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Abstract

Rheumatoid arthritis (RA) is one of the inflammatory joint diseases in a heterogeneous group of disorders that share features of the destruction of the extracellular matrices of articular cartilage and bone. Matrix metalloproteinase (MMP) enzymes (in particular MMP9), are crucial for RA. Given the limited investigation of the MMP9 inhibition by coumarin derivatives, the present study was taken up. A coumarin derivative (ethyl 6-[(4-methyl-2-oxo-2H-chromen-7-yl)oxy]hexanoate) was synthesized, characterized by spectral analysis (^{1}HNMR, ^{13}CNMR, IR, and MS), single crystal XRD and molecular docking was carried out. The title compound $C_{18}H_{22}O_5$ crystallizes in the monoclinic crystal system in $P2_1/c$ space group. The glide docking score for the title compound is -6.8, compared with -6.6 for co-crystal compound (LT4). The synthesis, characterization and crystal data are discussed.

Keywords: 7-hydroxy-4-methyl coumarin, crystal structure, MMP9, molecular docking, anti-rheumatoid arthritis.