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Synthesis and biological evaluation of novel anthraquinone derivatives as potential therapeutics against breast cancer: *In vitro* and *in silico* approaches

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Many traditional chemotherapeutic agents used for breast cancer cause systemic toxicity. Studies conducted on new-generation drug candidates have gained importance in recent years because of their low cytotoxicity and high anticancer effects. Anthraquinones and their derivatives are widely used for cancer treatment. In this study, we synthesized amino (5,7) and thioanthraquinone (3) derivatives. The effect of the compounds on cell viability was tested by the MTT assay using MCF-7 and MCF-10A cell lines. Compound 7 showed the highest inhibitory effect on cell proliferation MCF-7 with an IC_{50} value of 1.781 ± 1.4 and was therefore selected for further studies. The apoptotic effect of compound 7 was investigated using AnnexinV/Propidium Iodide (AV/PI) staining by flow cytometry, which revealed a significant increase in late apoptotic cells after 24h of treatment. Additionally, Caspase 3/7 activation was analyzed using fluorescence, which confirmed the induction of apoptosis by compound 7. In *silico* predictions of absorption, distribution, metabolism, and excretion (ADME) analysis confirmed the drug-likeness of compound 7. Molecular docking studies were conducted to understand interactions with target proteins. Compound 7 showed lower binding energy scores for Caspase 3, P53, Cytochrome C and Bax than the reference drugs These findings suggest that compound 7 holds promise as a potential therapeutic agent for breast cancer treatment. Further studies are warranted to elucidate its mechanism of action and explore its potential in clinical applications.

Keywords: Breast cancer, Anthraquinone derivates, Apoptosis, Molecular docking, ADME analysis