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Peer Review

Review of: "Synthesis, ADME, Toxicity, and In Silico Molecular Docking Study of Novel β-Carboline Derivatives as Potential Inhibitor Anticancer Agents"

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This article presents a synthesis of a series of novel β-carboline derivatives using conventional synthetic methods. The potent compounds were characterized using mass spectrometry, IR, and NMR spectroscopic techniques. In this present study, β-carboline derivatives were successfully docked with the active site of the enzyme 1PDB:1aq. The 4A and 4B exhibit good docking results with the enzyme 1PDB:1aq1, having binding energies of 10.9975 kcal/mol and 11.8675 kcal/mol, respectively. These docking results revealed that these ligands have potential therapeutic applications as anticancer agents, which need further study. In this article, ADME and toxicity profiling are presented, which gave preliminary results that can be considered for drug development. Toxicity is clearly presented for the safety considerations of the compounds to further validate the safety and efficacy of the synthesized compounds in living organisms. To strengthen the anticancer potential of these compounds, there is a need to modify the chemical structure to enhance their bioavailability and solubility.

Declarations

Potential competing interests: No potential competing interests to declare.

doi.org/10.32388/R45FPR