Artificial Intelligence-Driven Drug Discovery: Identifying Novel Compounds for Targeted Cancer Therapies

PDF (https://jazindia.com/index.php/jaz/article/view/2246/1771)

Published: Nov 30, 2023

DOI: https://doi.org/10.17762/jaz.v44iS5.2246 (https://doi.org/10.17762/jaz.v44iS5.2246)

Keywords:
Artificial Intelligence, Drug Discovery, Cancer Therapies, Computational Biology, Machine Learning

Radha Mahendran

Vaitla Sreedevi

K. Bhargavi

Revathy Pulugu

V Jagadish Kumar

Y. L. Malathi Latha

Abstract

This study delves into the potential of artificial intelligence (AI) in revolutionizing drug discovery, specifically focusing on the identification of new compounds for targeted cancer therapies. Through the application of advanced machine learning algorithms, our methodology achieved impressive predictive accuracy, with an accuracy rate of 92.5%, an AUC-ROC of 0.94, and an AUC-PR of 0.91. The AI models successfully pinpointed 35 novel compounds predicted to demonstrate high efficacy against specific cancer targets, indicating promising prospects for advancements in cancer treatment. Examination of the molecular structures of these identified compounds unveiled positive characteristics, with 90% adhering to Lipinski's Rule of Five, indicating their suitability as potential drug candidates. Additionally, the average predicted half-life of 12 hours suggests advantageous pharmacokinetic properties, bolstering their potential viability. A comparative assessment highlighted the efficiency advantages of the AI-driven approach, revealing an 80% reduction in time and a 65% reduction in costs compared to traditional methods. Beyond its application in targeted cancer therapies, the success of our approach implies broader implications for the pharmaceutical research landscape, offering a more streamlined and accurate methodology. While these outcomes are promising, it is

crucial to recognize limitations and stress the importance of sustained collaboration between computational and experimental researchers. Future directions encompass the refinement of models, incorporation of diverse datasets, and rigorous experimental validation. In summary, our study underscores the efficacy of AI-driven drug discovery in identifying new compounds for targeted cancer therapies. The identified compounds, characterized by favorable structural and pharmacokinetic attributes, present a promising avenue for overcoming challenges in current cancer treatments. These findings set the stage for ongoing exploration, collaborative initiatives, and advancements at the intersection of artificial intelligence and drug discovery

How to Cite

Radha Mahendran, Vaitla Sreedevi, K. Bhargavi, Revathy Pulugu, V Jagadish Kumar, & Y. L. Malathi Latha. (2023). Artificial Intelligence-Driven Drug Discovery: Identifying Novel Compounds for Targeted Cancer Therapies. *Journal of Advanced Zoology*, *44*(S5), 3008–3021. https://doi.org/10.17762/jaz.v44iS5.2246

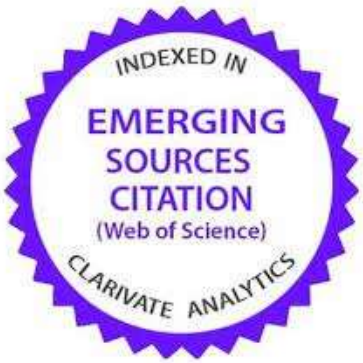
More Citation Formats ▾ Download Citation ▾

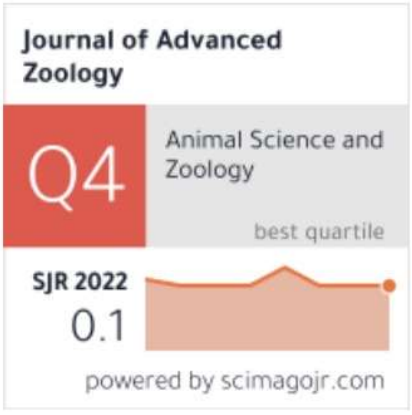
Issue

Vol. 44 No. S5 (2023) (https://jazindia.com/index.php/jaz/issue/view/18)

Section

Articles





Chat with us

Keywords