the structure it is only one alpha helix. In Figure 3, white color shows non-polar residues, blue shows basic residue and green shows polar residues. Figure 3, shows the final position of SP-B after 25 nsec it can be seen in figure only polar and non-polar residues make contact with carbon nanotube.

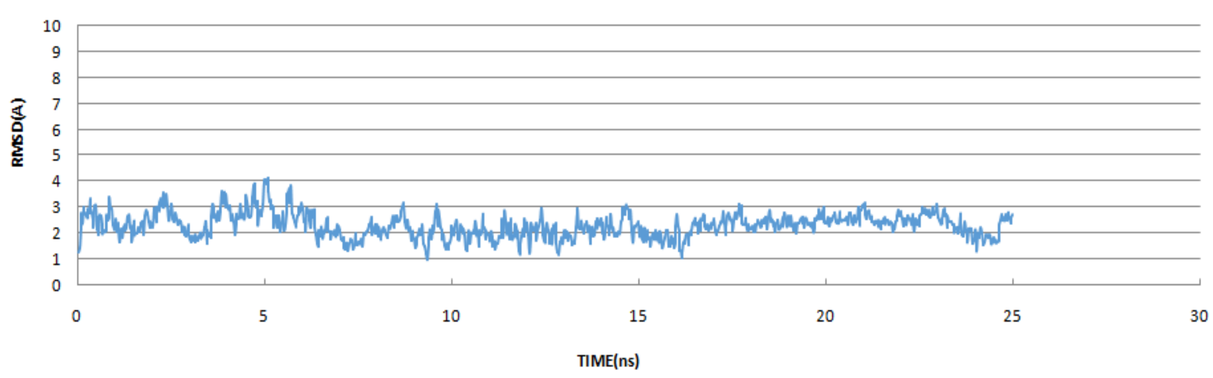

Figure 4: RMSD plot of SP-B for 25 nsec.

Conclusions and Future Work

Using NAMD and force field molecular dynamics it is clearly shown that protein molecules get absorbed on the surface of carbon nanotubes. Surface of carbon nanotube is hydrophobic and protein is also made up of both hydrophobic and hydrophilic residues.

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