**Experimental And Theoritical Studies Of Synthetic Biomaterial 1- Acetyl-2-(4-Isopropoxy-3-Methoxyphenyl) Cyclopropane**

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**Abstract**

Quantum chemical computations are excellent methods in the design of biological and pharmcetical molecules and help to predict some properties of the new materials The present works deals with the vibrational spectra and the molecular structural analysis of 1- Acetyl 2-44 Isopropoxy 3- Methoxyphenyl) Cyclopropane have been analyzed. The equilibrium geometry, harmonic vibrational wavenumbers of 1-Acetyl-2-(4-Isopropoxy-3-Methoxyphenyl) Cyclopropane investigated with the help of density functional theory (DFT) method. The calculated vibrational are well agreement with experimental spectra. The value of HOMO-LUMO energy was also calculated, it confirm its Charge transfer interation and the bio activity of the molecule. The possible interaction present in the molecule is analyzed using Natural Bond Brbital (NBO) analysis. The mulliken and natural charge of the compound were calculated and analyzed

Keywords: DFT, Optimized geometry, NBO, HOMO-LUMO, Biomaterial