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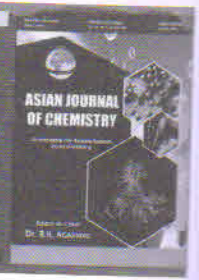

Design, Synthesis, *in silico* Analysis and Pharmacological Evaluation of Coumarin Derived Mercaptotriazole Derivatives as MCL-1 Inhibitors

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Design and synthesis of new series of 4-amino-5-mercapto-4*H*-1,2,4-triazoles connected to coumarin ring and assessed for cytotoxity and the study of docking studies was done against MDA-MB-231 cell lines. Using substituted diols, a series of new coumarin linked 4-amino-5-mercapto-4*H*-1,2,4-triazoles derivatives were synthesized from substituted diols. Moreover, the elucidation of the newly synthesized mercaptotriazole derivatives was achieved by spectral data. An MTT assay was employed to evaluate the antineoplastic activity against triple-negative breast cancer (TNBC) and the synthesized compounds demonstrated promising, potent, and innovative inhibitory effects, highlighting their potential for the development of new anticancer therapies. Compounds **8h**, **8d**, **8e**, **8b**, **8i**, **8j** and **8a** exhibit high binding energies with target receptor MCL-1 enzyme of the MDA-MB231 cells, where remaining compounds exhibit good binding interactions with target protein. *In silico* Docking studies verified the uncompetitive inhibition of MCL-1 enzyme.

Keywords: Coumarins, Mercaptotriazole, Chromen-2-one derivatives, MCL-1 enzyme, Antineoplastic activity, *In silico* studies.