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Role of Temperature Variation on the Dynamics of Carbon Nanotube and Protein Interactions

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ABSTRACT

3CLN (Calcium Modulated Protein) protein plays an important role in the calcium signalling inside the eukaryotic cell structure [1, 2]. Temperature dependent conformation changes in the Calmodulin protein are studied with detailed molecular dynamics simulations by using VMD and NAMD software. The quantitative comparison of the simulation data with analysis shows the different aspects of the folding process can help with correctness of the calculations. It can also provide a detailed structural interpretation for the experimental observations as well as physical interpretation for theoretical concept without actual experimentation. Earlier these kinds of studies were also performed experimentally using fluorescence measurements as in [3]. Dynamics approach was used before the time to study the temperature dependent conformation change of Calmodulin protein [4]. In this work, we perform molecular dynamics simulations of 100 ns each to study the interaction of 3CLN with carbon nanotube at 300 K, 500K, 550K, 600K and 650 K. A carbon nanotube (CNT) has a cylindrical structure with a nanoscale diameter and appears like a rolled graphene sheet [7, 8]. A remarkable dependence of the temperature is observed on the overall dynamics of the protein and carbon nanotube as found in our earlier study [5, 6]. This interaction will be helpful in drug delivery. Need of this interaction will give a pathway for further research and also it will help to study the role of environmental conditions on the dynamics of a specified protein.

Keywords: Carbon nanotube, VMD; NAMD; Simulation; Eukaryotic cell; Calmodulin Protein

1. INTRODUCTION

Biophysics will play an important role in the medical science as it will help in the treatment with much better ways. A carbon nanotube (CNT) has a cylindrical structure with a nanoscale diameter and appears like a rolled graphene sheet [7, 8]. Interaction between a carbon nanotube and 3CLN (Calmodulin) protein was studied [9, 10] with the help of software's VMD and NAMD. This interaction will be helpful in drug delivery. Need of this interaction will give a pathway for further research also as it will help to study the role of environmental conditions on a specified protein. It will definitely a play important role in the drugs delivery as CNT is a very small tube of nano scale diameter that will make it to easily pass through the organs.

The interaction between the carbon nanotube and the protein is therefore an important aspect to study for its application in drug delivery systems. Protein are made up of different types of amino acid. Some proteins can be found in the cytoplasm of all eukaryotic cells. Amino acid availability is a good regulator for muscle protein synthesis [11]. Proteins are large and complex molecules that play various important and critical role in our body. Proteins do most of the work in cell and are required for function, structure and regulation of body tissue and organ in proper way. Proteins are made up of various number of small units of amino acids that are attached so that they form a long chain. Proteins performs various functions like as an antibody, as an enzyme, as a messengers, as a growth hormone, as a structural component, as a transporter and for storage etc. For a particular type of drug delivery through CNT its interaction with

the protein needs to studied under different environmental condition like pH and temperature etc. Earlier work is done on the interaction of CNT and proteins [12] but the effect of environmental conditions is not studied in detail.

2. METHODOLOGY

2.1 Visual molecular dynamics (VMD)

VMD is a software with molecular modelling and visualization computer programing. It is designed for the display and analysis of molecular assemblies, in particular biopolymers such as proteins and nucleic acids. VMD can simultaneously display any number of structures using a wide variety of rendering styles and colouring methods. VMD developed as a tool to observe and analyze the results of molecular dynamics simulations. It includes tools for observing volumetric and sequence of data, also for arbitrary graphics objects. Figure 1 shows the structures of a CNT and CNT interacting with protein created with the help of VMD program.

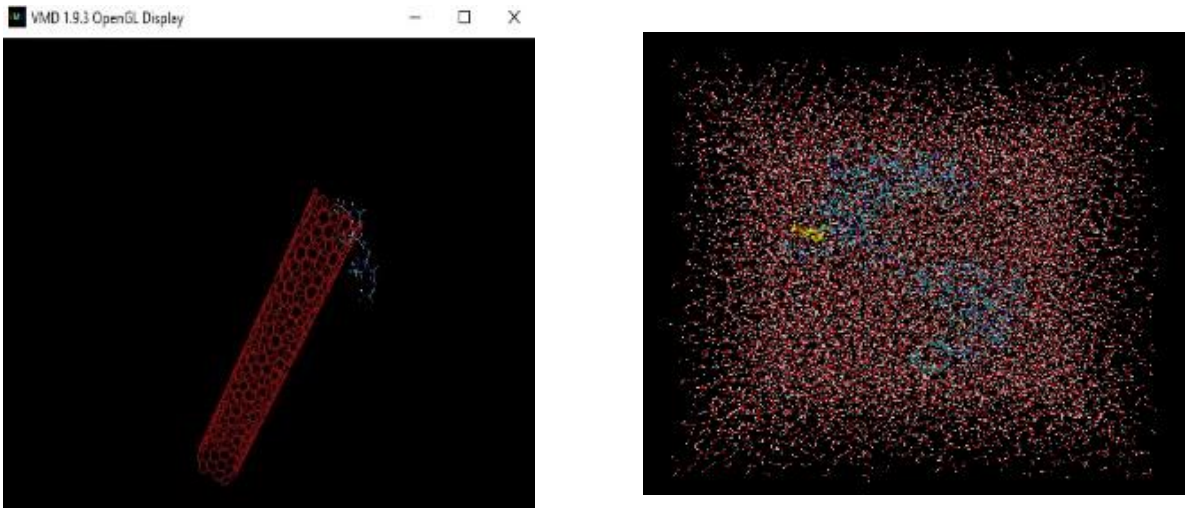

Fig. 1. (a); Structure of 3CLN protein with Carbon nanotube (b) Structure of 3CLN Protein with CNT in a water box

VMD supports computers running MacOS X, Unix, or Windows, is distributed free of charge, and includes source code.

2.2 Nanoscale Molecular Dynamics (NAMD)

NAMD is used to run efficiently on parallel machines for simulating large molecules. NAMD helps in an interactive simulation tool with the Visual Molecular Dynamics (VMD) molecular as a software. NAMD is a parallel designed software for high-performance simulation of large biomolecule systems. NAMD scales to hundreds of processors on high-end parallel platforms, as well as tens of processors on low-cost commodity clusters, and also runs on individual desktop and laptop computers. NAMD has an interface to quantum chemistry packages ORCA and MOPAC, as well as a scripted interface to many other quantum packages. Together with VMD and QwikMD, NAMD's interface provides access to hybrid QM/MM simulations in an integrated, comprehensive, customizable, and easy-to-use suite

NAMD is available as freeware for non-commercial use by individuals, academic institutions, and corporations for in-house business uses.

3. RESULTS AND DISCSSION

In this work we have performed five sets of simulations at 300 K, 500K, 550K, 600K and 650 K to study the interaction of CNT with 3CLN protein. Kinetic energy and temperature are found to be stable at 300K, 500 K and 550K as shown in Figure 2. The root mean square deviation (RMSD) is as shown in Figure 3 for 300 K. At this temperature RMSD is found to be variable not stable from 0 to 100ns as observed from Figure 3. A stable dynamic is observed between the CNT and the protein at 300 K as seen in the Figure 4 (as clearly observed from snapshot given in figure 4 that CNT is remain close to the protein during whole of the period from 0-100ns).

At higher temperatures such as 500K, 550 K, a dynamic interaction is observed between the protein and carbon nanotube. At 500K, RMSD is found to be nearly stable from 20 ns to 100 ns with slight variation as shown in Figure 5. At this temperature the protein is observed to come in the close proximity of the carbon nanotube around 60 ns. Around 85 ns the protein nearly wraps around the CNT as shown in Figure 6.

At 550 K, RMSD is found to be nearly slight variation from 20 ns to 80 ns in an increasing manner with slight variation and from 80 ns to 90 ns in deceasing manner after that it shows stability as shown in Figure 7. At this temperature the protein is observed to come in the wrapping proximity of the carbon nanotube at around 65 ns. Around 85 ns the protein wrapped around the CNT as shown in Figure 8.

At 600 K, RMSD is found to be nearly stable from 5 ns to 90 ns and from 90 ns to 100 ns in an increasing manner with slight stability as shown in Figure 9. At this temperature the protein is observed not to come nearly of the carbon nanotube from starts to 100 ns as shown in Figure 10, means no interaction at this temperature i.e. some destruction occurs at this temperature.

At 650 K, RMSD is found to be nearly shows stable variation from 10 ns to 80 ns and from 80 ns to 100 ns in a decreasing manner with slight stability as shown in Figure 11. At this temperature the protein is observed not to come nearly of the carbon nanotube from starts to 100 ns as shown in Figure 12, means no interaction at this temperature i.e. some destruction occurs at this temperature. This interaction is important from the point of view of applications in drug delivery.

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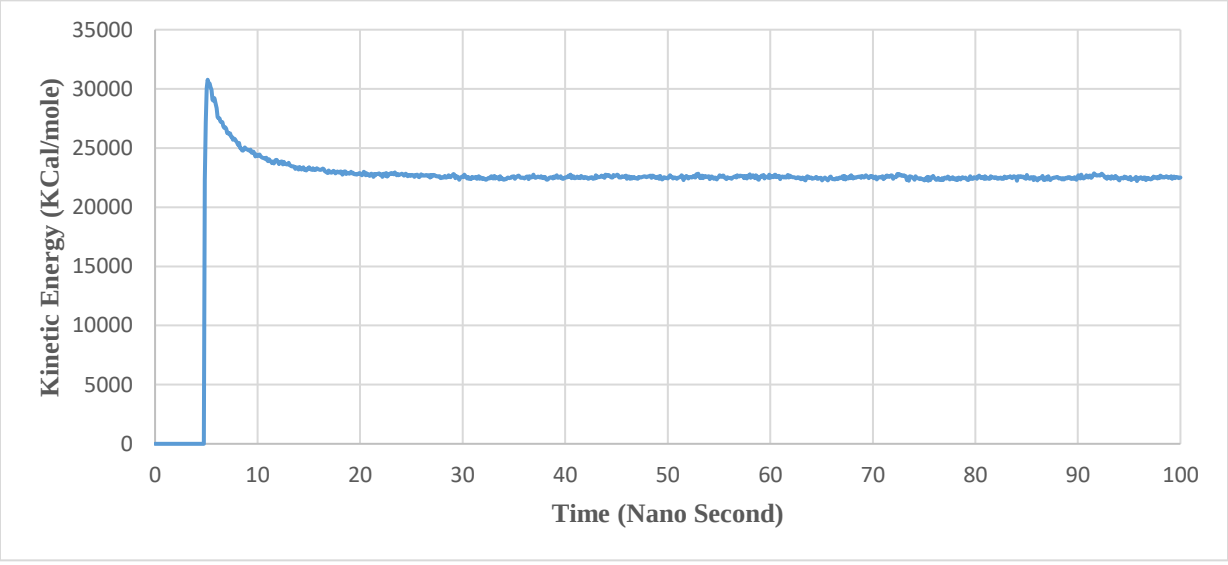


Fig.2. (a) Kinetic energy as a function of time at 300K

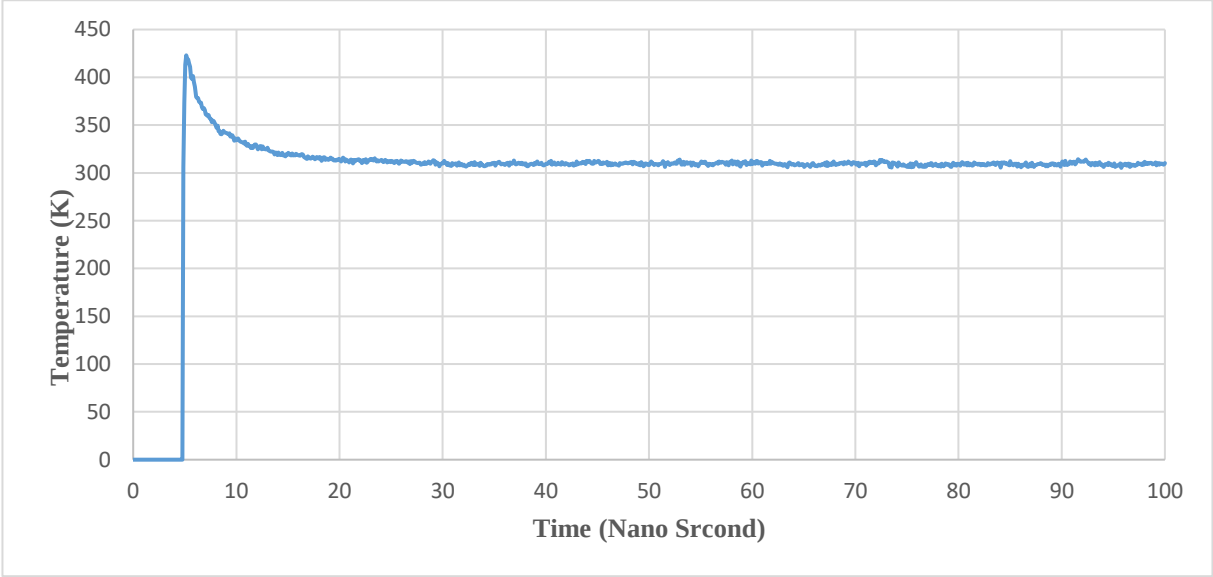


Fig. 2. (b) Temperature as a function of time at 550K

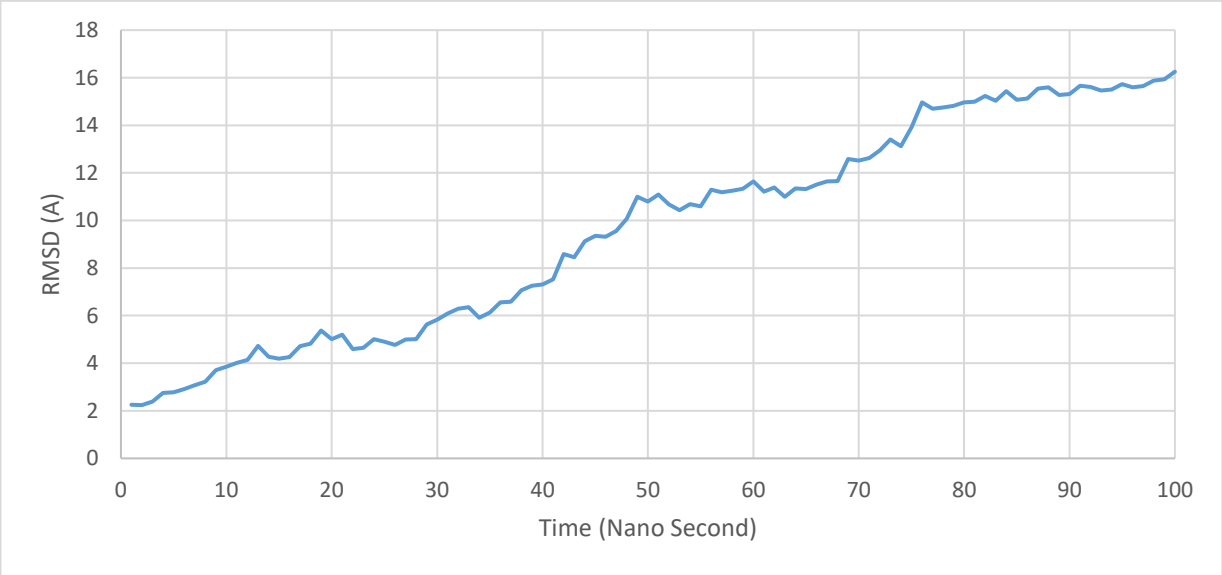
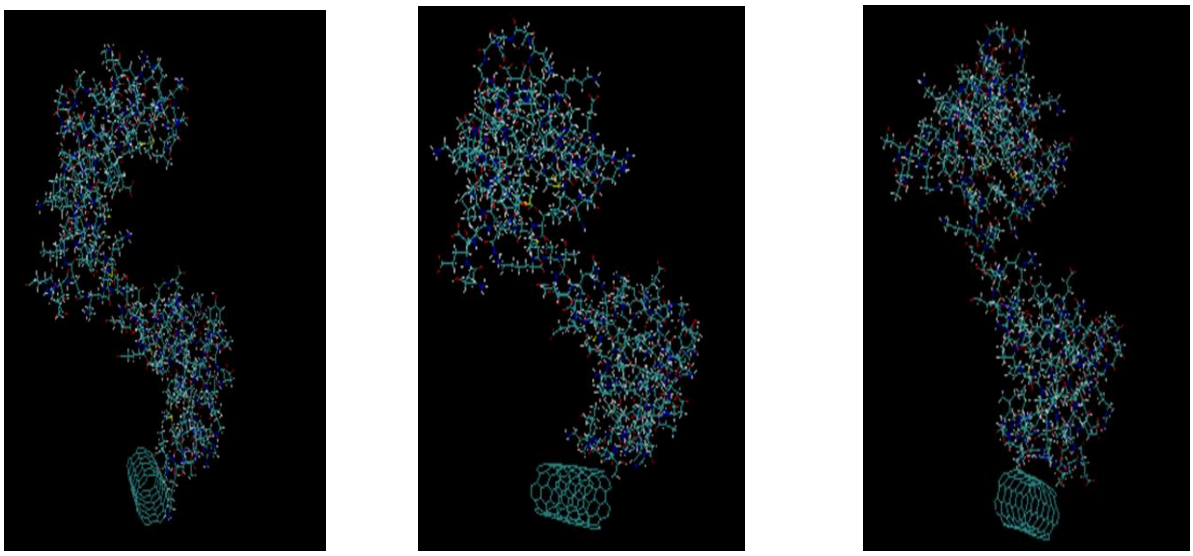


Fig. 3. Root Mean Square Deviation (RMSD) as a function of Time at 300 K



At 10ns At 50ns At 100ns

Fig. 4. Snapshots at different time showing a stable interaction between the CNT and protein at 300 K

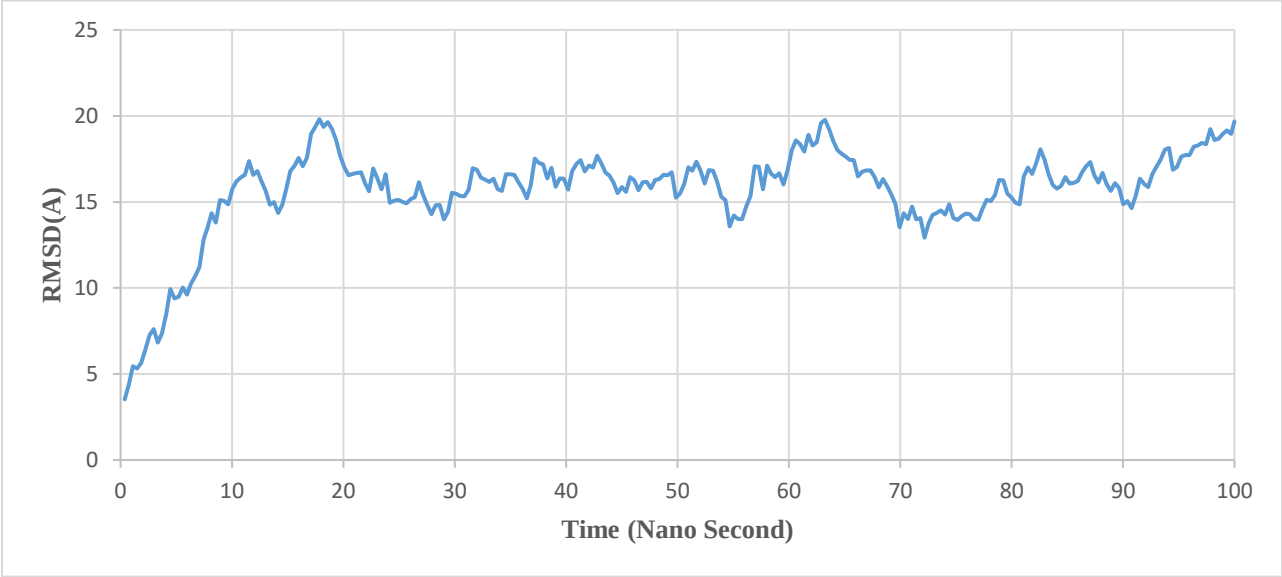


Fig.5. Root Mean Square Deviation (RMSD) as a function of Time at 500 K

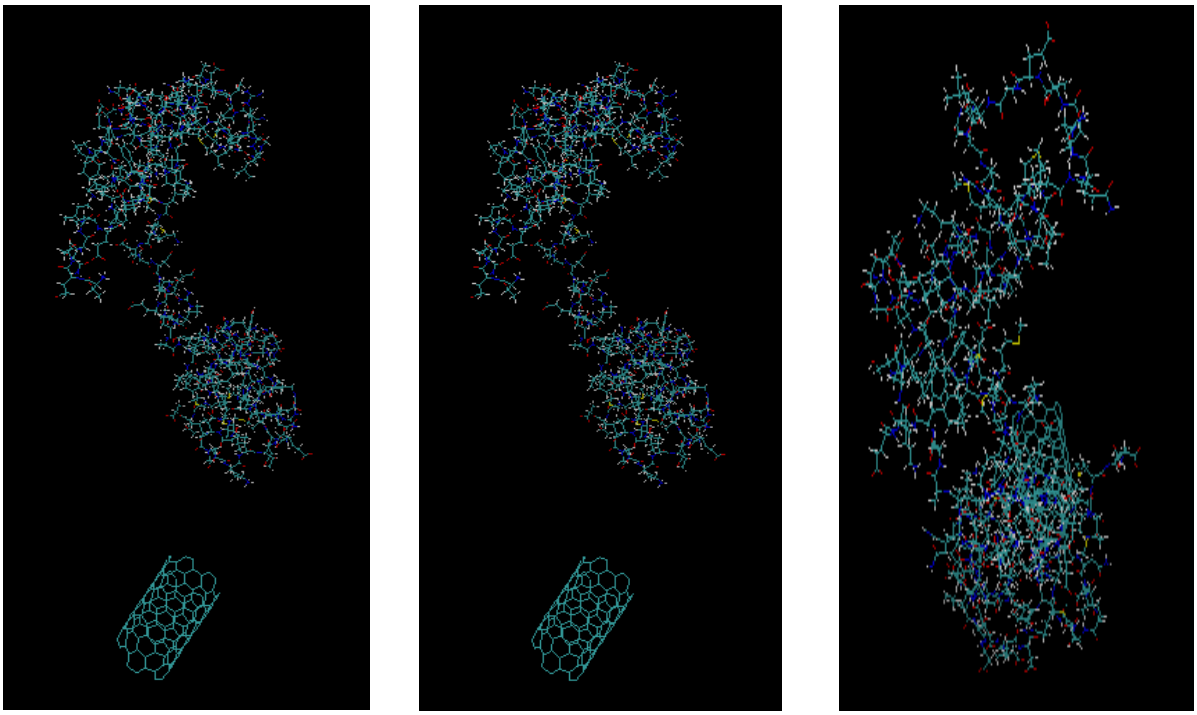


Fig. 6. Snapshots at different time showing a dynamic interaction between the CNT and protein at 500 K

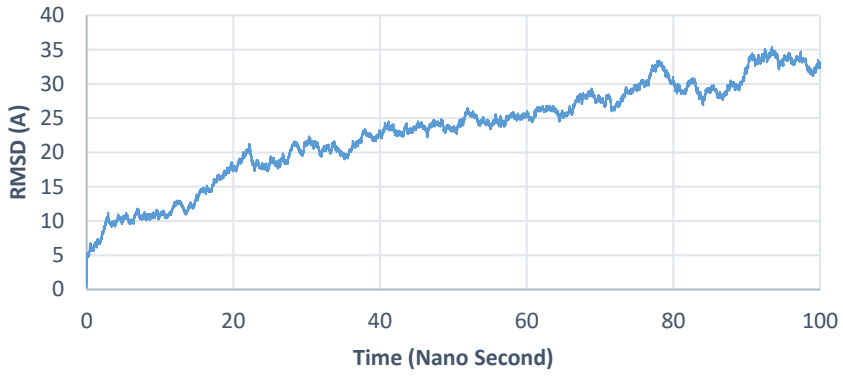
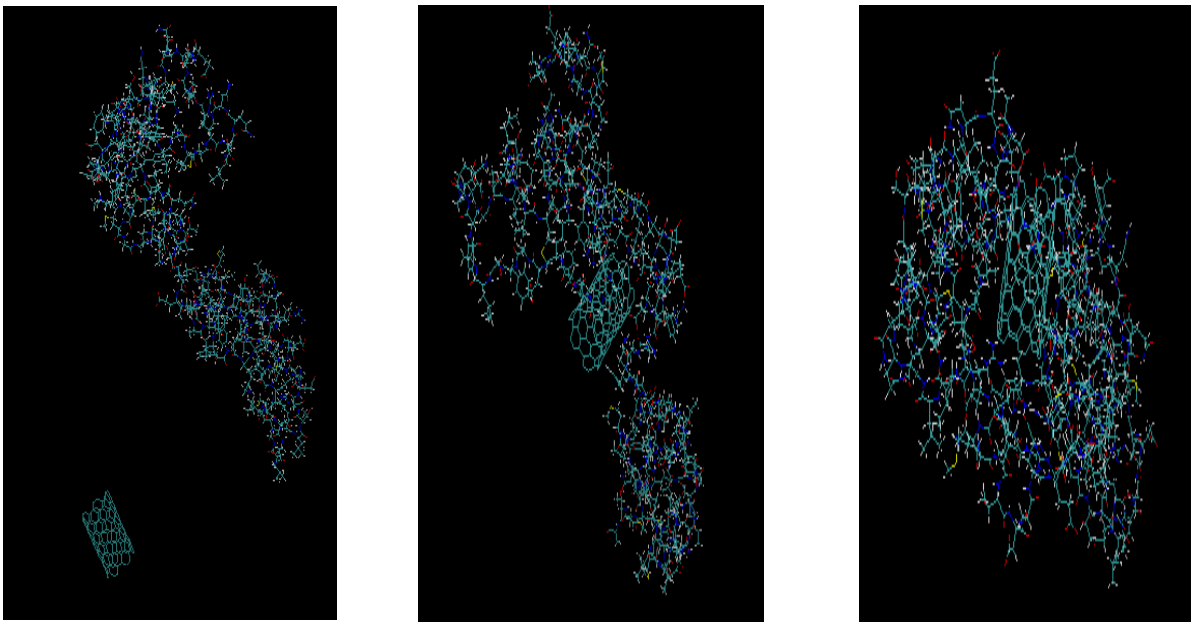


Fig. 7. Root Mean Square Deviation (RMSD) as a function of Time at 550 K



At 8ns At 65ns At 85ns

Fig. 8. Snapshots at different time showing a dynamic interaction between the CNT and protein at 550 K

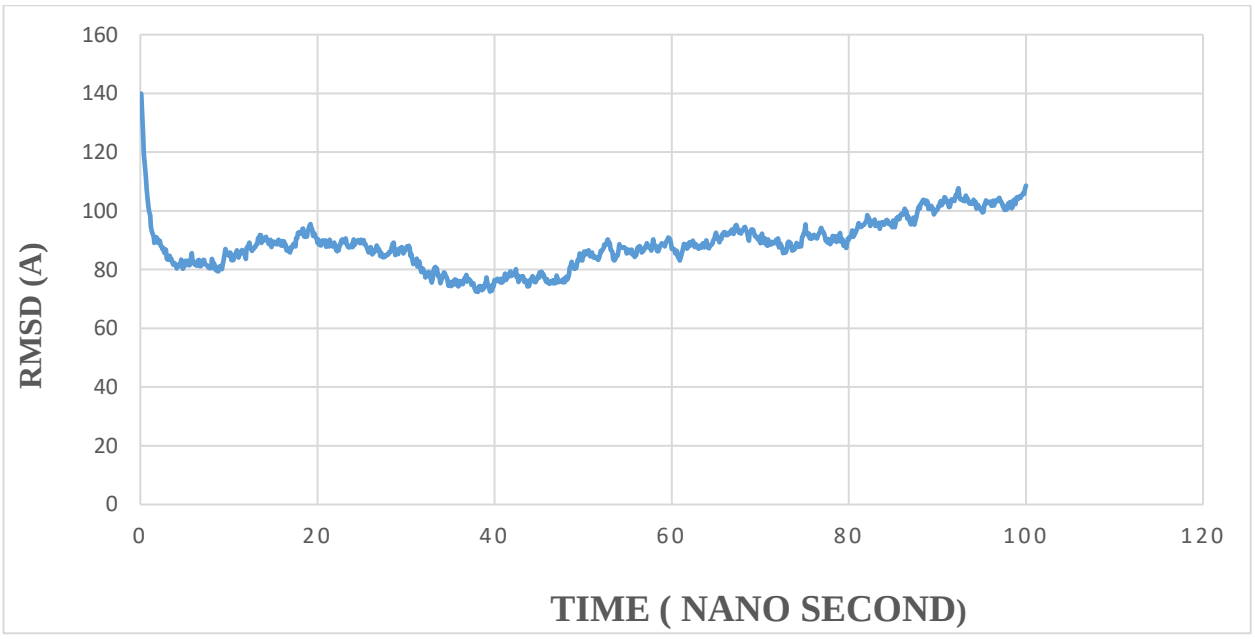


Fig.9. Root Mean Square Deviation (RMSD) as a function of Time at 600 K

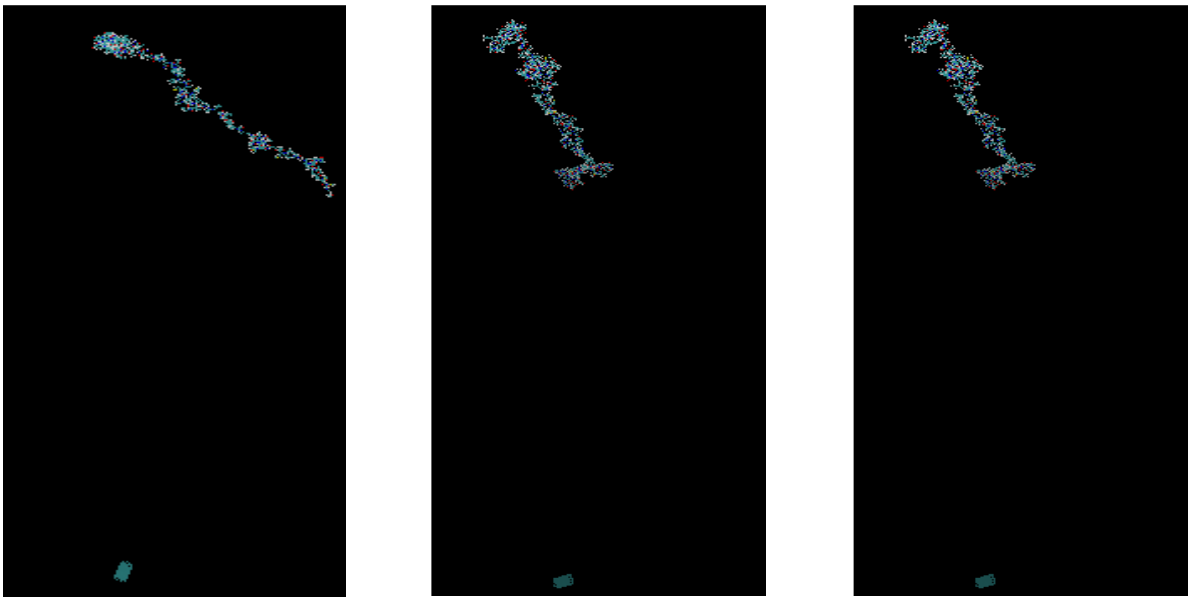


Fig.10. Snapshots of CNT and 3CLN protein simulation at 600 K

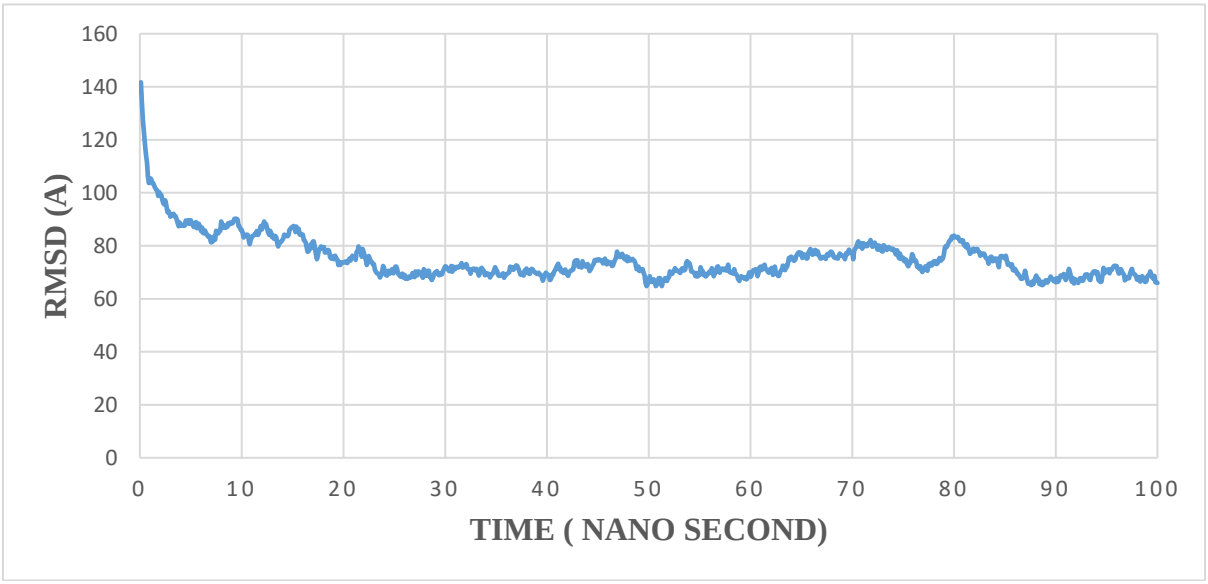


Fig.11. Root Mean Square Deviation (RMSD) as a function of Time at 650 K

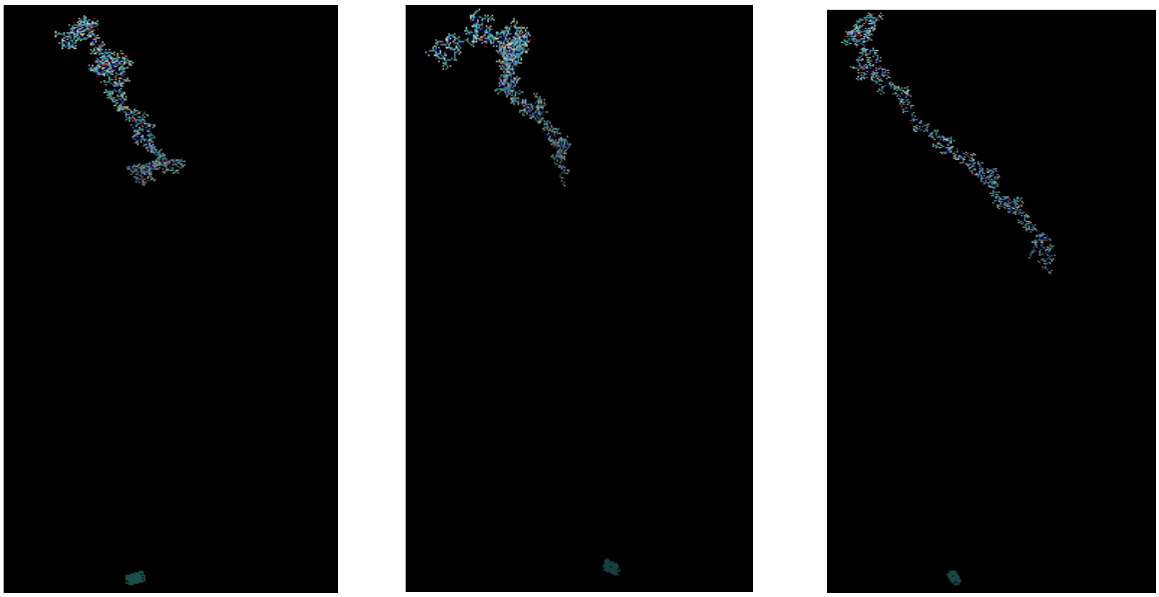


Fig.12. Snapshot of CNT and 3CLN protein at 650K

4. SUMMARY AND CONCLSION

Molecular dynamics simulations of 100 ns are performed with the help of software's such as NAMD and VMD to study the interaction of 3CLN protein with carbon nanotube at different temperature 300 K, 500 K, 550K, 600K and at 650K. A remarkable dependence of the temperature is observed on the overall dynamics of the protein and carbon nanotube as reported in our earlier study. At 300 K the structures are found to be showing a stable dynamic. Whereas at higher temperatures such as 500K and at 550K, a dynamic interaction is observed between the protein and carbon nanotube in which the protein is observed to wrap around the CNT structure towards the end of the simulation. But at temperatures 600K and 650K, no interaction is observed between protein and carbon nanotube as protein is observed not to come close to the carbon nanotube till the end of the simulation. Overall conclusion is that from temperature 300K to 500K proteins shows great interaction with carbon nanotube but from 600K to 650K no interaction shows between protein with carbon nanotube. This interaction will be helpful in the applications of such systems for the drug delivery purposes.

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