QUANTUM-CHEMICAL MODELING OF DOXORUBICIN-FULLERENOL AGENTS OF CANCER THERAPY

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In order to therapeutically destroy neoplasms chemotherapy or radiotherapy is usually applied, and in isotope medicine – short-lived radio nuclides are injected into the tumor (^{59}Fe, ^{90}Y, ^{95}Zr, ^{99m}Tc, ^{106}Ru, ^{114*}In, ^{147}Eu, ^{148}Eu, ^{155}Eu, ^{170}Tm, ^{177m}Lu, ^{188}Re, ^{210}Po, ^{222}Rn, ^{230}U, ^{237}Pu, ^{240}Cm, ^{241}Cm, ^{253}Es). Binary (or neutron capture therapy) − a technology developed for the selective effect on malignant tumors and using drugs tropic to tumors containing non-radioactive nuclides (^{10}B, ^{113}Cd, ^{157}Gd at al.). Triadic - the sequential introduction into the body of a combination of two or more separately inactive and harmless components, tropic to tumor tissues and capable of selectively accumulating in them or entering into chemical interaction with each other and destroying tumor neoplasms under the influence of certain sensitizing external influences. The aim of this work is quantum-chemical simulation of the electronic structure and analysis of the thermodynamic stability of new doxorubicin-fullerenol agents for the treatment of tumor neoplasms. The need for preliminary studies of modeling such objects is due to the extremely high labor intensity, cost and complexity of their practical production. Previously, we presented data on quantum chemical modeling of the structure and electronic structure of chemotherapy drug methotrexate [1] and cortisone fullerenol clusters [2, 3].

The need for preliminary modeling of such objects is due to the extremely high labor intensity and complexity of their production. In this work, *ab initio* quantum-chemical calculations of a number of potential agents for the diagnosis and therapy of cancer diseases, C_{60} fullerenol derivatives, are applied. Connection calculations were carried out by the DFT method using the B3LYP1/MIDI theory level using the GAMESS software package and the MIDI basis set. To increase the effectiveness of these drugs, it is promising to introduce into the composition of their molecules structural fragments of known dosage forms, for example, doxorubicin. This report presents the results of quantum-chemical modeling of the structure and electronic structure of endohedral doxorubicin-fullerenol clusters.

^{90}Y, ^{210}Po and ^{222}Rn were chosen as endohedral components of inclusion in the inner spheres of clusters. Emphasis on these supramolecular objects of inclusion in the inner cavities of both fullerenol itself and monodoxorubicin-fullerenol or bisdoxorubicin-fullerenol clusters is due to the fact, that radionuclides are sources of therapeutic ionizing α-radiation [4].

References

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