Indian Journal of Heterocyclic Chemistry
Vol. 35 - Number 01 (Jan-Mar 2025) 77-84
https://connectjournals.com/01951.2025.35.77
https://doi.org/10.59467/IJHC.2025.35.77

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

Design, synthesis, molecular docking, anticancer and antibacterial activities of some new 4,4'-((((phenylmethylene)bis(4,1-phenylene))bis(oxy)) bis(methylene)) bis(1-butyl-1*H*-1,2,3-triazoles

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ABSTRACT Some new 4,4'-((((phenylmethylene)bis(4,1-phenylene))bis(oxy)) bis(methylene))bis(1-butyl-1*H*-1,2,3-triazoles) (**4a-4g**) were synthesized by the reaction of 4,4'-(phenylmethylene)bis((prop-2-yn-1-yloxy)benzenes) (**2a-2g**) with butyl azide in the presence of sodium ascorbate $CuSO_4.5H_2O$ in DMF. The newly synthesized triazoles demonstrated anticancer efficacy through docking with the C-met tyrosine kinase receptor protein, evidenced by docking scores ranging from −7.58 to −8.60 to Kcal/mol, in comparison to the control Crizotinib value of −6.86 Kcal/mol. These triazoles **4a-4g** were also assessed for their *in vitro* cytotoxic activities and tested against the hepG2 cell line. The synthesized compounds exhibited significant cytotoxic action against the MCF-7 cell line while demonstrating no cytotoxicity toward the normal WRL68 cell line. Compared to normal cells, the study revealed a considerable selectivity of the newly synthesized triazoles for cancer cells. The study showed a good correlation between molecular docking and *in vitro* results for synthesized compounds toward the c-met tyrosine kinase receptor protein.

KEY WORDS Anticancer, Antibacterial, Molecular docking, Triazole.

How to cite this article: Abdulridha, M.M. and Mohammed, M.N. Design, synthesis, molecular docking, anticancer and antibacterial activities of some new 4,4'-((((phenylmethylene)bis(4,1-phenylene))bis(oxy)) bis(methylene))bis(1-butyl-1*H*-1,2,3-triazoles, *Indian J. Heterocycl. Chem.*, **2025**, *35*, 77–84. *https://doi.org/10.59467/IJHC.2025.35.77*