Abstract

The cancer treatment has been as a purpose and concern in medical science. Noteworthy developments in improving the chemotherapy using various nano-carriers has been performed for targeted and controlled delivery the anti-cancer agents. Boron-nitride single-walled nano-tubes are one of the effective tools in the cancer treatment. In this study, the possible confirmations of the breast cancer drug (letrozole) have been performed by density functional theory. The calculations in level (B3LYP) have been carried out using the Gaussian09 software. Also, to better understand the molecular and sub-molecular orbital theory of natural bond nature of the link and the atom in the molecule were used. Harmonic vibrational frequency calculations were performed on the same level. Molecular orbital calculations, including the highest occupied molecular orbital and density functional theory and method lowest unoccupied molecular orbital level in order to investigate parameters such as hardness, softness, and chemical potential was conducted. Conformations charge density distribution and chemically active sites studied by the electrostatic potential was optimized level. To investigate the effect of solvent molecules on the electronic and structural properties of the solvent continuum model was used. So, the boron-nitride nanotubes can be used as a drug carrier and also to remove the drug side effects and significantly reduce the amount of drug

Keywords:
Single-walled nanotubes, boron -Nytryd, breast cancer, letrozole, computational chemistry,

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