Artificial Intelligence in Drug Discovery: Integrating Bioinformatics and System Biology for Next- Generation Therapeutics.

Purva Bobhate[1], Harshad Tambekar[1], Dr. Trupti Deshpande[1]

[1]Department of pharmacy, JSPM RSCOPR Tathawade, Pune, India.

Corresponding author: Purva.kbobhate@gmail.com, truptideshpande06@gmail.com
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ABSTARCT :

Integrating bioinformatics, systems biology and drug discovery, artificial intelligence (AI) has become a pivotal force in the advancement of biomedical research. Bioinformatics, typically, analyses huge data-sets and organizes them in such a way that the disease-associated genes, proteins, biomarkers and molecular signatures can be identified. On the other hand, systems biology goes a step further and with the help of combined multi-omics data, it can expose the complicated molecular networks, mechanisms of diseases and also show the ways to potential drug-targets. AI technologies, including machine learning, deep learning, artificial neural networks, graph neural networks, large language models, generative AI and reinforcement learning, significantly enhance these domains by improving pattern recognition, predictive modelling and biological data integration. Their applications span genomics, transcriptomics, protein structure prediction, pathway analysis, disease modelling, precision medicine and digital twin technologies, ultimately facilitates therapeutic target identification, virtual screening, lead optimization, ADMET prediction, de novo drug design and drug repurposing. This review highlights the unified role of AI in integrating bioinformatics and systems biology to enable faster, more accurate and cost-effective drug discovery. It also discusses current limitation, including data quality, model interpretability, ethical considerations and clinical validation, while presenting the future perspectives for AI-driven precision therapeutics and personalized medicine.

Keywords:- Artificial intelligence, Bioinformatics, System biology, Drug discovery, Integration, Drug discovery pipeline.

1] INTRODUCTION :

A lot of drugs don't make it to market during clinical development, which is one of the reasons why drug discovery remains a very expensive and time-consuming process usually lasting over a decade [1] [2] . Traditional methods do not only take more time, but also are less effective, especially with complicated diseases because they mainly depend on slowly and painfully screening and testing one by one [3] [4] . Due to next-generation sequencing, multi-omics and computational biology, enormous biological datasets have been created and with the support of bioinformatics, it has become feasible to study these databanks in order to identify genes, proteins and disease biomarkers [5]. Systems biology examine together multi-omics data to locate druggable targets and molecular interactions [6] . Also, artificial intelligence is a combination of machine learning, deep learning, graph neural networks and generative AI that together facilitate target identification, lead optimization, ADMET prediction and personalized medicine, over other applications. So, this ultimately leads to higher accuracy, lower costs and a quicker, safer drug creation process.[7]

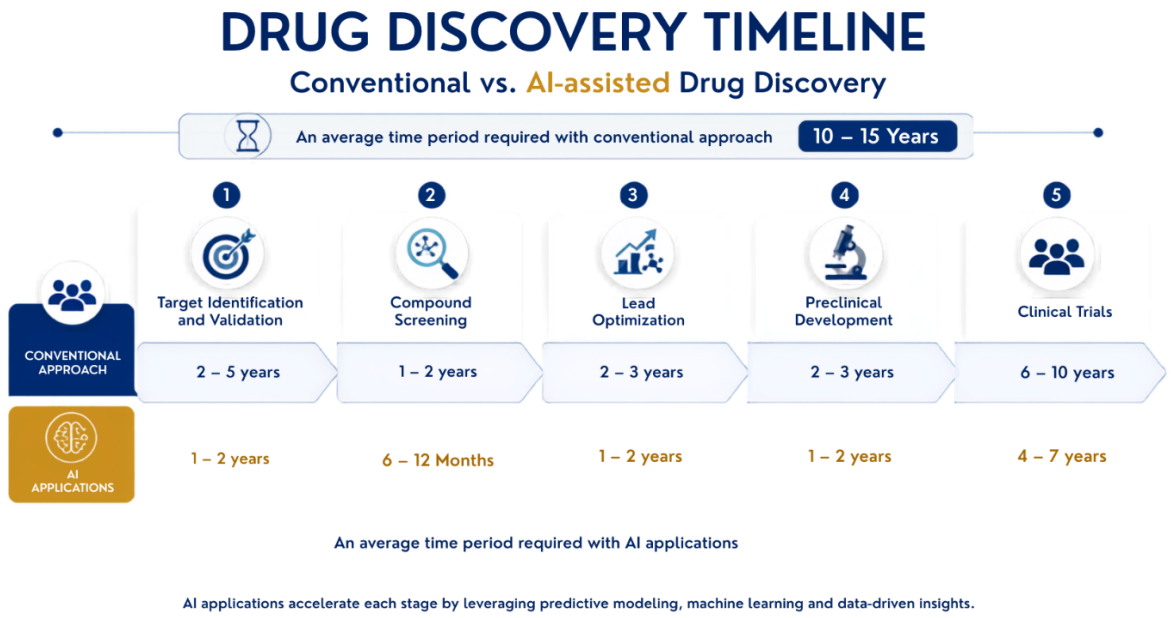

Figure 1: Title- Drug Discovery Timeline

2] AI Technologies Enabling Bioinformatics, Systems Biology, and Drug Discovery :

Artificial intelligence (AI) is a term that covers many different programming techniques that allow machines to understand biological data at a deep level, find patterns and make predictions. In the field of biomedicine, AI is a must-have tool for handling the enormous amount of data coming from genome studies, gene expression analysis, protein studies, metabolite research and clinical trials [8] . Differently from the old-style statistical methods, AI techniques are able to uncover concealed connections in datasets with many variables, thus enabling informed decisions at each step of drug discovery

Following are some AI technologies used in these domains:

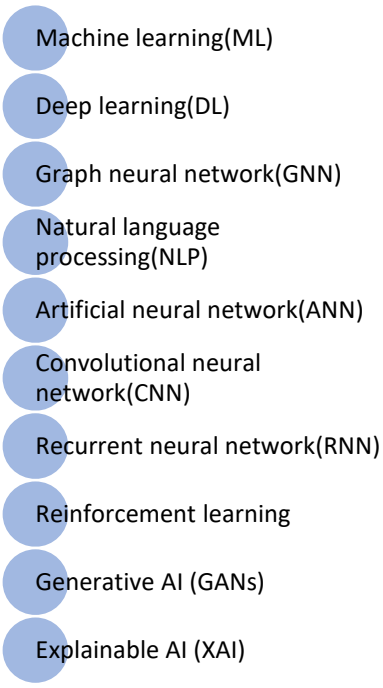

Figure 2: Title- AI technology used in bioinformatics, system biology, drug discovery.

2.1} Machine learning (ML)

Helps computer systems to automatically improve their performance based on experience, without being explicitly programmed. They are used for identifying diseases, discovering new biomarkers, predicting molecular properties and even drug repurposing. [4] [9]

2.2} Deep learning (DL)

Deep learning is a type of ML that works with neural networks having multiple layers. The applications of deep learning include prediction of protein structures, processing of medical images and creation of new drugs [10] [11]

2.3} Artificial neural networks (ANNs)

It have been extensively utilized for QSAR modelling, toxicity prediction and lead optimization. Graph neural networks (GNNs) take the molecular graphs as input to predict molecular property and drug-target interaction. [12] [13]

2.4} Transformer architectures, large language models (LLMs), generative AI and reinforcement learning

They are making the contributions to biomedical knowledge extraction, protein sequence analysis, as well as the design and optimization of novel therapeutic molecules even stronger. [14] [15]

3] AI in Bioinformatics :

Definition:

Bioinformatics is a multidisciplinary field that uses computer science, statistics, mathematics and biology to collect, store, analyse and interpret biological data, such as DNA, RNA, proteins and gene expression in order to understand living systems and support innovation in agriculture, biotechnology and medicine. [16]

3.1} Introduction:

Artificial intelligence (AI) is one of the leading technologies transforming bioinformatics nowadays. It has elevated the field from simply analysing biological data to a powerful system capable of designing, interpreting and predicting. Bioinformatics involves managing huge and intricate data sets such as RNA expression profiles, DNA sequences, protein structures and cell information. Since biology is a data-rich science, traditional methods are just not sufficient [17] . Understanding data patterns and making accurate predictions are some of the ways AI helps.

3.2} APPLICATIONS:

3.2.1] AI in Transcriptomics and Single-Cell Analysis

Another very important area where AI is influencing a lot is transcriptomics and single cell analysis. Single-cell technologies allow scientists to study gene expression at a single cell level, nevertheless the data resulting from these technologies are usually complicated, noisy and extremely high-dimensional [18] . AI tools can help to classify cell types, discover gene expression patterns, integrate data from various experiments and even forecast cellular responses [19] . These capabilities provide the researchers with a better understanding of the functioning of tissues, their development and diseases as well.

3.2.2] AI in Genomics and DNA Sequence Analysis

Genomics and DNA sequence analysis is one of the fastest growing areas of AI in bioinformatics. AI algorithms can find complicated patterns in the genome, such as promoters, splice sites, enhancers and transcription factor binding regions. This application of AI is especially needed because many genetic changes related to diseases occur in non-coding regions of DNA[20] These regions are difficult to understand using regular methods. AI can also predict if and how a DNA change might affect gene regulation and expression. [21]

3.2.3] AI in Variant Calling and Mutation Interpretation

In the area of variant calling and mutation interpretation, AI has shown that it can be a very useful tool. Among millions of genetic variants in human genomes, only few are dangerous. AI helps distinguish which mutations

cause disease and which are harmless by analysing sequencing data and predicting their biological effects [22] . Accurate mutation interpretation is key in medicine tailored to individual patients. It can improve diagnosis and treatment decisions. [23]

3.2.4] AI in Protein Structure Prediction

AI's role in addressing the protein folding problem has showcased its impact on bioinformatics. Since a protein's function largely depends on its three-dimensional structure, AI has allowed researchers to predict structures with accuracy that was once thought impossible from amino acid sequences [24] . This not only helps in molecular biology research but also opens new opportunities in drug discovery and the understanding of various diseases. [25]

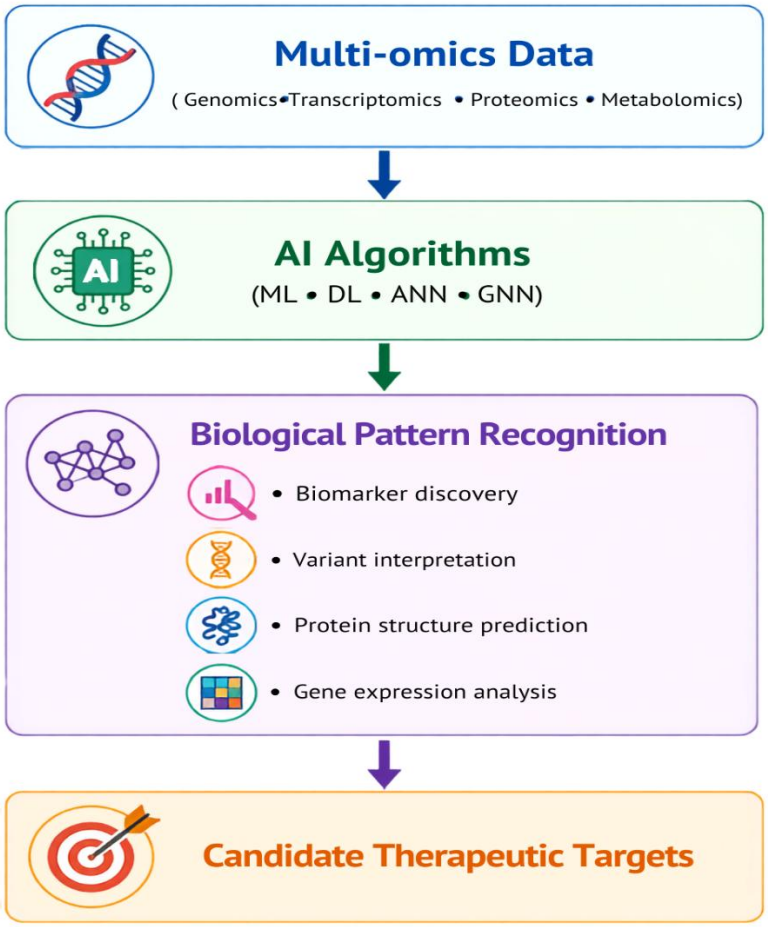

Figure 3: Title-AI driven workflow for therapeutic target identification.

4] AI in Systems Biology :

Definition:
Systems biology considers living organisms as interconnected entities instead of as parts. It applies a set of disciplines such as biology, genetics, computer science, mathematics, statistics and more recently, engineering to gain an insight into the way genes, proteins, metabolites, cells, tissues and organs interact to perform functions in the biology and cause diseases [26] [27]

Introduction:
In the context of systems biology, the use of artificial intelligence is an integration of AI, omics data and network science for the purpose of modelling living phenomena as a series of processes interactively involved [28] . This method can be used for identification of disease mechanisms, treatment prediction, biomarker identification and

precision medicine by means of pathway analysis, single-cell data study and generation of digital twin technologies. [28] [29]

APPLICATION:

Biomolecular pathway investigation

It is the role of pathway analysis in systems biology to convert vast genomic datasets into interpretable mechanisms [30]. While some studies may focus on genes or proteins alone, this approach identifies the concerted pathway-wise changes in apoptosis, for instance, inflammation, regulation of the cell-cycle, metabolism, DNA repair and immune signalling. AI aids this method in terms of finding subtle molecular patterns and combining various layers of data such as transcriptomics, proteomics, genomics, metabolomics, single-cell data and spatial omics to map their relations to the biology in these pathways as well [31]

Modelling of disease mechanisms

The modelling of disease mechanisms provides an understanding of how at a molecular level changes cause disease symptoms. According to systems biology, disease is the result of a kind of a malfunction at the level of the whole network made of proteins, genes, tissues, cells, etc. and even the environment [32]. ML can recognize disease subgroups, identify the likely evolution of the illness, and help search for reliable indicators [32] . AI in conjunction with CRISPR perturbation and single-cell sequencing helps us identify which changes in the genome are actually triggering the diseases and which are just associated. [33]

Investing in the omics of single cells

Single-cell omics is centred on the analysis of individual cells instead of the averaging of signals from the mixture of cells in tissues [34] . Methods such as single-cell RNA sequencing, CITE-seq, single-cell ATAC-seq and spatial transcriptomics open up ways to look at the rare cell types, tumor subclones, immune statuses, different paths of differentiation and also interactions within tissues [34] . AI-based methods can help with the assignment of cell types, correction of different data batches, inference of development path (trajectory), analysis of inter-cellular communication and prediction of impacts of either genetic or drug manipulations [35]

Digital twin models

A biomedical digital twin is a personalized computational model of a patient, organ, tissue or disease process, it can integrate imaging, omics, electronic health records, laboratory results, wearable data and treatment history [36]. Digital twins may simulate predict drug response, disease progression, compare virtual treatment options and update as new patient data become available. They hold promise for precision health but require protection of privacy, validation and ethical governance. [37]

Precision medicine

Precision medicine is giving the right treatment to the right patient at the right time. Artificial intelligence biology facilitates this goal by integrating clinical variables, molecular profiles, drug-response data and pathway activity [38] . It can identify molecular disease subtypes, mechanisms of treatment resistance, predictive biomarkers and patient specific therapeutic targets. [39]

5] AI in Drug Discovery :

Definition:

Drug discovery is the scientific process of identifying and developing potential therapeutic compounds that can be used to prevent, treat or manage diseases. It involves target identification, compound screening, lead optimization and preclinical evaluation before clinical testing begins. [40]

AI plays a key role in Drug discovery pipeline:-

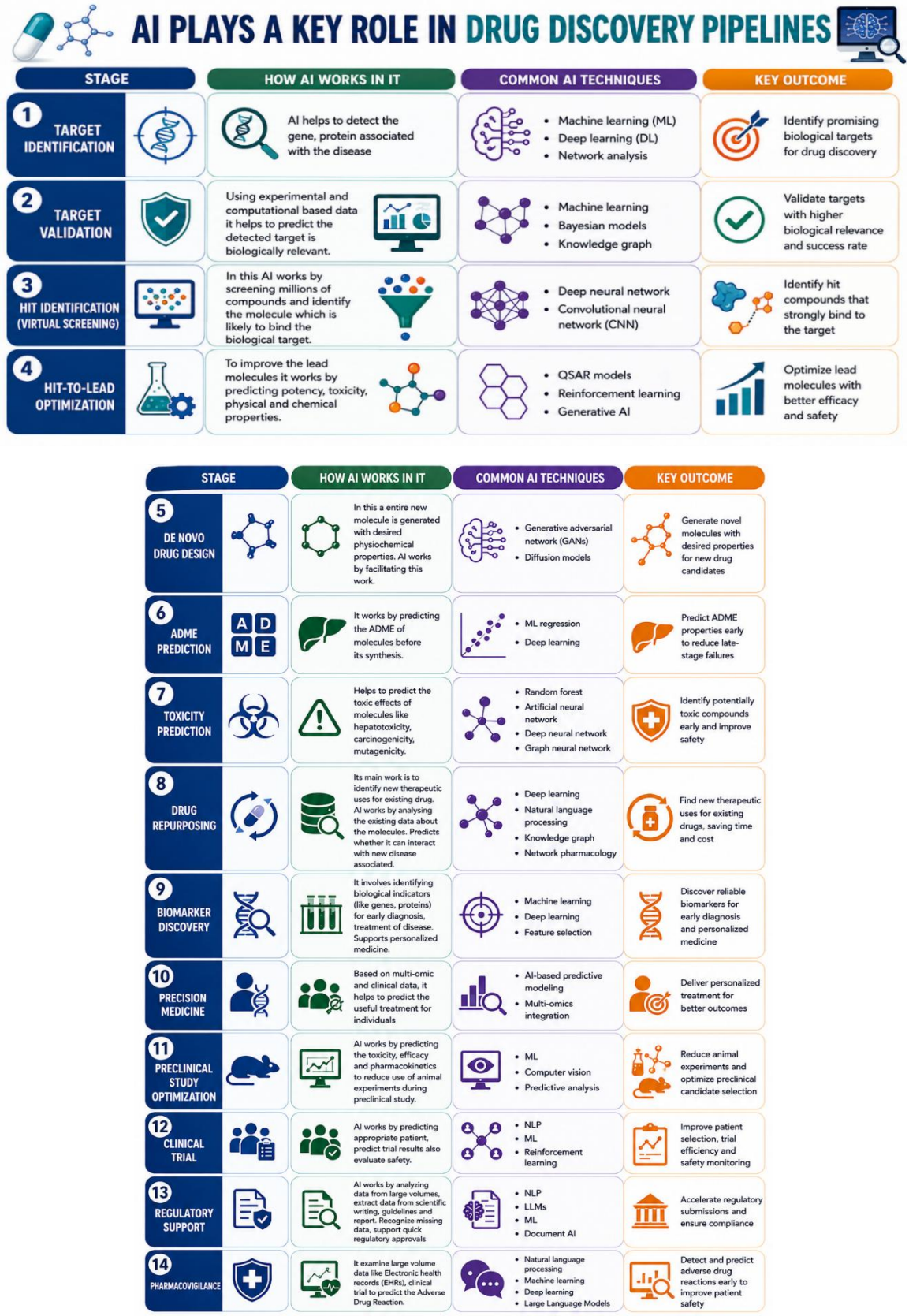

Figure 4: Title- AI driven workflow for Drug discovery pipeline [40] [41]

6] INTEGRATION OF AI, BIOINFORMATICS, SYSTEM BIOLOGY, AND DRUG DISCOVERY:

The real potential of artificial intelligence (AI) in drug discovery today, goes beyond the fact that it can be used for certain tasks only. Its true power is in combining bioinformatics and systems biology into one single, data-driven platform. These fields complement each other very well, bioinformatics produces and analyse huge biological datasets, systems biology gives an overview of molecular interaction at network level and AI changes these different pieces of information into models that can predict and direct drug discovery. [42]

The first step in combining these fields is through bioinformatics that depends on the use of many high-throughput technologies to generate multi-omics datasets which include genomic, transcriptomic, proteomic, metabolomic and epigenomic information [42] . AI systems are used to dissect these datasets in order to identify genes associated with diseases, biomarkers, genetic variants and protein structures. These findings provide the molecular basis for understanding disease mechanisms

Pathways to disease derived from bioinformatics data are represented in systems biology, where AI reconstructs gene regulatory networks, protein-protein interaction networks and signalling pathways to reveal how individual molecular changes influence cellular behaviour and disease progression. By studying these complex biological interactions at a systems level, AI can point to the most important nodes of regulation and predict therapeutic interventions with a level of accuracy that surpasses traditional methods.

Ultimately, the biological knowledge so confirmed is turned into the drug discovery pipeline where AI facilitates various tasks such as therapeutic target identification, virtual screening, molecular property prediction, lead optimization, ADMET assessment, de novo drug design and drug repurposing [43] . This integration into a single pipeline reduces experimental workload, increases prediction fidelity and leads to personalized medicine.

All in all, the convergence of AI, bioinformatics and systems biology is a drastic change in thinking about drug development - from trial and error to a predictive and systems-oriented approach. By connecting biological data with computational intelligence and therapeutic innovation, AI leads to drug development that is faster, less expensive and more precise, thus improving patient outcomes and moving the field of precision therapeutics forward. [42] [43]

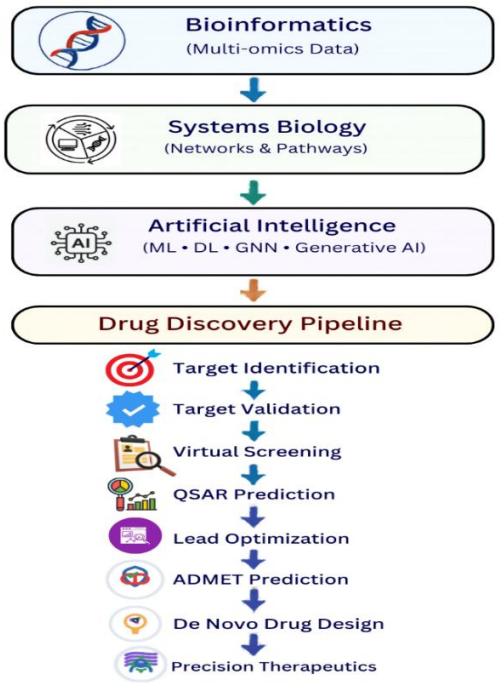

Figure 5: Title- AI based pipeline for integration of bioinformatics, system biology, drug discovery.

Challenges and Future Perspectives:

Integration of artificial intelligence (AI), bioinformatics, systems biology and drug discovery still deals with several scientific, technical and regulatory challenges apart from its significant benefits. The scope, diversity and extensiveness of biological datasets have a significant effect on the reliability of AI models. Many publicly available datasets have problem like missing data, inconsistencies and population biases which can lead to poor model performance and limit the wide applicability of prediction results

Table 1:

CHALLENGES	EFFECT	FUTURE PERSPECTIVE
Limited or biased datasets [44]	Reduced prediction accuracy [44]	Diverse, high-quality multi-omics databases
Poor model interpretability [45] [46]	Low clinical trust [45] [46]	Explainable AI (XAI)
Heterogeneous data sources [44]	Difficult integration [44]	Standardized formats and interoperable databases
Ethical and privacy concerns [44]	Restricted data sharing [44]	Privacy-preserving AI and clear regulatory frameworks.

Conclusion:

Artificial intelligence (AI) is rapidly becoming a game changer in biomedical research by combining bioinformatics, systems biology and drug discovery into one integrated platform for precision therapeutics. AI's capacity to crunch intricate multi-omics data, among other things, lead to the discovery of biomarkers linked with diseases, therapeutic targets and molecular interaction networks responsible for disease progression. Merged with systems-level modelling, these understandings give impetus to the drug discovery lanes from initiation to target identification, virtual screening, lead optimization, ADMET prediction and de novo drug design.

In the last few years, breakthroughs in machine learning, deep learning, graph neural networks and generative AI have dramatically increased the pace and accuracy of developing new drugs; at the same time, these technologies have lowered the costs and risks of failures related to drug development. Despite this, challenges such as data quality issues, model explainability, ethical concerns and clinical validation still remain significant hurdles for the large-scale adoption of AI in this domain.

It is predicted that, with the ongoing association of AI with bioinformatics and systems biology, the landscape of drug discovery will be tremendously changed in the near future leading to more predictive, personalized and data-based therapeutic solutions.

More efforts towards facilitating such multidisciplinary scientific dialogues, enhancing data quality and progressing explainable AI techniques will help the field of AI-augmented precision therapeutics to come to its fullest potential and turn computational breakthroughs into real clinical gains.

Reference:

1. Paul, S. M., Mytelka, D. S., Dunwiddie, C. T., Persinger, C. C., Munos, B. H., Lindborg, S. R., & Schacht, A. L. (2010). How to improve R&D productivity: The pharmaceutical industry's grand challenge. *Nature Reviews Drug Discovery*, *9*(3), 203–214. https://doi.org/10.1038/nrd3078
2. DiMasi, J. A., Grabowski, H. G., & Hansen, R. W. (2016). Innovation in the pharmaceutical industry: New estimates of R&D costs. *Journal of Health Economics*, *47*, 20–33. https://doi.org/10.1016/j.jhealeco.2016.01.012
3. Vamathevan, J., Clark, D., Czodrowski, P., Dunham, I., Ferran, E., Lee, G., Li, B., Madabhushi, A., Shah, P., Spitzer, M., & Zhao, S. (2019). Applications of machine learning in drug discovery and development. *Nature Reviews Drug Discovery*, *18*(6), 463–477. https://doi.org/10.1038/s41573-019-0024-5

4. Paul, D., Sanap, G., Shenoy, S., Kalyane, D., Kalia, K., & Tekade, R. K. (2021). Artificial intelligence in drug discovery and development. *Drug Discovery Today*, *26*(1), 80–93. https://doi.org/10.1016/j.drudis.2020.10.010
5. Min, S., Lee, B., & Yoon, S. (2017). Deep learning in bioinformatics. *Briefings in Bioinformatics*, *18*(5), 851–869. https://doi.org/10.1093/bib/bbw068
6. Hasin, Y., Seldin, M., & Lusis, A. (2017). Multi-omics approaches to disease. *Genome Biology*, *18*, Article 83. https://doi.org/10.1186/s13059-017-1215-1
7. Ekins, S., Puhl, A. C., Zorn, K. M., Lane, T. R., Russo, D. P., Klein, J. J., Hickey, A. J., & Clark, A. M. (2019). Exploiting machine learning for end-to-end drug discovery and development. *Nature Materials*, *18*(5), 435–441. https://doi.org/10.1038/s41563-019-0338-z
8. Acosta, J. N., Shapiro, J. S., Fletcher, P. K., Koch, L. M., Nixon, T. C., & Allen, M. A. (2022). Multimodal biomedical AI. *Nature Medicine*, *28*(9), 1773–1784. https://doi.org/10.1038/s41591-022-01981-2
9. Dara, S., Dhamercherla, S., Jadav, S. S., Babu, C. M., & Ahsan, M. J. (2021). Machine learning in drug discovery: A review. *Artificial Intelligence Review*, *54*, 1–33. https://doi.org/10.1007/s10462-021-10058-4
10. Torrisi, M., Pollastri, G., & Le, Q. (2020). Deep learning methods in protein structure prediction. *Computational and Structural Biotechnology Journal*, *18*, 1301–1310. https://doi.org/10.1016/j.csbj.2019.12.011
11. Zhou, S. K., Greenspan, H., & Shen, D. (2017). Deep learning for medical image analysis. *Annual Review of Biomedical Engineering*, *19*, 221–248. https://doi.org/10.1146/annurev-bioeng-071516-044442
12. Zhang, Z., Liu, Q., & Wang, H. (2022). Graph neural network approaches for drug-target interactions. *Current Opinion in Structural Biology*, *73*, 102327. https://doi.org/10.1016/j.sbi.2021.102327
13. Lim, J., Ryu, S., Park, K., Choe, Y. J., Ham, J., & Kim, W. Y. (2019). Predicting drug-target interaction using a novel graph neural network with 3D structure-embedded graph representation. *Journal of Chemical Information and Modeling*, *59*(9), 3981–3988. https://doi.org/10.1021/acs.jcim.9b00387
14. Madan, S., Sethi, K., et al. (2024). Transformer models in biomedicine. *Briefings in Bioinformatics*, *25*(4), bbae269. https://doi.org/10.1093/bib/bbae269
15. Zhang, Y., Wang, J., & Chen, Y. (2024). Generative artificial intelligence for small molecule drug design. *Current Opinion in Structural Biology*. https://doi.org/10.1016/j.sbi.2024.102509
16. Luscombe, N. M., Greenbaum, D., & Gerstein, M. (2001). What is bioinformatics? A proposed definition and overview of the field. *Methods of Information in Medicine*, *40*(4), 346–358. https://doi.org/10.1055/s-0038-1634381
17. Jamialahmadi, H., et al. (2024). Artificial intelligence and bioinformatics: A journey from data analysis to predictive modeling. *Current Bioinformatics*. https://doi.org/10.2174/011570669X30409240909192054
18. Brendel, M., Su, C., Bai, Z., Zhang, H., Elemento, O., & Wang, F. (2023). Application of deep learning on single-cell RNA sequencing data analysis: A review. *Briefings in Bioinformatics*, *24*(1), bbac492. https://doi.org/10.1093/bib/bbac492
19. Zhang, J., Niu, X., et al. (2021). Machine intelligence in single-cell data analysis: Advances and new challenges. *Frontiers in Genetics*, *12*, 655536. https://doi.org/10.3389/fgene.2021.655536
20. Wang, X., Zhang, Y., et al. (2024). Deep learning approaches for non-coding genetic variant effect prediction. *Briefings in Bioinformatics*, *25*(5), bbae446. https://doi.org/10.1093/bib/bbae446

21. Zhou, J., Troyanskaya, O. G., et al. (2021). A semi-supervised deep learning approach for predicting the functional effects of genomic non-coding variations. *BMC Bioinformatics, 22*, Article 307. https://doi.org/10.1186/s12859-021-03999-8
22. Poplin, R., Chang, P.-C., Alexander, D., Schwartz, S., Colthurst, T., Köse, K., et al. (2018). A universal SNP and small-indel variant caller using deep neural networks. *Nature Biotechnology, 36*(10), 983–987. https://doi.org/10.1038/nbt.4235
23. Cheng, J., et al. (2023). Predicting variant pathogenicity with AlphaMissense. *Nature Reviews Genetics, 24*, 681–683. https://doi.org/10.1038/s41576-023-00668-9
24. Jumper, J., Evans, R., Pritzel, A., Green, T., Figurnov, M., Ronneberger, O., et al. (2021). Highly accurate protein structure prediction with AlphaFold. *Nature, 596*(7873), 583–589. https://doi.org/10.1038/s41586-021-03819-2
25. Torrisi, M., Pollastri, G., & Le, Q. (2020). Deep learning methods in protein structure prediction. *Computational and Structural Biotechnology Journal, 18*, 1301–1310. https://doi.org/10.1016/j.csbj.2019.12.011
26. Kitano, H. (2002). Systems biology: A brief overview. *Science, 295*(5560), 1662–1664. https://doi.org/10.1126/science.1069492
27. Westerhoff, H. V., & Palsson, B. O. (2004). The evolution of molecular biology into systems biology. *Nature Biotechnology, 22*(10), 1249–1252. https://doi.org/10.1038/nbt1018
28. Kumar, P., et al. (2024). Harnessing artificial intelligence in multimodal omics data integration: Paving the path for the next frontier in precision medicine. *Annual Review of Biomedical Data Science, 7*(1), 225–250. https://doi.org/10.1146/annurev-biodatasci-102523-103801
29. Altucci, L., et al. (2025). Artificial intelligence and network medicine: Path to precision medicine. *PMC article*. https://doi.org/10.1056/aira2401229
30. Draghici, S., Khatri, P., Tarca, A. L., Amin, K., Done, A., Voichita, C., Georgescu, C., & Romero, R. (2007). A systems biology approach for pathway level analysis. *Genome Research, 17*(10), 1537–1545. https://doi.org/10.1101/gr.6202607
31. Nam, Y., Kim, J., Jung, S.-H., Woerner, J., Suh, E. H., Lee, D.-G., Shivakumar, M., Lee, M. E., & Kim, D. (2024). Harnessing artificial intelligence in multimodal omics data integration: Paving the path for the next frontier in precision medicine. *Annual Review of Biomedical Data Science, 7*(1), 225–250. https://doi.org/10.1146/annurev-biodatasci-102523-103801
32. Barabási, A.-L., Gulbahce, N., & Loscalzo, J. (2011). Network medicine: A network-based approach to human disease. *Nature Reviews Genetics, 12*(1), 56–68. https://doi.org/10.1038/nrg2918
33. Tejada-Lapuerta, A., Bertin, P., Bauer, S., Aliee, H., Bengio, Y., & Theis, F. J. (2023). Causal machine learning for single-cell genomics. *arXiv*. https://doi.org/10.48550/arXiv.2310.14935
34. Kong, Y., et al. (2024). Advances in single-cell omics and multiomics for high-resolution molecular profiling. *Experimental & Molecular Medicine, 56*(3), 515–526. https://doi.org/10.1038/s12276-024-01186-2
35. Ngassam, B. T., Niu, H., Pang, S., Shydlouskaya, V., & Andrews, T. S. (2026). Applications of AI to single-cell and spatial transcriptomics: Current state-of-the-art and challenges. *Frontiers in Bioinformatics, 5*, 1715821. https://doi.org/10.3389/fbinf.2025.1715821

36. Katsoulakis, E., et al. (2024). Digital twins for health: A scoping review. *NPJ Digital Medicine, 7*, Article 29. https://doi.org/10.1038/s41746-024-01073-0
37. Sadée, C., Testa, S., Barba, T., et al. (2025). Medical digital twins: Enabling precision medicine and medical artificial intelligence. *The Lancet Digital Health, 7*(7), 100864. https://doi.org/10.1016/j.landig.2025.02.004
38. Chen, Y.-M., et al. (2025). Unlocking precision medicine: Clinical applications of integrating artificial intelligence with health records, genetics, and immunology data. *BMC Medical Informatics and Decision Making, 25*, Article 54. https://doi.org/10.1186/s12911-024-02236-8
39. Wang, X., et al. (2025). Advancing precision medicine: The transformative role of artificial intelligence in immunogenomics, radiomics, and pathomics for biomarker discovery and immunotherapy optimization. *Cancer Biology & Medicine, 22*(1), 33–47. https://doi.org/10.20892/j.issn.2095-3941.2024.0376
40. DiMasi, J. A., Grabowski, H. G., & Hansen, R. W. (2016). Innovation in the pharmaceutical industry: New estimates of R&D costs. *Journal of Health Economics, 47*, 20–33. https://doi.org/10.1016/j.jhealeco.2016.01.012
41. Kola, I., & Landis, J. (2004). Can the pharmaceutical industry reduce attrition rates? *Nature Reviews Drug Discovery, 3*(8), 711–715. https://doi.org/10.1038/nrd1470
42. Jamialahmadi, H., et al. (2024). Artificial intelligence and bioinformatics: A journey from genome sequencing to personalized medicine. *Computational and Structural Biotechnology Journal, 22*, 4469–4487. https://doi.org/10.1016/j.csbj.2024.08.010
43. Ocana, A., et al. (2025). Integrating artificial intelligence in drug discovery and early development: Challenges and opportunities. *Molecular Cancer, 24*, Article 38. https://doi.org/10.1186/s12943-025-02131-6
44. Bender, A., et al. (2024). Data-centric challenges with the application and adoption of artificial intelligence for drug discovery. *Drug Discovery Today, 29*(12), 103958. https://doi.org/10.1016/j.drudis.2024.103958
45. Pereira, A. C., et al. (2023). Explainability and white box in drug discovery. *Chemical Biology & Drug Design, 102*(1), 217–233. https://doi.org/10.1111/cbdd.14262
46. Jiménez-Luna, J., Grisoni, F., & Schneider, G. (2020). Drug discovery with explainable artificial intelligence. *Nature Machine Intelligence, 2*, 573–584. https://doi.org/10.1038/s42256-020-00236-4