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The study of force fields molecular mechanics and molecular quantum on the interaction with drugs of the alkylating agent with SWCNT-BNNT in different solvents and at different temperatures

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The present study investigates the interaction between two alkylating agent drugs, cyclophosphamide (CP) and mechlorethamine (MC), with Single-Wall carbon nanotubes (SWCNTs) and Boron Nitride nanotubes (BNNTs). Calculations have been performed by using methods of quantum mechanics and molecular mechanics. The effects of different solvents on the interaction of CP and MC with SWCNTs and BNNTs within the Onsager self-consistent reaction field (SCRF) model, as well as the effects of temperature on the stability of the interactions between the compounds in various solvents have been investigated. Thermodynamic parameters, Frontier Molecular Orbitals (FMOs), and Total Density of States (DOS) of the title compounds have been evaluated by using theoretical calculations. Moreover, the interaction of CP and MC with SWCNTs and BNNTs have been examined through AMBER, OPLS, CHARMM, and MM+ force fields through the molecular mechanic (MM) method. The Monte Carlo simulation of CP and MC structures connected to carbon and boron nitride nanotubes in Water, Methanol, Ethanol, DMSO, and Chloroform solvents showed that Chloroform is the most stable solvent for simulation with the lowest energy, which is directly attributed to dielectric constant. Studies show that the results of Monte Carlo, molecular mechanics, and quantum mechanics are consistent with each other in terms of thermodynamic properties and conformer populations.

Keywords: Quantum Monte Carlo (QMC), Single-Wall carbon nanotubes (SWCNTs), Boron Nitride nanotubes (BNNTs), Alkylating agent, Force field