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Spectroscopic Analysis (FT-IR, FT-Raman) with HOMO-LUMO, ADMET and Molecular Docking Studies of β(3E)-4-(2, 6, 6-Trimethylcyclohex-1-en-1-yl) but-3-en-2-one against Lung Cancer: A potential Inhibition of ATP Synthase

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ABSTRACT

Investigations (experimental and theoretical) on the molecular structure and vibrational characteristics of β-ionone: (3E)-4-(2, 6, 6-Trimethylcyclohex-1-en-1-yl) but-3-en-2-one is reported in this work. In comparison, experimental FT-IR and FT-Raman spectral data were in good agreement with the results obtained from the computational method. The equilibrium geometry and vibrational spectra are calculated by using DFT (B3LYP) with a 6-311G (d, p) basis set using GAUSSIAN 09.Quantum chemical calculations of the equilibrium geometry and the complete vibrational assignments of wavenumbers using potential energy distribution (PED) were carried out. The HOMO-LUMO energies show that the chemical activity of the molecule and molecular electrostatic potential maps (MEPs) activity confirm the superiority of the material.. Electrophilic and nucleophilic interactions were predicted from the Fukui function

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