DOI:10.31557/RRO.2025.11.1.161

LETTER TO EDITOR

# Accelerating Cancer Drug Discovery: The Urgent Need for True Interdisciplinary Convergence of Computational Science and Organic Synthesis

**Farzaneh Shomoossi[1], Seyed Alireza Javadinia[2], Elaheh Emadi[3]**

[1]Faculty of Science, Imam Khomeini International University, Qazvin, Iran. [2]Non-Communicable Diseases Research Center, Sabzevar University of Medical Sciences, Sabzevar, Iran. [3]Cellular and Molecular Research Center, Sabzevar University of Medical Sciences, Sabzevar, Iran.

## Abstract

Cancer drug discovery remains a slow, costly, and resource-intensive process, limiting the timely development of effective anticancer therapies. The convergence of computational modeling, artificial intelligence (AI), and organic synthesis has the potential to transform the field from empirical screening to rational, mechanism-based, and increasingly personalized drug design. Advances in machine learning, quantitative structure–activity relationship (QSAR) modeling, structure-based drug design (SBDD), molecular generative models, and AI-assisted retrosynthetic planning now enable the rapid identification of cancer-specific molecular targets and the design of synthetically feasible compounds with optimized efficacy, selectivity, and safety profiles. Despite these advances, several critical challenges continue to impede clinical translation, including the limited synthetic accessibility of many computationally generated candidates, fragmented and non-standardized datasets, insufficient experimental validation, and a persistent skills gap between computational scientists and synthetic chemists. Overcoming these barriers will require integrated drug discovery platforms that combine AI-driven molecular design, automated or robotic synthesis, high-throughput biological screening, and iterative experimental feedback. Continued investment in data infrastructure, interdisciplinary collaboration, and workforce training will be essential to fully realize the potential of this convergence. Ultimately, integrating computational intelligence with modern synthetic chemistry may accelerate the development of safer, more effective, and increasingly personalized anticancer therapeutics.

**Keywords:** artificial intelligence, computational drug design, machine learning, organic synthesis, cancer therapeutics

*Rep Radiother Oncol*, **11 (1)**, 161-162 Submission Date: 09/01/2025 Acceptance Date: 10/02/2025

## Introduction

Cancer continues to impose a substantial and growing global health burden, underscoring the urgent need for more efficient strategies for anticancer drug discovery [1]. Conventional drug development pipelines, which rely heavily on high-throughput screening and iterative experimental optimization, often require more than a decade of research and billions of dollars to bring a single anticancer agent to market [2]. The convergence of computational modeling, artificial intelligence (AI), and modern organic synthesis offers a transformative opportunity to shift drug discovery from empirical screening toward rational, mechanism-based, and cost-effective design [3, 4].

Recent advances in machine learning and deep learning have enabled the integration of genomic, transcriptomic, and proteomic data to identify actionable molecular targets and predictive biomarkers, facilitating the development of increasingly precise targeted therapies [5]. At the molecular level, quantitative structure–activity relationship (QSAR) modeling and structure-based drug design (SBDD) have substantially improved the prediction of receptor–ligand interactions, pharmacokinetic properties, toxicity, and drug selectivity, thereby reducing the number of compounds requiring experimental validation [6, 7]. In parallel, AI-assisted retrosynthetic planning has emerged as a powerful tool for translating

**Corresponding Author:**
Dr. Elaheh Emadi
Cellular and Molecular Research Center, Sabzevar University of Medical Sciences, Sabzevar, Iran.
Email: elahehemadi@yahoo.com

computationally designed molecules into synthetically accessible chemical structures, narrowing the gap between virtual design and laboratory synthesis [4, 8, 9].

Despite these advances, several critical challenges continue to limit the translation of computational discoveries into clinically useful anticancer agents. First, many compounds identified through in silico optimization remain difficult or impractical to synthesize, emphasizing the need for synthesizability-aware molecular design algorithms developed in close collaboration with synthetic chemists [4, 9]. Second, the performance and generalizability of AI models remain constrained by fragmented, heterogeneous, and insufficiently standardized datasets, which compromise reproducibility and predictive accuracy [2]. Third, a persistent shortage of researchers with interdisciplinary expertise spanning computational science, medicinal chemistry, synthetic organic chemistry, and cancer biology continues to impede effective collaboration and innovation [10].

Addressing these limitations will require the development of fully integrated drug discovery ecosystems in which AI-driven molecular design, automated or robotic synthesis, and high-throughput biological screening operate within a continuous iterative workflow. In such closed-loop platforms, computational models generate candidate molecules tailored to specific tumor subtypes, robotic systems synthesize the proposed compounds, and experimental assays provide rapid biological feedback that is used to refine subsequent rounds of molecular optimization [9, 10]. This iterative framework has the potential to substantially shorten development timelines while facilitating the discovery of increasingly personalized anticancer therapeutics.

Realizing this vision will require coordinated investment in infrastructure, interdisciplinary education, and collaborative research. Priority should be given to establishing dedicated translational laboratories that integrate computational and synthetic expertise, developing training programs that cultivate cross-disciplinary competencies, and implementing funding mechanisms that actively promote collaborative rather than discipline-specific research. Through these efforts, the convergence of AI, computational drug design, and modern organic synthesis can evolve from a promising technological concept into a practical strategy for accelerating the development of safer, more effective, and personalized cancer therapies. The opportunity is clear; translating this potential into clinical benefit now depends on sustained scientific collaboration and strategic investment.

## Acknowledgements

Not applicable.

*Consent for Publication*

Not applicable.

*Funding*

Not applicable.

*Conflict of Interest*

The authors declare that they have no conflicts of interest related to this work.

## References

1. Siegel RL, Kratzer TB, Giaquinto AN, Sung H, Jemal A. Cancer statistics, 2025. CA: a cancer journal for clinicians. 2025;75(1):10-45. https://doi.org/10.3322/caac.21871
2. Ouma RBO, Ngari SM, Kibet JK. A review of the current trends in computational approaches in drug design and metabolism. Discover Public Health. 2024 09 27;21(1):108. https://doi.org/10.1186/s12982-024-00229-3
3. Sadybekov AV, Katritch V. Computational approaches streamlining drug discovery. Nature. 2023 04;616(7958):673-685. https://doi.org/10.1038/s41586-023-05905-z
4. Abbasi K, Razzaghi P, Gharizadeh A, Ghareyazi A, Dehnad A, Rabiee HR, Mofrad MRK. Computational drug design in the artificial intelligence era: A systematic review of molecular representations, generative architectures, and performance assessment. Pharmacological Reviews. 2026 01;78(1):100095. https://doi.org/10.1016/j.pharmr.2025.100095
5. M'rhar K, Chadi M-A, Mousannif H. Exploring deep learning approaches in anticancer drug design: a review of recent advances. Frontiers in Drug Discovery. 2025;5:1713308. https://doi.org/10.3389/fddsv.2025.1713308..
6. Vasilev B, Atanasova M. A (Comprehensive) Review of the Application of Quantitative Structure–Activity Relationship (QSAR) in the Prediction of New Compounds with Anti-Breast Cancer Activity. Applied Sciences. 2025;15(3):1206. 2026 03 19;. https://doi.org/10.3390/app15031206
7. Liu H, Ma Y, Chen W, Gu X, Sun J, Li P. Strategies for the drug development of cancer therapeutics. Frontiers in Pharmacology. 2025;16:1656012. https://doi.org/10.3389/fphar.2025.1656012
8. Sutanto H, Fetarayani D. Integrating artificial intelligence into small molecule development for precision cancer immunomodulation therapy. Npj Drug Discovery. 2025 Oct 01;2(1):25. https://doi.org/10.1038/s44386-025-00029-y
9. Fu C, Chen Q. The future of pharmaceuticals: Artificial intelligence in drug discovery and development. Journal of Pharmaceutical Analysis. 2025 08;15(8):101248. https://doi.org/10.1016/j.jpha.2025.101248
10. Lopes AB, Rodrigues CF, Silva FAM. From Algorithm to Medicine: AI in the Discovery and Development of New Drugs. AI. 2026 01;7(1):26. https://doi.org/10.3390/ai7010026