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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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The author prepared and evaluated a series of new 5-(9-benzyl-1-methyl-9H-pyrido[3,4-b] indol-3-yl)-1,3,4-oxadiazol-2-amine (**4a-b**). 1H NMR, IR, and mass spectral data were used to evaluate the structures of the synthesized compounds. Besides the in silico molecular docking, which has been done on these newly synthesized compounds in the active pocket of Protein kinase inhibition by staurosporine PDB:1aq1 complex, it shows a good binding interaction in the active pocket of the PDB:1aq1 enzyme. The ADME and cytotoxicity properties suggest that this compound is best for further studies.

I think the work is good and can be published in this journal after some modifications

1. In the abstract, the synthesized compounds are written as 4a-b; it should be 4a,b.
2. The number of the synthesized derivatives is low (2 compounds).
3. In the abstract, (were used to evaluate the structures) should be to elucidate the structure.
4. ^{13}C NMR should be used for further elucidation of the structure.
5. In the second paragraph of the introduction, talking about (**The development of new drugs for the treatment of cancer is facing several issues ……Hence, due to these limitations, very few classes of anticancer drugs have been developed**), this part should discuss **anticancer** drugs used, mentioning more recent references in this field like;

H.K. AbdEl-Mawgoud, A.M. AboulMagd, M.T.M. Nemr, M.M. Hemdan, A.I. Hassaballah, P. S. Farag, Design, synthesis and **cytotoxic** evaluation of new thieno[2,3-d]pyrimidine analogues as VEGFR-2/AKT dual inhibitors, apoptosis and autophagy inducers, Bioorg. Chem. 150 (**2024**) 107622. https://doi.org/10.1016/j.bioorg.2024.107622

M. T. M. Nemr, M. Teleb, A. M. AboulMagd, M. E. El-Naggar, N. Gouda, A. A. Abdel-Ghany, Y. A. M. M. Elshaier, Design, synthesis and chemoinformatic studies of new thiazolopyrimidine derivatives as potent **anticancer** agents via phosphodiesterase-5 inhibition and apoptotic inducing activity. J. Molecular structure, **2023**,1272, 134216. doi.org/10.1016/j.molstruc.2022.134216

W. A. A. Fadaly, Y. A. M. M. Elshaier, M. T. M. Nemr, K. R. A. Abdellatif, Design, synthesis, modeling studies and biological evaluation of pyrazole derivatives linked to oxime and nitrate moieties as nitric oxide donor selective COX-2 and

 doi.org/10.32388/5Z7WPR

aromatase inhibitors with dual anti-inflammatory and **anti-neoplastic** activities, Bioorg. Chem. 134 (**2023**) 106428.

M. T. M. Nemr, A. Elshewy, M. Labib, A. M. El Kerdawy, P. A. Halim, Design, synthesis, **antineoplastic** activity of new pyrazolo [3, 4-d] pyrimidine derivatives as dual CDK2/GSK3β kinase inhibitors; molecular docking study, and ADME prediction. Bioorg. Chem. 150 (**2024**) 107566.

M. T. M. Nemr, A. Sonousi, A. A. Marzouk, Design, synthesis and **antiproliferative** evaluation of new tricyclic fused thiazolopyrimidines targeting topoisomerase II: Molecular docking and apoptosis inducing activity. Bioorg. Chem. (105) (2020) 104446. doi.org/10.1016/j.bioorg.2020.104446

W. A. A. Fadaly, F. E. A. Mohamed, M. T. M. Nemr, A. M. Sayed, R. G. Khalil, T. H. Zidan, Novel benzenesulfonamide derivatives as potential selective carbonic anhydrase IX, XII inhibitors with **anti-proliferative** activity: Design, synthesis and in silico studies. Bioorg. Chem. (153) (**2024**) 107881. https://doi.org/10.1016/j.bioorg.2024.107881

M. T. M. Nemr, A. M. AboulMagd, New fused pyrimidine derivatives with **anticancer** activity: synthesis, topoisomerase II inhibition, apoptotic inducing activity and molecular modeling study. Bioorg. Chem. (103) (2020) 104134. doi.org/10.1016/j.bioorg.2020.104134

M. T. M. Nemr, A. M. AboulMagd, H. M. Hassan, A. A. Hamed, M. I. A. Hamed, M. T. Elsaadi "Design, synthesis and mechanistic study of new benzenesulfonamide derivatives as **anticancer** and antimicrobial agents via carbonic anhydrase IX inhibition" RSC Advances 11, 2021, P. 26241-26257. DOI: 10.1039/d1ra05277b.

W. A. A. Fadaly, M. T. M. Nemr, T. H. Zidan, F. E. A. Mohamed, M. M. Abdelhakeem, N. N. Abu Jayab, H. A Omar, K. R. A. Abdellatif, New 1,2,3-triazole/1,2,4-triazole hybrids linked to oxime moiety as nitric oxide donor selective COX-2, aromatase, B-RAFV^{600E} and EGFR inhibitors celecoxib analogs: design, synthesis, anti-inflammatory/**anti-proliferative** activities, apoptosis and molecular modeling study. Journal of Enzyme Inhibition and Medicinal Chemistry 38 (1), 2290461 (**2023**).

W. A. A. Fadaly, M. T. M. Nemr, N. M. Kahk, Discovery of Novel Pyrazole Based Urea/Thiourea Derivatives as Multiple Targeting VEGFR-2, EGFRWT, EGFRT790M Tyrosine Kinases and COX-2 Inhibitors, with **Anti-cancer** and Anti-inflammatory Activities. Bioorg. Chem. 147 (**2024**) 107403.

W. A. A. Fadaly, T. H. Zidan, N. M. Kahk, F. E. A. Mohamed, M. M. Abdelhakeem, R. G. Khalil, M. T. M. Nemr, New Pyrazolyl-Thiazolidinone/Thiazole Derivatives as Celecoxib/Dasatinib Analogues with Selective COX-2, HER-2 and EGFR Inhibitory Effects: Design, Synthesis, Anti-inflammatory/**Anti-proliferative** Activities, Apoptosis, Molecular Modeling and ADME Studies. Journal of Enzyme Inhibition and Medicinal Chemistry 38 (1), 2281262 (**2023**).

Declarations

Potential competing interests: No potential competing interests to declare.