Adsorption and encapsulation of melittin on covalently functionalized carbon nanotubes; a molecular dynamics simulation study

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Introduction

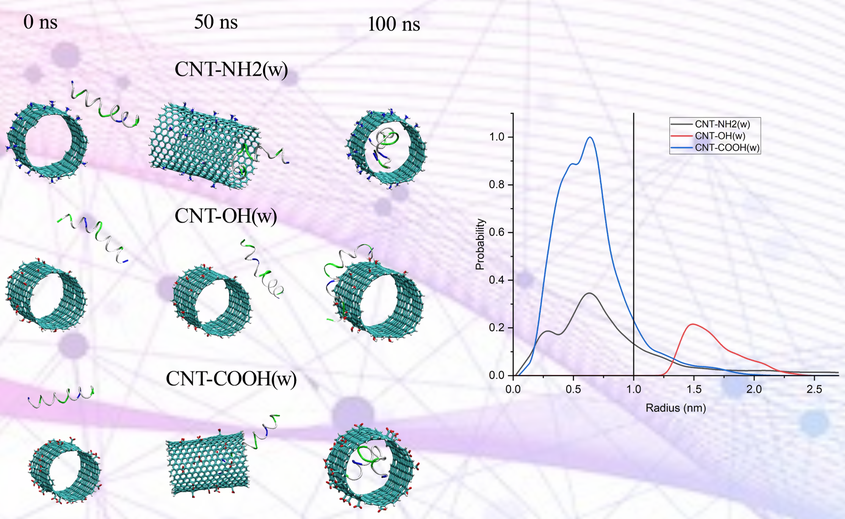
Anticancer peptides (ACPs) have been identified with the development of molecular biology. The positive charge, the length of about 30 residues, and the alpha helix and beta sheet structures are the common characteristics of ACP [1]. Melittin, an amphiphilic peptide with 26 amino acids, is the major component of bee venom. Melittin is a membrane-active peptide and causes cell death by pore formation in the cell membrane, and for this reason, it is known as an anti-cancer peptide. The toxicity and hemolytic activity of melittin require a drug delivery system to be considered [2].

Model and Method

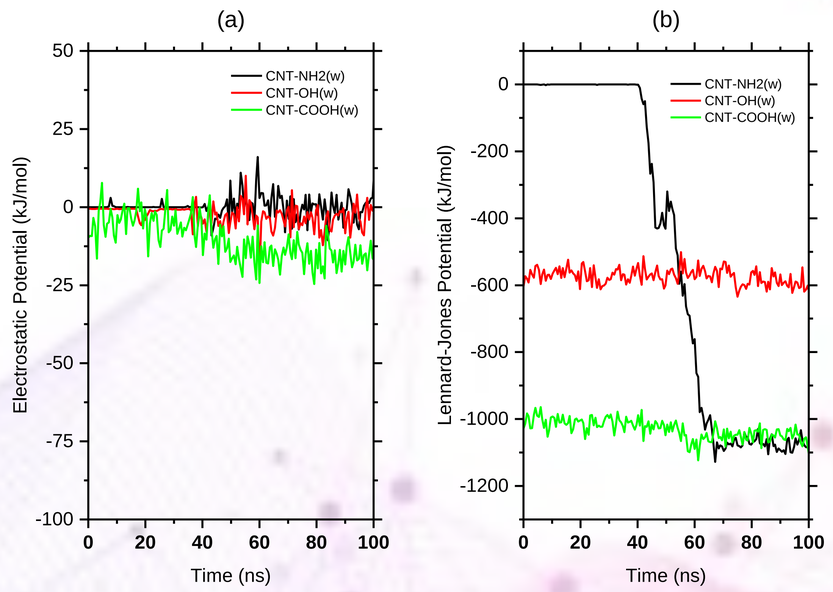
An armchair (15,15) single-wall CNT (SWCNT) was built with the Nanotube Modeler Package. The functionalization was perfumed with carboxyl, hydroxyl, and amine groups and terminal, wall, terminal, and wall of CNT.

Result and Discussion

The snapshots of the interaction between melittin and wall fCNTs during simulation time are shown below. First, melittin is located at a distance from the fCNTs. The comparison of final snapshots elucidates that melittin is encapsulated inside the CNT-COOH(w) and CNT-NH2(w) while it is adsorbed on the surface of CNT-OH(w). Encapsulation of melittin was also proved by the RDF plot below Figure, which indicated that the RDF peak of melittin on CNT-COOH(w) and CNT-NH2(w) was observed at a distance of less than 1 nm. By wall functionalization, the adsorption sites on the CNT surface decreased, facilitating the observed encapsulation.



The LJ and electrostatic potentials between melittin and wall fCNTs are represented in the below Figure. The obtained results indicated that encapsulated melittin has a strong LJ potential with fCNT compared to the state that adsorbed on the fCNT surface. Spontaneous encapsulation of proteins inside the CNT reported previously [3].



The peptide conformation determines its biological activity, and peptide adsorption on the nanocarrier should not significantly change the peptide structure. Therefore, the carrier will be the best choice for the peptide to retain its confirmation and remain stable after adsorption. For this purpose, the conformation of melittin in water has been compared with the one adsorbed on the fCNTs.

Conclusion

The results showed that when only the CNT terminal is functionalized, the peptide tends to be adsorbed on the outer surface of the nanotube. In contrast, when the wall and terminals of the CNTs are functionalized, melittin is encapsulated inside the space of the nanotube. The structural changes were investigated with parameters such as RMSF and Rg. The results showed that the amine functional group is unsuitable and has caused significant structural changes in the peptide. As a result, melittin has a more stable structure in a nanotube filled with hydroxyl and carboxyl. This result will be useful for the design of peptide carriers.

References

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