CHIRALITY BASED SEPERATION OF CARBON NANOTUBES BY ANALYZING THE SPECIFIC INTERACTION WITH THE AMB-1 FLAGELLIN DERIVED TRIPEPTIDE.

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ABSTRACT

Isaac *et. al* (2015) studied the interaction between the flagellum of AMB-1 and different chirality CNTs (m-CNT and s-CNT). The observations through Molecular Dynamics simulations demonstrated that the glycine residues in D3 domain of flagellum interacts with m-CNT whereas such an interaction with s-CNT is absent. The specific interaction of glycine with m-CNT can lead to the development of a biological method for chirality based CNT sorting. Hence, further studies were required to determine the effect of the residues flanking glycine on it's interaction with m-CNT. The type of interactions and the extent of interaction of different combinations of polar and non-polar amino acid residues flanking glycine were conducted. Hence, the role of glycine with two flanking amino acid residues (tripeptide) is substantiated to determine it's specific interaction with m-CNT through the study of **interaction energy** and **RMSD** of the middle glycine and the flanking residues towards the adsorption of the tripeptide onto m-CNT.

INTRODUCTION

Chirality based sorting of a mixture of carbon nanotubes (CNT's) into individual m-CNT and s-CNT is carried out through tedious centrifugation and electrophoresis techniques. Many such techniques of separation such as gel chromatography and DNA sequencing have been reported for chirality based separation[1] without receiving widespread acceptance. Hence, studies were conducted to determine an easy and safer approach for chirality based separation. The biological method of chirality based sorting of a CNT mixture was then simulated by Isaac *et.al* involving residue specific interaction between a bacterial flagellum and CNT. Glycine showed specific interaction with m-CNT, which is a topic further studied upon in the current work.

METHODS

Molecular Dynamics based simulations were carried out using VMD [2] and NAMD [3]. R-type falgellin pdb (1UCU) file was obtained from the Protein Data Bank. Glycine residues with two flanking amino acid residues (forming a tri-peptide) were extracted from the D3 domain of R-type flagellin pdb file. Simulations were carried out between m-CNT and various combinations of tri-peptide with glycine in the middle of the two flanking residues for a period of 50 ns. All simulations used the CHARRM force field, TIP3 water model [4] and a 0.05 mol/l neutralizing NaCl concentration. Temperature was maintained at 300 K at a pressure of 1 atm.

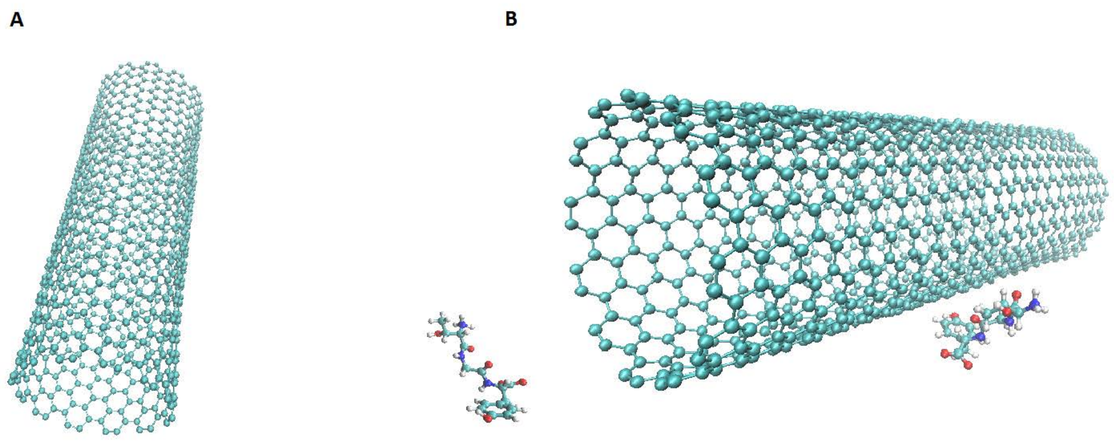
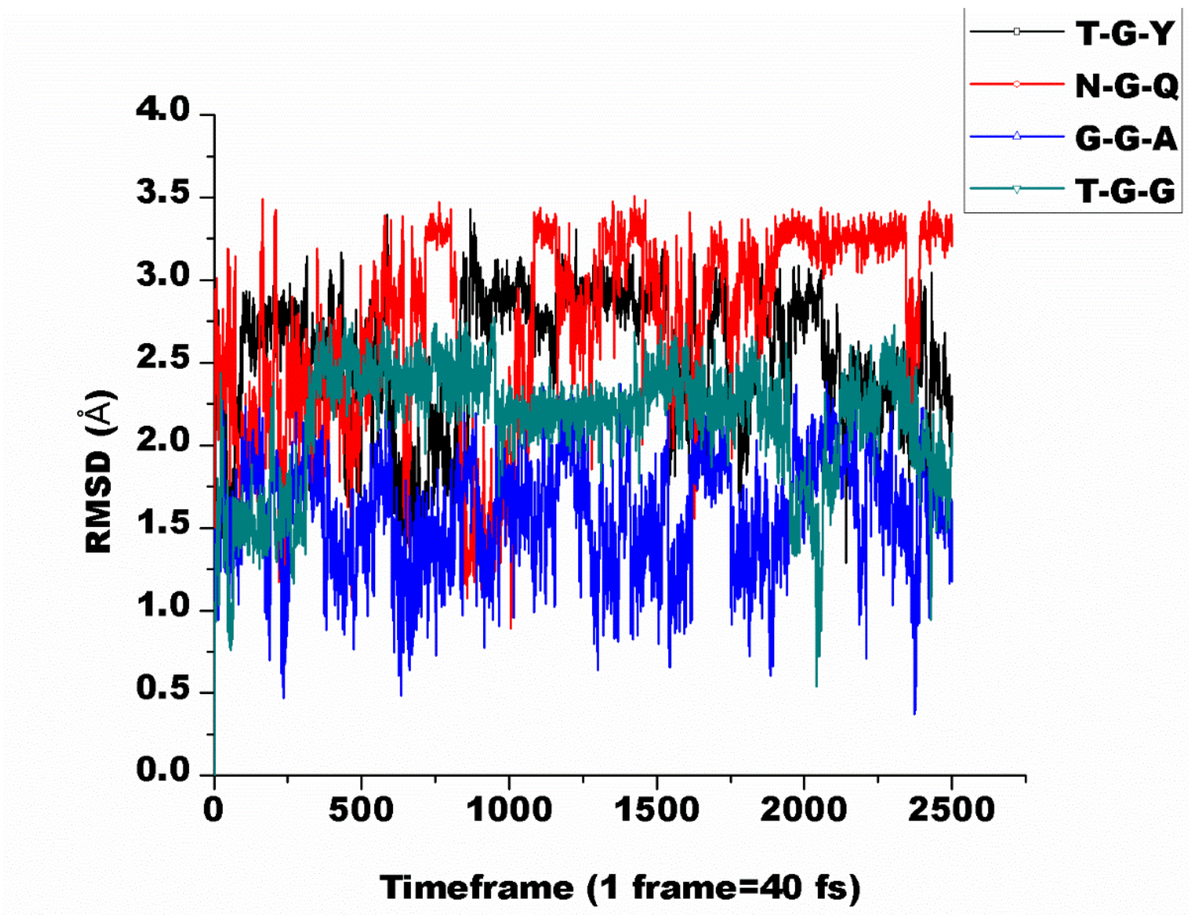
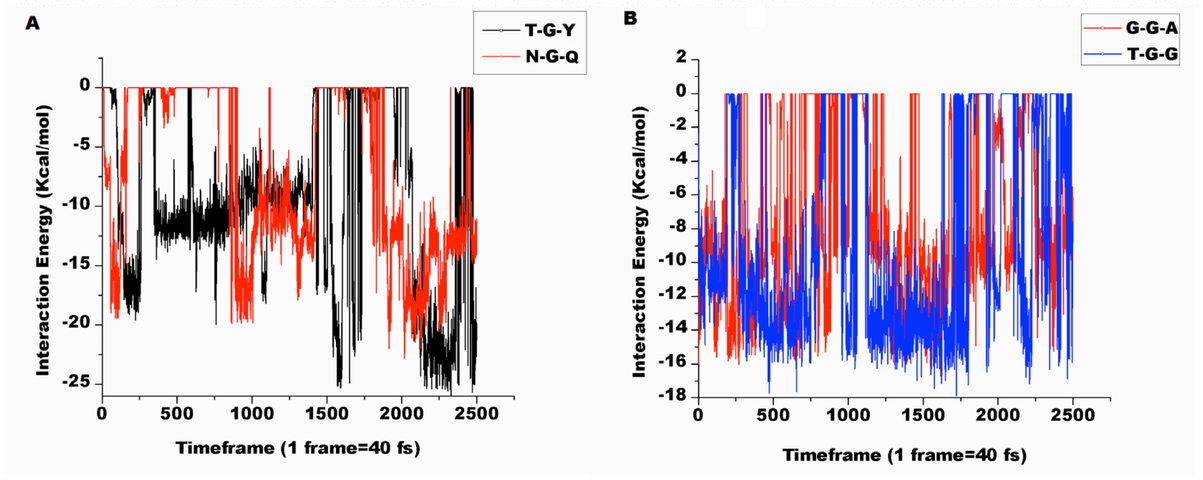


Figure 1: CPK representation of CNT and tripeptide at 0 ns (Fig A.) and 50ns (Fig B).

RESULTS





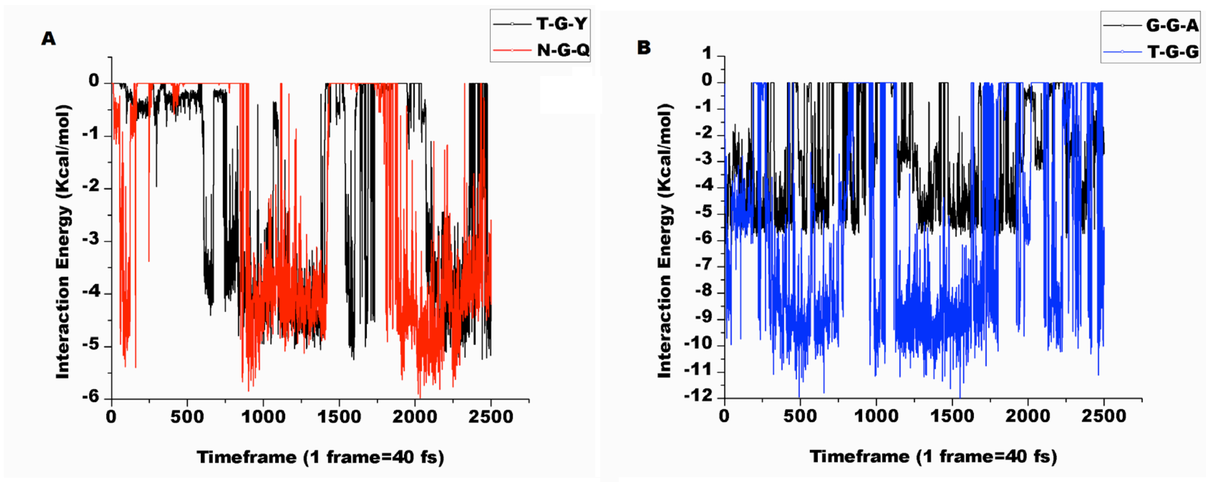


Figure 2: Root Mean Square Deviation (RMSD) between m-CNT and four combination of tri-peptides with glycine in the middle flanked by two residues. on either side.
Figure 3: Interaction energy between m-CNT and tri-peptide THR-GLY-TYR, ASN-GLY-GLU (Fig A) and GLY-GLY-ALA, THR-GLY-GLY (Fig B).
Figure 4: Interaction energy between m-CNT and the middle GLY residue for the different combinations of tri-peptide mentioned above.

The combination of tri-peptides with a middle glycine residue flanked by two amino acid residues were: THR-GLY-TYR, ASN-GLY-GLU, GLY-GLY-ALA and THR-GLY-GLY. Of the above mentioned amino acid residues, TYR and ALA are non-polar in nature. THR, ASN and GLU are polar whereas GLY has a omnipotent behavior. Figure 4 demonstrated that GLY interacts with m-CNT as previously proposed with a large interaction energy. The presence of polar residues give a higher interaction energy suggesting that the surrounding water causes a better interaction between the tri-peptide and m-CNT. The RMSD (Fig 1) of the tri-peptides suggest the same with a more stable and larger RMSD with the polar flanking residues.

CONCLUSION

The study of specific interactions between glycine and m-CNT can provide an in-depth analysis on the overall specific interaction of D3 domain of AMB-1 flagellin with m-CNT. Once established that glycine in D3 domain specifically interacts with m-CNT, the use of AMB-1 flagellin for chirality based separation of CNT mixtures can be further explored.

REFERENCES

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