PHYSICOCHEMICAL AND ANTIBACTERIAL PROPERTIES OF ORNIDAZOLE-BASED NANOCOMPOSITES FOR MEDICAL APPLICATION

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The rapid adaptation of bacteria to widely used medical drugs and the insufficient development of new antibacterial agents create a global problem of forming microorganisms with multiple drug resistance. This issue drives the search for innovative approaches, among which the development of drug-loaded nanocomposite materials is considered a promising strategy for combating multidrug-resistant bacterial strains [1]. One effective method for obtaining such materials is modifying silica surfaces with biologically active substances, which enhances their bioavailability and ensures controlled drug release, thereby reducing the risk of resistance development in pathogenic microorganisms [1, 2]. This study analyzed nanocomposites with ornidazole – an antimicrobial agent effective against anaerobic bacteria and protozoa. Investigating the physicochemical characteristics of the obtained nanocomposites enables the assessment of their stability, morphology, and interactions with biological systems. Also, studying the antimicrobial properties of these materials helps determine their effectiveness against pathogenic microorganisms and their potential for improving antibacterial therapy.

Considering the above, this study aimed to investigate the physicochemical and antibacterial properties of silica-based nanocomposites modified with ornidazole using quantum chemical calculations, scanning electron microscopy, the physical adsorption method, and biological methods. Quantum chemical calculations have demonstrated that the interaction between the ornidazole molecule and the silica surface is thermodynamically feasible during adsorption from the gas phase and from an aqueous solution. It was established that the energy of intermolecular interaction in the gas-phase approach (ΔG_{int}) and the energetic effect of the water molecule displacement reaction by ornidazole for silica are -80.9 kJ/mol and -33.5 kJ/mol, respectively. The hydration energy (ΔG_{hydr}) of ornidazole is lower (-103.1 kJ/mol) compared to the corresponding value for silica (-180.6 kJ/mol).

The physical adsorption method confirmed that the specific surface area of silica modified with ornidazole decreased compared to the initial silica, depending on the percentage content of the drug. Morphological and structural analysis of the nanocomposites using SEM confirmed the uniform distribution of ornidazole on the silica surface.

It is important to study the adsorption and desorption processes to predict the ability to control the release of the active substance. The adsorption isotherm of ornidazole on silica corresponds to the S-type, indicating weak interaction with the surface and competition with the solvent for active sites. The bioavailability assessment of the active substance demonstrated that ornidazole from the nanocomposite is released significantly faster than pure ornidazole, achieving a higher solubility level within the same time frame. This is explained by the transition of ornidazole into an amorphous state, as confirmed by X-ray phase analysis.

The assessment of antibacterial activity showed that nanocomposites modified with ornidazole exhibited a more pronounced inhibitory effect on Gram-positive (*S. aureus*) and Gram-negative (*E. coli*) bacterial strains compared to initial silica, which displayed weak antibacterial activity.

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