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Ab-Initio Study of Structural and Vibrational Properties of Latifolin

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Aim of the study: Alzheimer's disease (AD), which is a chronic neurodegenerative disease, usually starts slowly and gets worse over time. The patients with alzheimer have memory loss and other insufficiently intellectual abilities to interfere with daily life. They give rise to the dementia occuring with the range of 60% - 70% . Amyloid beta (Aβ) peptides are noticeably involved in Alzheimer's disease, because the main component of the amyloid plaques founded in the brains of Alzheimer patients. Latifolin is a substance which inhibits to Aβ. Some quantum-chemical properties of latifolin molecule are limited in the literature. Our main aim to calculate some spectroscopic properties of title molecule by using ab-initio method, in this study.

Material and Methods: In this work, the ab-initio calculations based on Density Functional Theory (DFT) with the basis set of 6-31G(d,p) are performed to determine the molecular structural properties of latifolin. Molecular structure is optimized to get the global minima of the molecule by considering C1-symmetry (no symmetry constraint). The vibrational spectra is predicted by using the optimized structure. The 1H and 13C NMR shielding constants are obtained by applying the Gauge-Including Atomic Orbitals (GIAO) method in the ambient of ethanol. VEDA 4 (Vibrational Energy Distribution Analysis) package program has been used to calculate Potential Energy Distribution (PED) for the vibrational frequency. We have used the scaled factor as 0.961 for DFT/B3LYP. Moreover, the observed vibrational wavenumbers of FT-IR are analyzed and assigned to different normal modes of the molecule.

Results: DFT calculations of the latifolin, which can be used for constructing new drug design to remedy Alzheimer's disease, are presented in this work. The NMR spectrum, FT-IR spectrum, PED analysis and complete molecular structural parameters such as bond lengths, bond angles and dihedral angles of the molecules have been investigated by using the DFT/B3LYP/6-31G(d,p) method.

Keywords: *DFT, Coumarin, Latifolin, NMR, FT-IR*