Poster Presentation

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Synthesis and Single Crystal Study of 7-Hydroxy-3-(4-nitrophenyl)-Coumarin

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Coumarin derivative, 7-hydroxy-3-(4-nitrophenyl)-coumarin (C15H9N1O5) was synthesized by knoevenagel condensation reaction by using 2,4-Dihydroxybenzladehyde and 4-nitrophenylacetonitrile. The title compound was characterized by FT-IR, NMR and LCMS spectral studies and finally, the structure was confirmed by X-ray diffraction studies. The crystal structure of the title compound displays a two-dimensional architecture. The compound exhibits both inter and intra-molecular hydrogen bonds of type O—H…O and C—H…O. In addition, DFT calculations and Hirshfeld surface analysis were carried to analyze nature of hydrogen bonding, inter-molecular interaction in crystal, and to examine the molecular shapes. The overlapping of atomic orbital along with their predicted energy is explained on the basis of HOMO-LUMO energy gap calculations. Molecular electrostatic potential map was studied for predicting the reactive sites.

[1] Harishkumar, H. N., Mahadevan, K. M., Jagadeesh, N. M. & Kirankumar, H. C. (2012). Org. Commun., 5(4), 196-208.
[2] Sheldrick, G. M. (2008). Acta Cryst., A64, 112.
[3] Spackman, M. A. & Jayatilaka, D. (2009). CrystEngComm., 11, 1932.

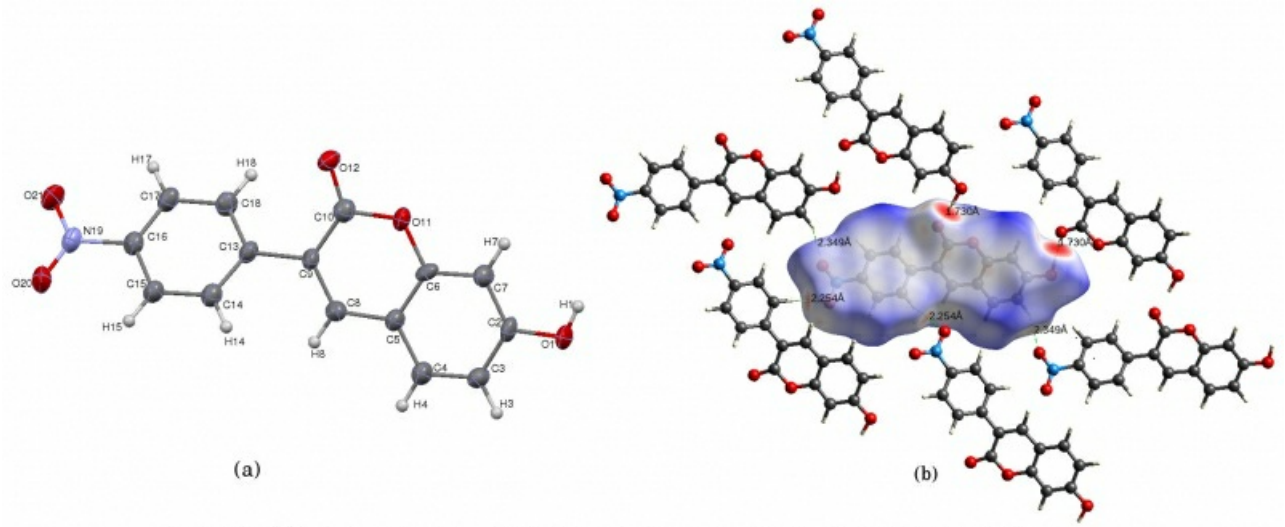

Figure: (a) Molecular structure and (b) intermolecular interactions of the title compound.

Keywords: Coumarin derivative, X-ray diffraction, Hirshfeld surface