Poster Presentation

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Structure and in vitro activity of coumarin derivative

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The compound Ethyl 2-(4-methyl-2-oxo-chromen-7-yl)oxyacetate (C14H14O5) was synthesized using 7-hydroxy-4-methyl-coumarin and ethyl chloroacetate. The structure was establised using IR, NMR and single crystal X-ray diffraction technique. The compound crystallizes in monoclinic crystal system and space group P21/n. The cell parameters are a = 12.502(3) Å, b = 8.324(2) Å, c = 13.477(3) Å, β = 115.558(15)°, V = 1265.3(5) Å3. The phenyl and the pyrone rings in the structure are planar and are in trigonal hybridization. These rings are in syn-periplanar (+sp) conformation. The molecular structure is stabilized by a weak inter and intramolecular interactions of the type C—H…O. They structure also exhibits strong π—π stackings. In the crystal packing C—H…O intermolecular hydrogen bonds link pairs of molecules to form inversion dimers forming R22(22) graph-set motif [1]. The intercontacts in the crystal structure are studied using Hirshfeld surface analysis [2]. The newly synthesized compound was screened for its antibacterial activity against two gram-positive and two gram-negative bacteria.

[1] Bernstein, J. et al. (1995) Angew. Chem. Int. Ed. 34(15), 1555–1573.
[2] Spackman, M. A. et al. (2009) Cryst. Eng. Comm. 11, 19–32.

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