

DFT, wavefunction and toxicity analyses of Megazol

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Megazol is a drug molecule used to treat acid-related diseases of the stomach. The B3LYP/6-311++G(d,p) level of theoretical calculations frequently employs Gaussian 16W software. In the present work electronic structure analysis, FMO, NBO, MEP, Mulliken charge, vibrational frequency analyses, and electronic excitation determination through the IEFPCM model in various solvents have been obtained. NBO analysis explains that this is a stable molecule. By using Multiwfn 3.8 software, NCI, a shaded surface map, and hole electron interaction (HEI) with inter-fragment charge transfer analyses have been determined. In the S6 excited state, electrons can move across π -linkers from an electron donor to an electron acceptor, according to HEI analysis. Heat maps are generated and discussed for the lowest six excitation states. Simulated scanning tunneling microscope analysis has also been performed. Using the Sermo software, the impact of temperature on S, CV and CP has also been ascertained. Theoretical UV-Vis and IR have been discussed. The toxicity of the molecule is explained.

Keywords: Megazol, DFT, Hole-electron transfer, NBO, MEP