Accepted Manuscript

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PII: S0005-2736(17)30348-6
DOI: doi:10.1016/j.bbamem.2017.10.030
Reference: BBAMEM 82630

To appear in:

Received date: 20 July 2017
Revised date: 19 October 2017
Accepted date: 27 October 2017

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Keywords: carbon nanotube; membrane; nanoidentation; phospholipid bilayer; MD simulations

ABSTRACT:
The influence of the single-walled carbon nanotubes on the phospholipid bilayer has been studied using steered molecular dynamics (SMD) simulations. The impact of different nanotubes on the phospholipid bilayer structure is discussed as well as the speed of indentation. Additionally, a series of simulations with pulling out of the nanotubes from the membrane were performed. The deflection of the membrane in both nanoindenation and extraction processes is also discussed. The self-sealing ability of membrane during this process is examined. Complete degradation of the bilayer was not observed even for the most invasive nanoindentation process studied. The obtained results show that carbon nanotubes can be regarded as potential drug carriers for targeted therapy.

1. Introduction

The living cell is basic component of all living organisms on Earth. The interior of a cell is protected by the cell membrane, an efficient barrier for external molecules, proteins and particles. This membrane is considerably complex molecular system in terms of its structural, mechanical and physical properties [1–3]. An important component of this system is phospholipid bilayer, composed of phospholipid and cholesterol molecules, which are essential to regulate membrane fluidity.

During last decades, much attention has been paid on the so called targeted therapy based on delivering drugs, encapsulated inside some nanocarriers, into the living cells [4–8]. The promising candidates for such containers seem to be carbon nanotubes (CNTs) [9–13]. The major advantage is their potential to reduce the side effects of taking a drug, for example highly toxic anticancer drugs. Carbon nanotube has been suggested as such a carrier to deliver drugs to a specific site in cancer treatments (drugs like cisplatin, paclitaxel or doxorubicin) [14,15]. CNTs biocompatibility can be increased by their modifications with various biological and bioactive species [16,17]. Some drugs and even DNA molecule could be spontaneously inserted into CNT in a water solute environment [18,19]. The long-term integration of cells with inorganic materials provides the basis for novel delivery and sensing platforms. Nanotubes can be used as a part of bioimplants, to deliver glucose and insulin to organism [20]. The interactions of CNTs with biologically-important substances such like cholesterol, homocysteine, dimethyl sulphoxide, peptides, proteins or DNA segments are intensively studied [21–26].

Our earlier simulations [22,27–29] as well as experimental studies [30–36] suggest that CNTs quite efficiently penetrate into the cells, but the mechanism of this process is still not well known.