Indian Journal of Heterocyclic Chemistry
Vol. 35 - Number 01 (Jan-Mar 2025) 49-55
https://connectjournals.com/01951.2025.35.49
https://doi.org/10.59467/IJHC.2025.35.49

ISSN (Print) : 0971-1627
ISSN (Online) : 2456-4311

Design, synthesis, antibacterial activity, anticancer activity, and molecular docking study of some appocynin derivatives

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ABSTRACT This study includes the synthesis of some apocynin derivatives $\mathbf{A_2}$-$\mathbf{A_5}$. The first step involves synthesizing compound **A1** by alkylation reaction of apocynin with 1,4-dichlorobutane. The derivatives **A2-A5** were synthesized through the cyclization reaction of compound **A1** with different aldehydes (4-methoxybenzaldehyde, thiophene-2-carbaldehyde, 4-chlorobenzaldehyde, 4-*N, N*-dimethylbenzaldehyde), ethyl cyanoacetate in the present ammonium acetate. The synthesized compounds **A2-A5** were tested for their antibacterial activities against Gram-positive + (***Staphylococcus aureus***) and Gram-negative–(***Escherichia coli***). Anticancer of appocynin derivatives **A2 and A4** were examined using MTT assay and esophagus cancer cell line SK-GT4. Molecular docking studies of the prepared compounds **A2 and A4** confirmed that the binding mode involved the active site of DNA *gyrase* B PDB ID: 6kzv.

KEYWORDS Appocynin, Pyridine-2-one, Antibacterial, Anticancer.

How to cite this article: Mekky, A.H., Hamed, F.M. and Hassan, B.A. Design, synthesis, antibacterial activity, anticancer activity, and molecular docking study of some appocynin derivatives, *Indian J. Heterocycl. Chem.*, **2025**, *35*, 49–55. *https://doi.org/10.59467/IJHC.2025.35.49*