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 established 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.


Keywords: graph-set motif, antibacterial