Structural analysis and biological profile of a novel hydroxy-chalcone

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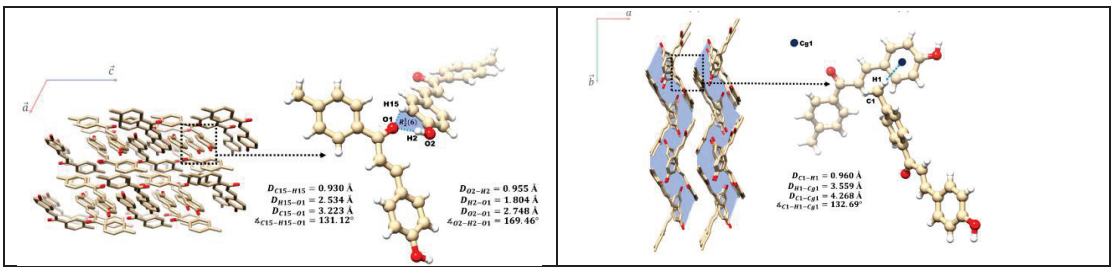
In the past few years, chalcones have shown an impressive array of biological activities like anticancer, antimalarial, antimicrobial, antitubercular, antimutagenic, anti-inflammatory and anti-diabetic effects. Considering this wide range of applications, this paper presents the synthesis and characterization of a new chalcone (*E*)-3-(4-hydroxyphenyl)-1-p-tolylprop-2-en-1-one (HXC). The molecular structure was analyzed from Single Crystal X-ray Diffraction [Final indexes R_1 = 0.0494 and wR_2 = 0.1262) [1] and Hirshfeld surfaces (Figure 1). HXC was optimazed at MP2/6-311++G(d,p) theory level by using Gaussian 09 [2] software in order to determine both the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) energies and the Gap energy between them. Additionally, the biological potential of HXC was evaluated from molecular modeling methods. The main results showed that HXC has a non-planar conformation, while its crystal packing is stabilized by classical hydrogen bonds and weak C–H···O and C–H···π interactions. The molecular electrostatic potential map showed the main electrophilic and nucleophilic sites of HXC concentrated in hydroxyl and carbonyl groups, respectively. Finally, molecular docking simulations evidenced that HXC establishes intermolecular interactions with Trp20 and Trp111, from the active sites of *M. tuberculosis* InhA (A) and human AR (B). These results indicate a good biological potential for HXC against tuberculosis.



(a) (b)

Figure 1: (a) Front view of HXC crystal packing and observed C–H···O and O–H···O interactions; (b) side view of HXC crystal packing and observed C–H···π interaction. Cg1 is formed by atoms C11, C12, C13, C14, C15 and C16.

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