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Molecular Docking, Synthesis & Biological Evaluation of Benzopyran Derivatives

[1]Dr. Kazi Mehraj Abukalam, [1]Mr. Awinash Subhash Chavan, [1]Dr. Amjadkhan A. Pathan
[1]Department of Pharmacy
Shri Jagdish Prasad Jhabarmal Tibrewala University, Vidyanagari, Jhunjhunu, Rajasthan
Corresponding Author: Mr. Awinash Subhash Chavan
avichavan4741@gmail.com

Abstract: *A series of 2-(3'-aminesubstituted)-7- hydroxyl-4H-1-benzopyran-4-one derivatives has been designed and synthesized through Claisen-Schmidt condensation reaction by condensation of 2,4-Dihydroxyacetophene (1.40 ml) and 3-Chlorobenzaldehyde (0.01 mole). After molecular simulation study of 25 benzopyran derivatives we select 10 molecular for synthesis having good docking score. Recent researches on Benzopyran derivatives received an added impulse with the discovery on Anticancer by several mechanisms, but the most important mechanism is the inhibition of aromatase generating enzyme.*

All the synthesized compounds was confirmed by their physicochemical properties and spectral studies. Novel benzopyran derivatives were assess for anticancer activity by using SRB assay on MCF-7 cell line. Novel benzopyran derivatives were performed to establish correlation between biological activity & molecular properties. Among the synthesized compounds (a, b, c, k, l) showed good anticancer activity; whereas compounds (t, v, w, k) shows good anti- inflammatory activity comparable to the reference drug Fadrazole and Celecoxib respectively. Thus, the conclusion can be made that the benzopyran moiety can exhibit a good anticancer as well as good anti-inflammatory activity..

Keywords: Benzopyran, Synthetic benzopyran derivatives, Claisen-Schmidt Condensation Reaction, Molecular docking, Anticancer

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