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Bionanomaterials for drug delivery: computational and experimental study of MoS2-based nanocomposites with anticancer drugs

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The development of effective new bionanomaterials for targeted drug delivery is one of the most pressing applied problems of modern nanoscience and nanotechnologies for biomedical applications. The contributions of computational biophysics, as well as combined experimental and theoretical nanobiophysical research, to the study of intermolecular interactions between nanocarriers and therapeutic molecules in the drug delivery nanobiosystems are difficult to overestimate. Among the variety of nanomaterials that have recently been proposed for use in drug delivery, 2D MoS2 nanosheets have caught our attention, due to the unique physicochemical properties of MoS2 that offer the possibility of utilizing this nanomaterial as a multifunctional drug delivery platform for anticancer drug delivery combined with photothermal therapy of tumors.

This report presents the results of our computational and mass spectrometry experimental characterization of nanobiocomposites of MoS2 nanosheets with a representative of set of anticancer drugs based on derivatives of DNA nitrogen bases 6-thiopurine (TP), 2-thioadenine (TA), 5-fluorouracil (FU), or with widely used anticancer medication doxorubicin (DOX).

Ab initio DFT/M06-2X computational modelling of nanobiohybrids of MoS2 nanosheet with a molecule of the mentioned anticancer drugs was performed to examine the possible structures of the MoS2-based drug delivery nanobiocomplexes. In particular, the structures of the covalent and noncovalent complexes of MoS2 particles with the drug molecules were determined, and the energies of such complexes were calculated. Based on the modelling results, the biologically significant peculiarities of the anticancer agents interactions with MoS2 nanosheets are discussed, and the nanomaterials applicability for drug delivery is estimated.

For the experimental study, binary nanocomposites (MoS2 + drug) for each anticancer agent were obtained via ultrasound treatment and examined by laser desorption/ionization (LDI) mass spectrometry. Analysis of the mass spectra obtained demonstrates the presence of peaks of intact molecular ions of the anticancer drugs in the spectra of the majority of the studied nanocomposites. It testifies to the preservation of the drug's molecular structure within the nanocomposites with MoS2, which is crucial for maintaining the drugs' therapeutic activity. At the same time, we revealed spectral confirmations of some chemical transformations (oxidation processes) of sulfur-containing anticancer drugs (TP, TA) induced by catalytically active MoS2. We believe that such chemical transformations of drug molecules can reduce their therapeutic activity, which is mostly related to the thio-groups of TP and TA.

We suppose that the current study results should be considered in the development and application of MoS2-based bionanomaterials.

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