

Abstract

Synthesis, In Silico and In Vitro Studies of 7-Methoxy-3-((4-phenyl piperazin-1-yl)methyl)-2H-chromen-2-one Analogues as Derivatives as Anti-Prostate Cancer Agents [†]

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Abstract: One of the most common diseases found among men in recent days is prostate cancer (PCa). The growth of cancer is generally due to the activation of the androgen receptor by androgens. Structural modification and molecular docking approaches were done with the protein (PDB ID: 3A49) to identify the novel 7-methoxy-3-((4-phenylpiperazin-1-yl)methyl)-2H-chromen-2-one derivatives. The compounds (5a-g) was synthesized and characterized well by IR, NMR, and LC-MS spectral techniques. The compound 5a and 5b were reconfirmed by single crystal XRD. The in vitro anticancer studies were carried out for the compounds (5a-g) against LNCaP, Pc3 and 3T3 cell line. Among them 5b showed highest cytotoxicity against LNCAP (10.45 ± 1.32 μ M, Pc3 (34.65 ± 1.36 μ M and reduced cell viability. For the compound 5b, simulations of molecular dynamics are conducted to test protein-ligand interactions. Drug similarity and pharma kinetic properties for all compounds were anticipated. The outcome of these results may give vital information in further development.



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