ISSN: 2320-5407
International Journal of Advanced Research
Publisher's Name: Jana Publication and Research LLP
www.journalijar.com
ISSN NO. 2320-5407

REVIEWER'S REPORT

Manuscript No.: IJAR- 51654 Date: 15/05/2025

Title: *Oxadiazole Derivatives as Potential EGFR Protein Kinase Inhibitors: Prediction of In-Silico ADMET Properties and Molecular Docking Study*

Recommendation:
✓ Accept as it is .....
Accept after minor revision.....
Accept after major revision .....
Do not accept (*Reasons below*) .....

Rating	Excel.	Good	Fair	Poor
Originality		✓		
Techn. Quality		✓		
Clarity		✓		
Significance	✓			

Reviewer Name: Dr. S. K. Nath Date: 15/05/2025

Reviewer's Comment for Publication:

This study offers a promising set of oxadiazole derivatives, especially compounds S10 and S23, with high in-silico binding affinity towards the EGFR kinase. The comprehensive computational analysis indicates their drug-likeness and favorable pharmacokinetic profiles, suggesting they could serve as leads for further development against hepatocellular carcinoma. However, the findings are preliminary, and necessary experimental validation—including synthesis, biological activity assays, and safety assessments—is crucial to progressing these compounds as potential therapeutic agents.

Reviewer's Comment / Report

Strengths

1. **Innovative Focus:** The study explores novel 1,3,4-oxadiazole derivatives as potential EGFR inhibitors, targeting hepatocellular carcinoma, which is a significant area in cancer research.
2. **Comprehensive In-Silico Approach:** Utilization of multiple computational techniques including molecular docking, ADMET prediction, and drug-likeness evaluations provides a robust preliminary screening of compounds.
3. **Identification of Lead Compounds:** The study successfully identifies compounds S10 and S23 as promising candidates with higher docking scores and favorable interactions with the EGFR target compared to the co-crystallized ligand and standard drug Afatinib.
4. **Detailed Methodology:** Clear description of the design and validation of docking protocols enhances reproducibility and confidence in the computational results.
5. **Potential for Future Development:** Findings serve as a good foundation for further in-vitro and in-vivo investigations to validate therapeutic efficacy and safety.

Weaknesses

1. **Lack of Experimental Validation:** The study is purely in-silico; no experimental or biological data are presented to back up the computational predictions.
2. **Limited Range of Compounds:** A library of only 30 compounds was designed, which might limit the scope for discovering more potent derivatives.

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3. **Absence of Synthesis Data:** The paper does not detail any synthetic pathways or practical considerations relating to the actual production of these molecules.
4. **Toxicity and Off-Target Effects:** Although ADMET predictions are provided, experimental toxicity and off-target effects are not confirmed, which are critical for drug development.
5. **Potential Bias in Docking Scores:** Docking scores alone do not always reliably predict biological activity; additional validation is needed.