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Synthesis, crystal structure, computational analysis, and *in silico* evaluation of 3-methyl-*N*-(2-oxo-4-(trifluoromethyl)-2*H*-chromen-7-yl)thiophene-2-carboxmide

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ABSTRACT A new coumarin derivative, 3-methyl-*N*-(2-oxo-4-(trifluoromethyl)-2*H*-chromen-7-yl)thiophene-2-carboxmide was synthesized by the reaction of 7-amino-4-(trifluromethyl)-2*H*-chromene-2-one with methyl-2-thenoyl chloride and characterized using spectroscopy techniques. The structure was confirmed by the X-ray diffraction method. The synthesized compound demonstrated intermolecular hydrogen bonding of the types N–H···O, C–H···F, and C–H···O, which contribute to the formation of supramolecular synthons. Hirshfeld surface analysis revealed that the predominant intermolecular interactions arise from F···H contacts. Structural characteristics of the compound were further examined through optimized geometry, intramolecular hydrogen bonding, and chemical reactivity studies using density functional theory with B3LYP hybrid functionals at 6–311+G(d,p) level basis set. In addition, molecular docking against epidermal growth factor receptors tyrosine kinase protein suggests a favorable binding score of −8.4 kcaL/moL, while absorption, distribution, metabolism, excretion, and toxicity analysis predicts acceptable drug-like properties.

KEY WORDS Coumarinylthiophene carboxamide, Crystal structure, Density functional theory studies, Hirshfeld surface, Molecular docking.

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