medical sciences forum

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Abstract

Thiazolopyrimidine as a Promising Anticancer Pharmacophore: In Silico Drug Design, Molecular Docking and ADMET Prediction Studies †

Omar A. El-Khouly [1,2,*], Dina I. A. Othman [1], Amany S. Mostafa [1] and Mohammed A. M. Massoud [1]

[1] Department of Pharmaceutical Organic Chemistry, Faculty of Pharmacy, Mansoura University, Mansoura 35516, Egypt
[2] Faculty of Pharmacy, New Mansoura University, New Mansoura 7723730, Egypt
* Correspondence: omarelkhouly99@gmail.com
† Presented at the 8th International Electronic Conference on Medicinal Chemistry, 1–30 November 2022; Available online: https://ecmc2022.sciforum.net/.

Abstract: Thiazolopyrimidines are well known to be designed to act as bio-isosteric analogues of purine nucleus. They proved to show a wide range of biological activities, such as anticancer, anti-inflammatory, antifungal, antiviral and antitubercular activity. In this study, a literature survey was thoroughly performed to elect the most active thiazolopyrimidine-containing scaffolds, acting as anticancer agents, to be subjected to extensive computational studies in order to explore the possible credible mode of their anticancer activity. First, drug-likeness was investigated for the most active derivatives, followed by molecular docking study against Cyclin-dependent kinases (CDK), Vascular endothelial growth factor receptor (VEGFR) and Phosphoinositide 3-kinases (PI3K) enzymes in order to assess their binding energy and propose the mode of action. Next, contact preference and surface mapping studies were carried out to explain the presence of remarkable affinity of certain analogues towards a specific enzyme, in addition to providing more information about their activity. Finally, physicochemical properties, Lipinski's rule of five and ADMET prediction studies were applied to predict the best route of administration and to suggest the pharmacokinetics of the most promising candidates.

Keywords: thiazolopyrimidines; anticancer; computational studies; molecular docking; ADMET prediction

Citation: El-Khouly, O.A.; Othman, D.I.A.; Mostafa, A.S.; Massoud, M.A.M. Thiazolopyrimidine as a Promising Anticancer Pharmacophore: In Silico Drug Design, Molecular Docking and ADMET Prediction Studies. *Med. Sci. Forum* **2022**, *14*, 4. https://doi.org/10.3390/ECMC2022-13313

Academic Editor: Maria Emília Sousa

Published: 1 November 2022

Supplementary Materials: The following are available online at https://www.mdpi.com/article/10.3390/ECMC2022-13313/s1.

Author Contributions: Conceptualization, A.S.M. and M.A.M.M.; methodology, D.I.A.O. and A.S.M.; software, O.A.E.-K.; validation, O.A.E.-K.; A.S.M. and D.I.A.O.; formal analysis, O.A.E.-K.; A.S.M. and D.I.A.O.; investigation, O.A.E.-K.; A.S.M. and D.I.A.O.; resources, O.A.E.-K.; A.S.M. and D.I.A.O.; data curation, O.A.E.-K.; A.S.M. and D.I.A.O.; writing—original draft preparation, O.A.E.-K.; writing—review and editing, A.S.M.; D.I.A.O. and M.A.M.M.; visualization, O.A.E.-K.; A.S.M. and D.I.A.O.; supervision, A.S.M.; D.I.A.O. and M.A.M.M.; project administration, M.A.M.M. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: All data are available at Supplementary Materials.

Conflicts of Interest: The authors declare no conflict of interest.