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6-(2-fluorobenzoyl)-3-(2-(4-(4-fluorophenyl)piperazin-1-yl)-2-oxoethyl)benzo[d]thiazol-2(3H)-one Drug Molecule Structure and Its Interaction with Atmospheric Pressure Plasma Jet

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Abstract

The structure, conformational stability and vibrational frequencies of 6-(2-fluorobenzoyl)-3-(2-(4-(4-fluorophenyl)piperazin-1-yl)-2-oxoethyl)benzo[d]thiazol-2(3H)-one (abbreviated as 6FOT) drug molecule in the ground state were computed by the density functional theory - DFT (B3LYP) and Hartree-Fock (HF) methods using different fundamental sets. The vibrational-Fourier transform infrared (FT-IR) spectra of the 6FOT molecule were examined for solid, liquid and gas phases. The four different stable conformations of the 6FOT drug molecule was obtained. The differences between the geometries as experimental and theoretical of the molecule exhibited that the X-ray parameters were quite compatible with the most stable conformer measured values as theoretically. The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) calculations were used to find the molecular energy gap, so the less band gap appears as ruther stable. The detailed structure of 6FOT molecule are given. In addition to these, the atmospheric pressure plasma treatment (APPT) was applied to the 6FOT molecule in liquid phase and then FT-IR and ultraviolet-visible (UV-Vis) spectra were analyzed. Even the plasma effects have been revealed. It is seen that some bonds of 6FOT molecule was broken. New photoproducts may