The effect of electron-donor/acceptor groups on structural/electronic properties of fluvoxamine drug to control covid-19

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October 6, 2022

Abstract

Studies have shown that fluvoxamine can be useful in preventing the spread of Covid-19 disease (in the early stages of the disease) by strengthening the body's immune system. For this purpose, in this work, the structural and electronic properties of fluvoxamine drug were investigated using quantum theory of atom in molecule (QTAIM) and Density-functional theory (DFT) at B3LYP-DFT/6-311G+ (at presence of water as solvent and the CPCM model) computational level. Also, in order to improve the electronic/pharmaceutical properties, the effect of electron donor/acceptor groups of NO2 and NH2 on fluvoxamine was studied. According to the results, electronic properties changed significantly in the presence of the NO2 group. So that (in the presence of NO2) cohesive energy, energy gap, dipole moment, adsorption energy, antioxidant properties, and recovery time improved by 20%, 70%, 84%, 48%, 48%, and 46% respectively. Although the electronic properties were improved in the presence of the NH2 group, the effect of the NO2 functional group was more noticeable. Therefore, it is expected that the presence of the NO2 electron-acceptor electron group will improve its medicinal function by changing the electronic properties of the drug fluvoxamine.

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