

Review

# AI In Drug Discovery: Anti-Cancer Drug Discovery Is A New Era of Therapeutics

Jyoti Mahadev Madar<sup>1\*</sup>, Murughendra Biradar<sup>2</sup>

<sup>1</sup>Department of Chemistry, K.R.C.E.S's G.G.D. Arts, B.M.P. Commerce and S.V.S. Science College Bailhongal, Karnataka, India.

<sup>2</sup>Department of Chemistry, Murarji Desai Residencial PU College, Nidasosi, Karnataka, India.

**Corresponding Author:**

Dr. Jyoti Mahadev Madar

**Email:** NA

**DOI:** 10.62896/ijmsi.2.s1.12

**Conflict of interest:** NIL

**Article History**

Received: 08/06/2026

Accepted: 16/06/2026

Published: 20/06/2026

**Abstract:**

Cancer disease continues to impose a substantial heavy burden on our global health systems, necessitating continuous innovation in therapeutic development. Earlier drug discovery strategies mainly depend on non-specific cytotoxic agents, associated with limited selectivity and adverse effects. On other hand, recent advances in molecular biology, genomics, and computational sciences have enabled a transition toward mechanism-driven and patient-specific therapeutic design. This review examines contemporary strategies in anti-cancer drug discovery, including targeted therapies, immunotherapeutic interventions, and precision-based approaches. Additionally, it highlights the integration of new technologies such as artificial intelligence and high-throughput methodologies. Current limitations and future prospects in oncology drug development are also discussed in this article.

**Keywords:** Anti-cancer drug discovery, immunotherapy, targeted therapy, artificial intelligence, biomedical.

This is an Open Access article that uses a funding model which does not charge readers or their institutions for access and distributed under the terms of the Creative Commons Attribution License (<http://creativecommons.org/licenses/by/4.0>) and the Budapest Open Access Initiative (<http://www.budapestopenaccessinitiative.org/read>), which permit unrestricted use, distribution, and reproduction in any medium, provided original work is properly credited.

## 1. Introduction

Cancer diseases arise from complex interactions involving genetic mutations, epigenetic dysregulation, and environmental influences, leading to uncontrolled cellular proliferation and metastasis. These diseases collectively represent a significant contributor to global mortality and healthcare burden (1, 2). Historically, these treatment modalities such as chemotherapy and radiotherapy have demonstrated limited, often affecting both cancerous and healthy tissues, thereby causing systemic toxicity (3). Recent progress in molecular oncology has facilitated a deeper understanding of tumor biology and its rapid growth, enabling the identification of actionable molecular targets (4).

Consequently, drug discovery efforts have shifted toward individualized therapeutic strategies aimed at enhancing efficacy while minimizing adverse outcomes (5, 6).

## 2. Evolution of Anti-Cancer Drug Discovery

Initially anti-cancer agents primarily functioned by stopping rapid cell division, targeting proliferating cells. Although these achieved clinical success in certain malignancies, but their lack of selectivity resulted treatment-related complications and in toxicity (7).

Despite advances in current anti-cancer treatment, challenges we face such as drug resistance, toxicity and tumor heterogeneity persist.

Several limitations we observe in traditional and single target drug with simple combination therapies are becoming challenging (7). Current advances in cancer genetics led to the discovery of oncogenic drivers and tumor suppressor pathways, paving the way for the development of specific targeted therapies. These interventions selectively reduce molecular components essential for tumor growth and survival (8, 9).

### 3. Contemporary Strategies in Drug Discovery

Cancer drug discovery become rapid transformation driven by advances in molecular biology, biotechnology, computational science, Nanotechnology and along with interdisciplinary research. (10) Tyrosine kinase inhibitors and monoclonal antibodies have significantly improved clinical outcomes in several malignancies (10, 11). Nanoparticles are engineered to recognize specific cancer cell and their selective mechanism contributes to improved safety profiles compared to traditional therapies.

Historically drug repurposing in oncology has largely derived by either by understanding of the disease pathway or through serendipitous findings. (13) The development of immunotherapy has introduced a paradigm shift in oncology. By developing the immune system's capacity to recognize tumor cells, therapies such as immune checkpoint inhibitors and adoptive cell transfer have demonstrated durable responses (12, 13). Engineered cellular therapies, including CAR-T cells, have further expanded treatment possibilities (14).

Precision oncology is another way to focus on tailoring treatments based on individual molecular and genetic profiles. The usage of such predictive biomarkers allows clinicians to select therapies that are more likely to benefit specific patient subgroups (15). This approach increases the therapeutic efficacy and reduces unnecessary ineffective treatments.

Biologically active compounds are derived from natural sources which are continue to play a vital role in oncology drug development. In parallel,

drug repurposing strategies aim to identify new therapeutic applications for existing pharmaceuticals, by reducing development time and even there cost (16, 17).

### 4. Technological Advancements Driving Drug Discovery

High-throughput sequencing and proteomic profiling techniques enable comprehensive characterization of tumor biology. These tools facilitate the identification of drug targets site and molecular signatures associated with disease improvement (18, 19).

Artificial intelligence is increasingly utilized nowadays to analyze complex 3D biological datasets, which predict molecular interactions, and optimize the drug patient. These computational approaches significantly improve their efficiency and reduce the time of drug development (20, 21).

Current screening analysis allows rapid evaluation of large chemical libraries, enabling the identification of promising therapeutic patients with improved accuracy (22).

### 5. Challenges in Anti-Cancer Drug Development

Anti cancer drug design has shown promising results, still it remains relatively underexplored area. By observing present data quality and availability present significant obstacles, anti cancer drug discovery is depends on biological and chemical datasets. Cancer cells can adapt to therapeutic pressure through genetic alterations and pathway reprogramming, leading to resistance and disease recurrence (23, 24).

Variability within and between tumors presents a major obstacle to effective treatment, necessitating more adaptive and personalized therapeutic strategies (25). Despite this, adverse effects remain a concern, and significant advancements, highlighting the need for safer and more selective therapeutic options (26). Drug development is often hindered by high costs, prolonged timelines, and stringent regulatory

requirements, limiting accessibility and innovation (27, 28).

## 6. Future Directions

Advanced computational tools, and personalized medicine is expected to further transform anti-cancer drug discovery. Emerging technologies such as gene editing and nanomedicine offer new avenues for targeted intervention and improved drug delivery systems (29, 30). Collaborative efforts across disciplines will be essential to accelerate progress and ensure equitable access to novel therapies.

## 7. Conclusion

Anti-cancer drug discovery has evolved into a highly sophisticated and interdisciplinary field. Advances in molecular biology, immunology, and computational sciences have significantly enhanced the development of targeted and personalized therapies. While challenges such as resistance and heterogeneity persist, ongoing innovation holds promise for more effective and safer cancer treatments in the future.

## Acknowledgments

I Dr. Jyoti M. Madar acknowledge my Husband Mr. Murughendra B. Biradar for his support and help and I also thank to our Institute, K.R.C.E.S's G.G.D. Arts, B.M.P. Commerce and S.V.S. Science College Bailhongal.

## References

1. Bray, F. et al. (2018). Global cancer statistics. *CA Cancer J Clin*, 68, 394–424.
2. Siegel, R.L. et al. (2020). Cancer statistics. *CA Cancer J Clin*, 70, 7–30.
3. Zhavoronkov, A. et al. (2019). AI for drug discovery. *Nat Biotechnol*, 37, 1038–1040.
4. Ashley, E.A. (2016). Towards precision medicine. *Nature Reviews Genetics*, 17, 507–522.
5. Collins, F.S. & Varmus, H. (2015). Precision medicine initiative. *N Engl J Med*, 372, 793–795.
6. Topol, E.J. (2019). AI in medicine. *Nat Med*, 25, 44–56.
7. Chabner, B.A. & Roberts, T.G. (2005). Chemotherapy and the war on cancer. *Nat Rev Cancer*, 5, 65–72.
8. Hanahan, D. & Weinberg, R.A. (2011). Hallmarks of cancer. *Cell*, 144, 646–674.
9. Sawyers, C. (2004). Targeted cancer therapy. *Nature*, 432, 294–297.
10. Druker, B.J. et al. (2001). Targeted therapy in leukemia. *N Engl J Med*, 344, 1031–1037.
11. Baselga, J. & Swain, S.M. (2009). Novel anticancer targets. *Oncogene*, 28, 161–170.
12. Pardoll, D.M. (2012). Immunotherapy. *Nat Rev Cancer*, 12, 252–264.
13. Sharma, P. & Allison, J.P. (2015). Checkpoint blockade. *Science*, 348, 56–61.
14. June, C.H. et al. (2018). CAR-T therapy. *Science*, 359, 1361–1365.
15. Dienstmann, R. et al. (2017). Precision oncology. *Nat Rev Clin Oncol*, 14, 635–648.
16. Newman, D.J. & Cragg, G.M. (2020). Natural products. *J Nat Prod*, 83, 770–803.
17. Pushpakom, S. et al. (2019). Drug repurposing. *Nat Rev Drug Discov*, 18, 41–58.
18. Mardis, E.R. (2008). Next-generation sequencing. *Annu Rev Genomics Hum Genet*, 9, 387–402.
19. Vogelstein, B. et al. (2013). Cancer genome landscapes. *Science*, 339, 1546–1558.
20. Zhavoronkov, A. et al. (2019). AI for drug discovery. *Nat Biotechnol*, 37, 1038–1040.
21. Topol, E.J. (2019). AI in medicine. *Nat Med*, 25, 44–56.
22. Macarron, R. et al. (2011). High-throughput screening. *Nat Rev Drug Discov*, 10, 188–195.
23. Holohan, C. et al. (2013). Drug resistance mechanisms. *Nat Rev Cancer*, 13, 714–726.
24. Vasan, N. et al. (2019). Resistance evolution. *Nature*, 575, 299–309.

International Journal of Multidisciplinary Science and Innovation (IJMSI)  
International Conference on Advances in Physical, Chemical and Mathematical Sciences  
for Sustainable Development

Organized by

D.M.S. Mandal's Bhaurao Kakatkar College, Belgaum, Karnataka, India

Website: <https://ijmsi.in/>

ISSN: 3107-5754 | Vol. 2, Special Issue 1, 2026 | Page No.: 108-111

25. Marusyk, A. et al. (2012). Tumor heterogeneity. *Nat Rev Cancer*, 12, 323–334.
26. Hutchinson, L. & Kirk, R. (2011). Drug attrition. *Nat Rev Clin Oncol*, 8, 189–190.
27. Mak, I.W. et al. (2014). Translation challenges. *J Transl Med*, 12, 173.
28. Paul, S.M. et al. (2010). R&D productivity. *Nat Rev Drug Discov*, 9, 203–214.
29. Doudna, J.A. & Charpentier, E. (2014). Genome editing. *Science*, 346, 1258096.
30. Shi, J. et al. (2017). Nanotechnology in oncology. *Nat Rev Cancer*, 17, 20–37.

\*\*\*\*\*