INSTITUTE OF PRIORITY TECHNOLOGIES

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STUDY OF THE POSSIBILITY OF CREATING A DRUG COATING FOR BILIARY STENTS BASED ON THE COPOLYMER "POLYLACTIC ACID-POLYCAPROLACTONE" MODIFIED WITH CARBON NANOTUBES AND DOXORUBICIN

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ABSTRACT

This article considers the possibility of creating an ultrathin drug coating for biliary stents. The article also presents theoretical calculations of the interaction of complexes of carrier polymers and copolymer "polylactic acid - polycaprolactone" modified by carbon nanotubes. This coating is proposed to improve biocompatibility during endobiliary stenting.

INTRODUCTION

Mechanical jaundice usually refers to a symptom complex that occurs when the outflow of bile through the bile ducts of the liver is disturbed. This disease is an indication for stenting. Unfortunately, over time, physicians noted a number of disadvantages of endobiliary stenting, the main of which was restenosis. Also, within the first few hours after the completion of stenting procedure, there may be a risk of serious complications such as thrombosis and restenosis. To reduce the risks of such complications, as well as to improve the future results of the operation, the use of stents with special drug-coated (DC) to provide local transportation, quality application of the drug substance on the surface of the biliary stent and prolonged drug release, a polymeric carrier complex is required.

THE STUDY PROPOSED AN ULTRAFINE DRUG COATING CONSISTING OF TWO POLYMERS (POLYCAPROLACTONE (PCL) AND POLYLACTIC ACID (PMC)), CARBON NANOTUBES (CNT) AFFECTING THE STABILITY AND PRESERVATION OF DRUG COATING ON THE STENT SURFACE DUE TO ITS UNIQUE SORPTION PROPERTIES, AND THE DRUG DOXORUBICIN (DOX), WHICH HAS PRONOUNCED ANTI-TUMOR ACTIVITY

Quantum-chemical calculations of the interaction of its main components, performed by the DFT method, were performed to prove the feasibility and effectiveness of the new ultrathin drug coating. The model of the complex "PCL+PMC+UNT+doxorubicin" is shown in Figure 1.

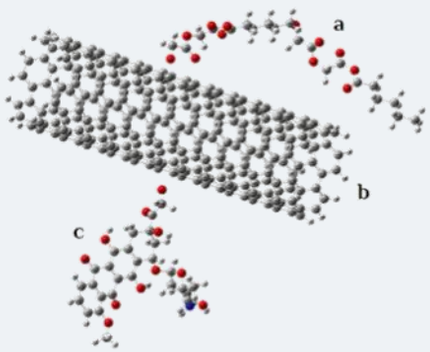

Fig. 1. Model of the complex "copolymer (PCL+PMK) (a) + CNT (b) + doxorubicin (c)"

Based on the analysis of the results of calculations of doxorubicin attachment to the "copolymer + CNT" complex, we plotted the dependence of the potential interaction energy of the coating components (Figure 2) .

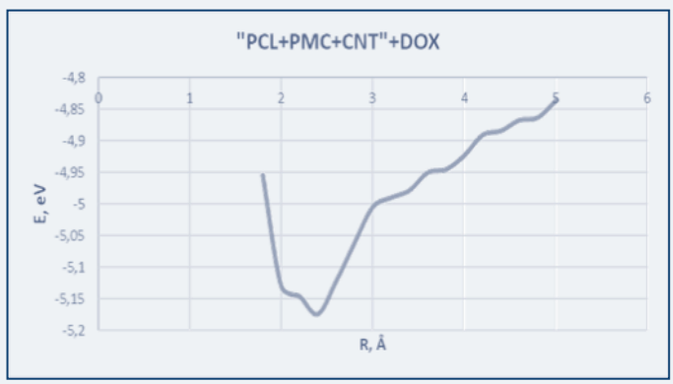

Fig. 2. Energy curve of adsorption energy (eV) versus distance (Å) of the complex structural complex "PCL+PMC+UNT" + DOX

CONCLUSIONS

The presence of the curve minimum at a distance of 2.4 Å, corresponding to the energy Eads = -5.17 eV and the distance of physical interaction between doxorubicin and the center of the complex consisting of copolymer and CNT, proves the possibility of fairly easy desorption of the drug from the carrier polymer and its gradual entry into the body.

The need to improve the technology of endobiliary stenting requires researchers to find effective ways to solve the problems of arising restenosis and thrombosis. Since the conduct of full-scale medical experiments requires detailed preparation and great time and economic expenses, as well as is associated with the risk of causing harm to human health, the most expedient is preliminary computer modeling of the materials under study. The nanocoating proposed in this paper is formed from the most effective materials for solving existing problems. On the one hand, these are polymers: polycaprolactone and polylactic acid, which improve mechanical and chemical properties of the stent; carbon nanotubes, whose unique features have long made them one of the in-demand materials of nanotechnology; and doxorubicin, a drug that allows to significantly reduce the risk of tumors.

During the model experiment, the mechanism of drug nanocoating formation was presented in detail, the most probable type of copolymer was determined, and the interaction of the obtained complex with the drug was presented.
The conducted studies theoretically prove the possibility of creating a drug nanocoating "PCL with PMC + CNT + DOX" with a copolymer of type A-B-A-B-A-B, which opens broad opportunities for the introduction of this material in medical practice.