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Experimental and Computational Analysis of 7-Isopropoxy-3-phenyl-4H-1-benzopyran-4-one

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Abstract

Non-hormonal isoflavone derivative 7-Isopropoxy-3-phenyl-4H-1-benzopyran-4-one (7I3P4H) is used for prevention and treatment of postmenopausal osteoporosis. It is also used for reducing bone loss caused by chronic kidney diseases and paralysis associated with stroke. Optimized geometry and Natural Bond Orbital (NBO) analysis of 7I3P4HB carried out to demonstrate the various intra-molecular interactions that are responsible for the stabilization of this molecule leading to its medicinal activity. Ultraviolet Absorption (UV) spectra have been recorded and analyzed. Energy gap has been calculated from Frontier Molecular Orbital Analysis with the help of B3LYP/6-311++G (d, p) method.

Keywords: Isoflavonoid, NBO, UV-Vis, HOMO-LUMO.

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