Abstract

Ab initio and density functional theory methods have been employed to study the molecular properties of the oxo-imino, oxo-amino and hydroxy-imino tautomers (including their rotamers) of imexon antitumor drug in different environments: gas, water and DMSO. Molecular geometries and energetics of the tautomeric forms (including their rotamers) in gaseous phase have been obtained using B3LYP and MP2 levels of theory. The results suggest that the oxo-imino tautomer may be the most stable form in the gas phase. Solvent effect is introduced by use of the conductor-like polarizable continuum model (CPCM) using universal force field (UFF) cavity. The structural and energetical parameters of all the conformers have been analyzed. The ^{1}H and ^{13}C NMR chemical shifts of imexon tautomers have been computed using gauge-independent atomic orbital (GIAO) method at B3LYP/6-311+G(2d,p) level of theory. The data obtained from this study were compared with the corresponding experimental results when available. From the calculated and experimental data, it can be concluded that in solution, the real existing structure of imexon should be the oxo-amino form