Abstract

Title: pH-Sensitive Co-Adsorption/Release of Doxorubicin and Paclitaxel by Carbon Nanotube, Fullerene, and Graphene Oxide in Combination with N-isopropylacrylamide: A Molecular Dynamics Study

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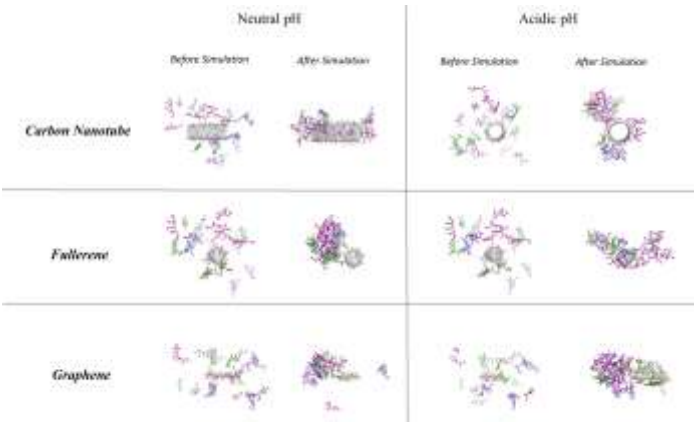
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I. Abstract Body (up to 250 words)

Nanotechnology based drug delivery systems for cancer therapy have been the topic of interest for many researchers and scientists. In this research, we have studied the pH sensitive co-adsorption and release of doxorubicin (DOX) and paclitaxel (PAX) by carbon nanotube (CNT), fullerene, and graphene oxide (GO) in combination with N-isopropylacrylamide (PIN). This simulation study has been performed by use of molecular dynamics. Interaction energies, hydrogen bond, and gyration radius were investigated. Results reveal that, compared with fullerene and GO, CNT is a better carrier for the co-adsorption and co-release of DOX and PAX. It can adsorb the drugs in plasma pH and release it in vicinity of cancerous tissues which have acidic pH. Investigating the number of hydrogen bonds revealed that PIN created many hydrogen bonds with water resulting in high hydrophilicity of PIN, hence making it more stable in the bloodstream while preventing from its accumulation. It is also concluded from this study that CNT and PIN would make a suitable combination for the delivery of DOX and PAX, because PIN makes abundant hydrogen bonds and CNT makes stable interactions with these drugs.

II. Image:



III. Reference:

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IV. **Biography:**

Milad Rezaian, MD from Shahid Beheshti University of Medical Sciences, School of medicine graduated as the number one student. I have silver medal from the 14th national Biology Olympiad of Iran. I've had publications in the fields of anatomy and pharmacology.

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