Synthesis and Anticancer Activity of Thiophene-2-carboxamide Derivatives and *In Silico* Docking Studies

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Abstract—A novel series of thiophene-2-carboxamide derivatives are designed and synthesized, and their structures are confirmed by ¹H and ¹³C NMR, and mass spectra. The synthesized compounds are evaluated for their *in vitro* cytotoxic activity by MTT assay. Among the tested compounds, the derivative with 4-Cl-phenyl ring exhibits potent inhibitory activity against MCF-7, K562, HepG2, and MDA-MB-231. The molecular docking study performed for the synthesized compounds against PTP1B exhibits essential key interactions.

Keywords: synthesis, thiophene-2-carboxamide, anticancer, molecular docking, protein tyrosine phosphatase inhibitor

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