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(57) Abstract :
The present invention relates to design of novel 9-aminoacridine derivatives by molecular docking studies with key breast cancer-related proteins including PARP 1, HER2, and ERa that exhibits strong binding affinities with these proteins, indicating their potential as effective inhibitors of breast cancer pathways. Then 10 novel 9-aminoacridine derivatives were synthesized, characterized and evaluation of in-vitro cytotoxic activity against MCF-7 cell line. Notably, compound A2MO showed particularly promising binding properties. Further pharmacological screening supported these findings, with A2MO demonstrating significant anti-cancer activity in DMBA-induced breast cancer models upon oral administration. In vitro studies, including cell viability assays and cell cycle analysis, confirmed the cytotoxic effects of A2MO on breast cancer cells, highlighting its potential to induce cell death and inhibit cancer cell proliferation. Furthermore, the invention shows potential for having A2MO as an alternative line of treatment having significant anti-cancer activity. This opens avenues for future research aimed at developing a targeted and effective therapeutic approach for breast cancer treatment.

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