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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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Reviewer Report

The manuscript entitled "Synthesis, ADME, Toxicity, and In Silico Molecular Docking Study of Novel β-Carboline Derivatives as Potential Inhibitor Anticancer Agents" presents a study on the synthesis, characterization, and computational evaluation of novel β-carboline derivatives. The work highlights their potential as anticancer agents through ADME (Absorption, Distribution, Metabolism, and Excretion) profiling, toxicity prediction, and molecular docking studies. The study is structured into a logical sequence, encompassing synthesis methods, computational tools, and the analysis of bioactivity parameters.

The focus on β-carboline derivatives addresses a relevant area in drug discovery, particularly targeting cancer treatment. The integration of experimental synthesis with computational evaluations (e.g., docking, ADME, and toxicity) provides a holistic assessment of the compounds. The compounds synthesized and tested are novel and show promising binding affinities in molecular docking studies with Protein kinase inhibition (PDB:1aq1). The manuscript is generally well-organized, with clear methodologies and appropriate figures and tables to support the data.

This study contributes valuable insights into β-carboline derivatives as potential anticancer agents. However, the manuscript requires additional experimental validation and a deeper analysis of the results to strengthen its conclusions. I recommend **minor revisions** to address the issues mentioned above before considering the manuscript for publication:

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1. While the synthetic procedures are outlined, more detailed reaction conditions, yields, and purification methods would enhance reproducibility.
2. The docking results, though promising, would benefit from a deeper analysis of the interactions and comparison with known inhibitors to contextualize the binding affinities.
3. The study lacks experimental validation of anticancer activity (e.g., in vitro or in vivo assays) for the synthesized compounds, which would substantiate the computational findings.
4. The toxicity predictions are discussed briefly, but the implications for therapeutic safety or optimization are not fully explored.
5. Authors should include preliminary biological activity tests, such as cytotoxicity assays on relevant cancer cell lines, to validate the computational predictions.

1. Authors should expand the discussion to compare the binding affinities and ADME properties with benchmark compounds in the same therapeutic class.
2. Authors should discuss potential limitations or uncertainties in computational predictions, especially regarding docking and ADME results.
3. Minor grammatical errors and typographical issues should be corrected for improved readability.

Declarations

Potential competing interests: No potential competing interests to declare.