Poster Presentation

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Synthesis and crystal structural studies of (E)-3-(3-methylthiophen-2-yl)-1-p-tolylprop-2-en-1-one

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The compound, (E)-3-(3-methylthiophen-2-yl)-1-p-tolylprop-2-en-1-one was synthesized by refluxing 3-methyl-2-thiophenecarboxaldehyde with 4-methylacetophenone in the presence of aqueous potassium hydroxide at room temperature. The title compound was characterized by NMR, FTIR and UV-Vis techniques and finally the structure was confirmed by X-ray diffraction studies. The olefinic double bond in the structure adopts an E conformation. The trans conformation of the C=C double bond in the central enone group is confirmed by the C=C-C-C torsion angle value of 178.1(3)°. The thiophene ring is affected by π conjugation. In the crystal, the molecules are linked via pairs of C--H...O hydrogen bonds forming inversion dimers with R22(10) ring motifs. The intermolecular contacts in the crystal structure were quantified using Hirshfeld surface analysis method. The majority contribution to the Hirshfeld surfaces is from H...H contacts. Further, the synthesized compound was also evaluated in-vitro for its antimicrobial and antioxidant susceptibilities, and these results will be presented.

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[2] Ahmad, M. R., Sastry, V. G. & Bano, N. (2011). International Journal of ChemTech Research, 3, 1462-1469.

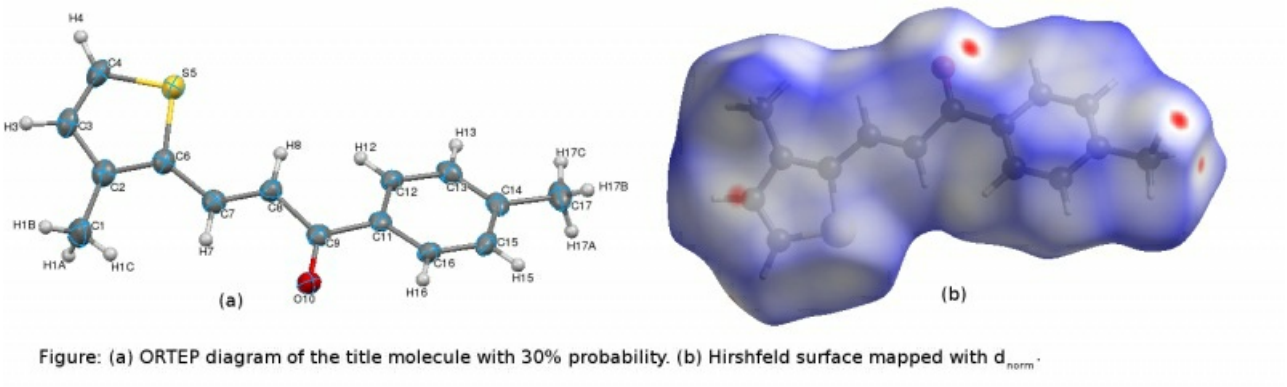

Figure: (a) ORTEP diagram of the title molecule with 30% probability. (b) Hirshfeld surface mapped with d_{norm}.

Keywords: X-ray diffraction studies, monoclinic, Hirshfield surface.