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Design, Synthesis, Characterization and Molecular Docking Evaluation of Dual-Imino Benzopyran Analogues as Potential VEGFR2 and EGFR Inhibitors for Breast Cancer Therapy

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The side effects associated with currently available chemotherapeutics for breast cancer treatments, intended present study to perform synthesis, characterization and molecular docking of novel benzopyrone analogues (NBPAs) against VEGFR2 (PDB: 6GQO) and EGFR (PDB: 3W32). The study involved the synthesis of some novel benzopyran analogues (NBPAs) by first treating 4-aminoacetophenone with a hydrazide derivative **5** of substituted benzopyrone (**1**), followed by treatment with different aromatic aldehydes to offer NBPAs (**6a-e**). NBPAs were characterized using ATR-IR, NMR (^{1}H & ^{13}C) and mass spectrometric analysis. The NBPAs were also subjected to molecular docking studies (using AutoDock 4.2) against VEGFR2 and EGFR. The results of the synthesis experiment and characterization study revealed successful synthesis of NBPAs and their structural elucidation. The docking study results also revealed NBPAs exhibit good binding affinity with 6GQO and 3W32. NBPAs exhibits good binding affinity against the targeted proteins 6GQO and 3W32. Present study concludes that synthesized novel NBPAs to exhibit high anticancer potential; however additional pre-clinical investigations are essential to support their clinical importance.

Keywords: Safety, Imino derivatives, Benzopyran derivatives, Anticancer activity, Docking studies.