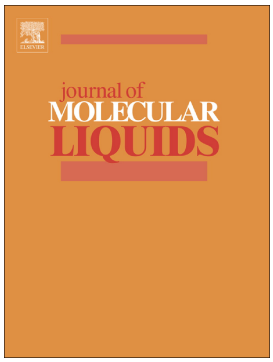

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Theoretical study of solvent and co-solvent effects on the interaction of Flutamide anticancer drug with Carbon nanotube as a drug delivery system

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Abstract

The current study describes the investigation of the solvent effects on the adsorption strength between Flutamide molecule and (5,5) single-walled carbon nanotube for different configurations in the water solution based on the density functional theory calculation. The negative values of the adsorption and solvation energies demonstrate that all designed configurations are stable and the interaction of the drug molecule with the nanotube sidewall is a spontaneous process. It is found that the polarity of the FLU/SWCNT complexes increases in the present of water solvent, suggesting the possibility of solvation and their disperses in the living system. The main and important parameters derived from Atoms-In-Molecule analysis, i.e., the positive and negative values of Laplacian and total electron energy density properties, respectively, reveal that the considered intermolecular interactions are a partial covalent character. The natural bond orbital calculations indicated that the drug molecule can be adsorbed on the nanotube with a charge transfer from the single-walled carbon nanotube to Flutamide molecule. Likewise, the interaction of the drug molecule and pristine nanotube on the basis of four reactivity descriptors such as the overall stabilization energy, charge transfer, the individual energy change of acceptor and the individual energy change of donor have been investigated.