Transportation of Glucose by the Cyclic Peptide Nanotube: Molecular Dynamics Simulations

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Abstract

Introduction: Nanotubes are formed through the self-assembly of many types of organic molecule. Peptide nanotubes (PNTs) are important due to their wide range of bio functionalities which leads to many potential uses in nanotechnology and biomedicine. Self-assembled cyclic peptide nanotubes (CPNs) show a potential use in drug delivery. Ghadiri et al. pioneered the design of PNTs based on the stacking of cyclic peptides containing even numbers of alternating D- and L- amino acids. Recently, self-assemblies of PNTs have appeared as one of the most interesting nanostructures to be explored in the field of nanotechnology. These smart assemblies can have diverse applications, such as in the design of sensors, electronics, and stimulus-responsive materials. In this study, a CPN with transferability was tested for the transport of glucose.

Methods and Results: To explore the transportation mechanism of CPNs, computational studies have been performed on the CPN models stacked by 7 subunits, including quantum calculations, conventional molecular dynamics (CMD) simulations, and steered molecular dynamics (SMD) simulations in the environment of hydrated dimyristoylphosphatidylcholine (DMPC) lipid bilayer, separately.

Conclusions:

The calculated interaction energy glucose with the cyclic peptide is -7.4 kcal/mol. The CMD simulation along the 30 ns demonstrated that CPN tilted with respect to the normal of the bilayer. The hydrogen bond network formed by the carbonyl and amide group of the backbone in CPN contributed to the stability and tilt of the tube. Some water molecules were found in the tube that preferred to reside in the middle zone of neighboring cyclic peptide subunits. The SMD simulation demonstrated that the glucose molecule was transported by hopping via different potential energy minimum distributed along subunits.

Key words: self-assembly; Cyclic Peptide Nanotube (CPNT); steered molecular dynamics (SMD)