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# Synthesis, anticancer evaluation, and molecular docking studies of vanillin-2,4-thiazolidinedione-triazole hybrid analogues

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Ten novel vanillin-2,4-thiazolidinedione-triazole hybrid analogues have been synthesized *via* Knoevenagel condensation and 1,3-dipolar cycloaddition. These have been tested for *in vitro* anticancer activity against various human cancer cell lines, including MDA-MB 231, MCF-7, A549, and FaDU. Compound **7f** (flouro and bromo substituted) shows notable inhibition of MDA-MB 231 (50.61%; IC30: 21.98 µm), while compound **7i** (di-flouro substituted) significantly inhibits FaDU (52.08%; IC30: 23.57 µm). *In silico* studies demonstrate that **7f** and **7i** have strong binding affinity with SDH (–16.7, –16.5), BCL-2 (–13.7, –13.7), BCL-XL (–16.2, –16.9) and BCL-W (–17.8, –17.7). These results suggest that such hybrid heterocyclic systems might be promising candidates for new anticancer therapies.

**Keywords**: Vanillin, 2,4-Thiazolidinedione, 1,2,3-Triazole, Anticancer activity, Molecular docking, Toxicity