INTERNATIONAL JOURNAL OF PHARMACEUTICAL SCIENCES
[ISSN: 0975-4725; CODEN(USA): IJPS00]
Journal Homepage: https://www.ijpsjournal.com

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Review Paper

Artificial Inteligence Used in Drug Discovery

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ARTICLE INFO

Published: 03 Mar. 2025
Keywords:
Artificial intelligence, machine learning, deep learning, drug discovery, target identification, compound screening, lead optimization
DOI:
10.5281/zenodo.14961715

ABSTRACT

The traditional drug discovery process is time consuming, costly and often yields limited success. Recent advancements in artificial intelligence (AI) have transformed the landscape of drug discovery, enabling faster, more accurate, and cost-effective identification of potential therapeutic candidates. AI powered approaches, such as machine learning (ML) and deep learning (DL), are being employed to analyze vast amounts of biological and chemical data, predict molecular interactions, and optimize lead compounds. This abstract review the current state of AI in drug discovery, highlighting its applications in target identification, compound screening, and lead optimization. We also discuss the challenges and future directions of AI driven drug discovery, emphasizing the potential for AI to revolutionize the development of novel therapeutics.

INTRODUCTION

AI is the ability of machines to interact with humans (through electronic output devices) without identifying themselves as non-human, with binary judgment being the primary criterion. One of the pioneers of artificial intelligence, Marvin Minky, described AI as the ability of machines to perform tasks that call for human intelligence. According to the symbolic school, artificial intelligence (AI) is the operation of symbols, with the most basic symbols representing physical entities. The research theories, techniques, technologies, and applications for mimicking, extending, and growing human intelligence are generally accepted to be at the heart of artificial intelligence (AI), despite the fact that different definitions exist. These days, the idea of artificial intelligence has a bigger and bigger influence on people's lives.[1] AI is the cornerstone of technology in the modern era and beyond, much like steam engines were in the Age of Steam, generators were in the Age of Electricity, and computers were in the Age of Information.[1]

The study of how to enable machines to competently carry out intelligent tasks without being specifically programmed for them is the

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Relevant conflicts of interest/financial disclosures: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

focus of artificial intelligence (AI) and its subfield of machine learning (ML). AI systems have recently come close to or even exceeded humans in a number of tasks, including image recognition and gaming, but these have usually been very specific and limited domains. However, artificial intelligence (AI) in all of its forms is now effectively used for difficult tasks in a wide range of fields, from robotics, image analysis, speech translation, and logistics to its continuous application in molecular design.[2]

The daily advancements in medicine made possible by artificial intelligence (AI) are astounding. AI is transforming the way we identify, treat, and prevent illnesses and opening up new medical possibilities. Cardiology is one area where AI has demonstrated remarkable promise. As the world's leading cause of death, cardiovascular diseases (CVD) present an increasingly difficult problem. Between 1990 and 2019, the number of people with CVD increased from 271 million to 523 million, while the number of deaths also increased from 12.1 million to 18.6 million.[3]

Application of Ai In Drug Discovery

A high-quality dataset is the key to applying AI to drug discovery. Advances in high-throughput sequencing and IT have boosted the generation of a series of free and open-access databases for drug discovery. These databases enable drug discovery to transit into the big data era and accelerate the drug discovery process.

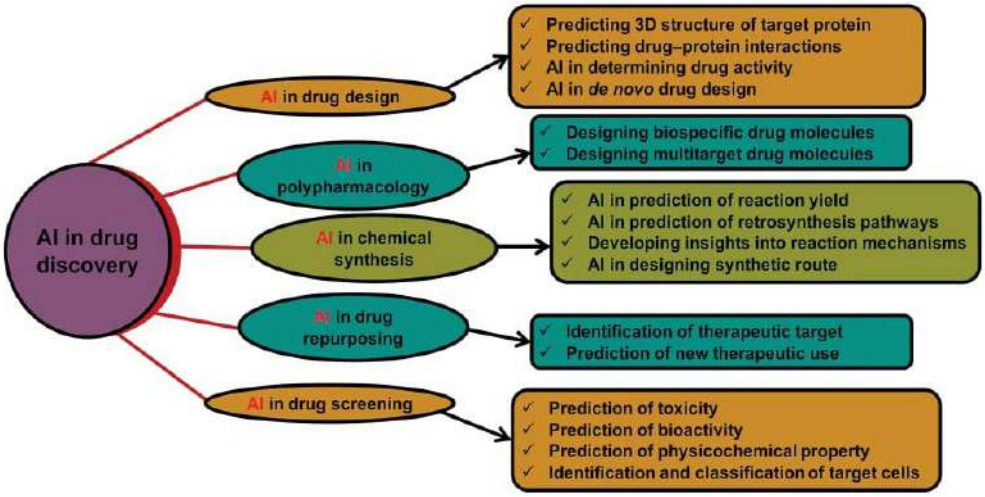

Fig. Applications of AI in Drug Discovery

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Introduction to Ai And Its Potential for Use in Drug Discovery

In recent years, there has been a lot of interest in medicinal chemistry's application of artificial

intelligence (AI) as a potential way to transform the pharmaceutical sector. The process of finding and creating new drugs, or drug discovery, is a difficult and drawn-out undertaking that has historically relied on time-consuming methods like high-throughput screening and trial-and-error testing. However, by making it possible to analyze vast amounts of data more accurately and efficiently, artificial intelligence (AI) techniques like machine learning (ML) and natural language processing have the potential to speed up and enhance this process. The authors recently described the successful application of deep learning (DL) to accurately predict the efficacy of drug compounds. The toxicity of potential medications has also been predicted by AI-based techniques. These and other studies have demonstrated AI's potential to increase the efficacy and efficiency of drug discovery procedures. But there are drawbacks and restrictions to using AI to create novel bioactive compounds. To completely comprehend the benefits and limitations of AI in this field, more research is required, and ethical considerations must be taken into account. Despite these obstacles, AI is anticipated to play a major role in the creation of novel drugs and treatments in the coming years.[4]

Limitations of The Current Methods in Drug Discovery

Large-scale testing procedures and a trial-and-error methodology are currently key components of medicinal chemistry methods. These methods entail looking at a lot of possible drug compounds to find those that have the desired qualities. These techniques, however, can be expensive, time-consuming, and frequently produce inaccurate results. They may also be constrained by the difficulty of precisely forecasting how they will behave in the body and the availability of appropriate test compounds. These issues may be resolved by a variety of AI-based algorithms, such as reinforcement learning, supervised and unsupervised learning techniques, and evolutionary or rule-based algorithms. These techniques usually rely on the analysis of vast quantities of data that can be used in a variety of ways. For example, these methods are more accurate and efficient than traditional methods in predicting the toxicity and efficacy of novel drug compounds. Additionally, new targets for drug development, like the precise proteins or genetic pathways implicated in diseases, can be found using AI-based algorithms. This may eventually result in the creation of new and more potent drugs by broadening the scope of drug discovery beyond the constraints of more traditional methods. Therefore, even though conventional pharmaceutical research techniques have historically been comparatively effective, they are constrained by their dependence on trial-and-error testing and their incapacity to precisely forecast the behavior of novel, potentially bioactive compounds. The development of more potent drugs, however, may result from AI-based methods that increase the efficacy and precision of drug discovery procedures.[5] The pharmaceutical industry is the primary beneficiary of artificial intelligence (AI), which has just begun to expand its use in many facets of society. This review emphasizes the significant application of AI in several pharmaceutical industry domains, including drug discovery and creation, repurposing of drugs, increasing pharmaceutical output, clinical trials, among other things, thereby decreasing the human workload as well as meeting deadlines and goals. Interaction between the tools and methods for implementing AI, continuous difficulties, and strategies to conquer them, as well as the prospects of artificial intelligence in the pharmaceutical industry is also covered. Artificial intelligence (AI) has been used more and more in many facets of society, most notably in the pharmaceutical sector. The use of AI in various

areas of the pharmaceutical industry, such as clinical trials, drug repurposing, drug discovery and development, and increasing pharmaceutical productivity, is highlighted in this review; it lowers the human workload as well as meeting deadlines and objectives. We also talk about the communication between the AI tools and methods, continuous difficulties, and solutions, as well as with the pharmaceutical industry's use of AI in the future.

Things to Be Aware of Regarding Artificial Intelligence:

The pharmaceutical industry has seen a sharp rise in data digitization in the last several years. The difficulty of gathering, evaluating, and using that knowledge to address intricate clinical issues, however, is a consequence of this digitization. This encourages the application of AI, because it has improved automation and can manage massive data volumes. Artificial Intelligence (AI) is a technology-based system that can simulate human intelligence using a variety of sophisticated tools and networks. However, it does not pose a threat to fully replace the physical presence of humans. Artificial Intelligence uses software and systems that can analyze and learn from the input data to make. [6]

Drug Discovery in The AI ERA:

AI has been used extensively in the search for new drugs. Machine learning models, like random forest (RF), have been used for VS and QSAR since the early 2000s. The deep learning era began in 2012 with AlexNet. Deep neural networks (DNNs) beat the conventional RF model in predicting molecular activities shortly after in the 2012 Merck Kaggle competition. Deep learning in chemistry is a rapidly developing field that has been aided by the success of AI techniques in computer vision and natural language processing in recent years. Researchers from Insilico Medicine found powerful inhibitors of discoidin domain receptor 1 (DDR1) in 21 days in 2019. Halicin is a novel antibiotic candidate that researchers at MIT discovered in 2020 to combat bacteria that are resistant to antibiotics. It should be noted that artificial intelligence (AI) can be used at various phases of drug discovery, from determining drug response to identifying and validating targets. The two core tasks of lead identification—the subject of this survey—are molecule generation and molecular property prediction. Predicting a molecule's property value based on its structure or learned representation is the fundamental function of molecular property prediction (VS). This can be used for a number of purposes, including toxicity prediction, drug-induced liver injury (DILI) prediction, and drug–target interaction (DTI) prediction.

There Are Two Levels of Tasks Involved in Molecule Generation, Which Is the Foundation of Drug Design:

1. Realistic molecule generation, which involves creating molecules within the limitations set by chemical rules,
2. Goal-directed molecule generation, which entails creating chemically valid molecules with desired properties.[4]

DRUG DISCOVERY

- Target identification
- Target validation
- Lead identification
- Lead optimization
- Product characterization
- Formulation and New Drug
- Preclinical research
- Investigational New Drug Application
- Approval

Target Identification

Deep learning-based techniques for predicting drug target interactions have gradually caught the interest of researchers in recent years. The prediction of drug-target association issues has greatly improved thanks to these techniques, but

they also face new Difficulties. In particular, it's common to think of drug target interaction prediction as a binary classification issue that calls for the extraction of reliable molecular fingerprint features or descriptors from a variety of intricate raw data.[9]

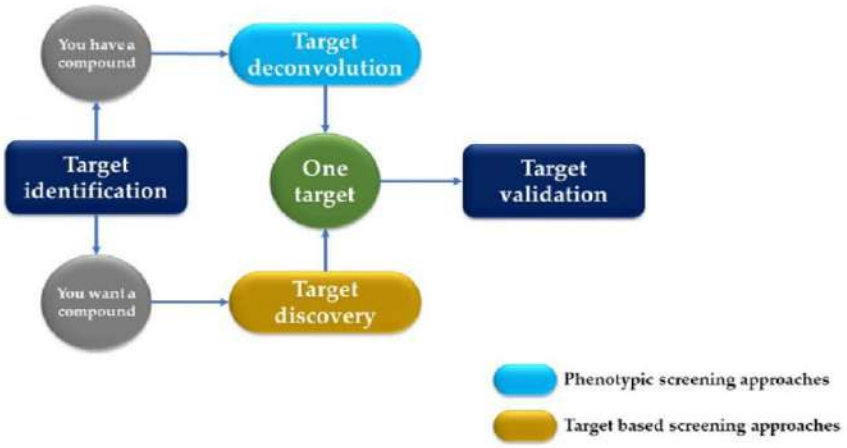

Fig. Process of Target Identification

Through the identification of promising compounds for additional development and refinement, structure-based virtual screening plays a crucial role in drug discovery. Screening the vast chemical space for lead discovery has gained popularity since the introduction of easily accessible chemical libraries containing billions of compounds. Only a small number of effective virtual screening campaigns utilizing ultra-large libraries have been documented, despite the advantages of screening these libraries. Moreover, physics-based docking methods find it more and more expensive and time-consuming to virtually screen an entire ultra-large library. The development of scalable virtual screening platforms to parallelize docking runs on high-performance computing clusters (HPC), deep learning guided chemical space exploration, or active learning techniques to only screen a small portion of the library for similar performance, hierarchical structure-based virtual screening, and GPU accelerated ligand docking are some of the methods that have been introduced in recent years to achieve the ultra-large library virtual screening.[10]

Discovery of The Lead Molecule

A lead molecule is any chemical compound that possesses pharmacological or biological properties with therapeutic qualities. It is difficult to find the lead molecule with good pharmacokinetic, efficiency, efficacy, and selectivity parameters. Sometimes a lead molecule that has been identified needs to have its structure changed in order to improve its biological qualities. We refer to this procedure as lead optimization. For the investigated lead molecule to function as a bioactive drug molecule, it must meet five requirements. These include duration, safety, potency, bioavailability, and pharmaceutical acceptability. Potency refers to a molecule's ability to display desired pharmacological characteristics in minuscule amounts.

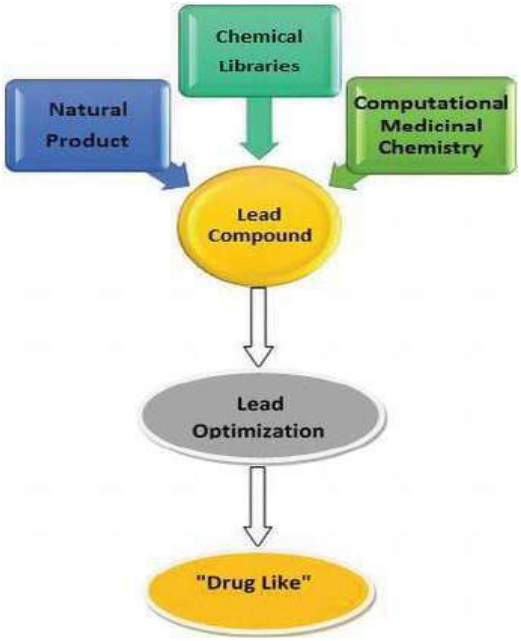

Fig. Discovery of Lead Compound

Bioavailability is the ability of drug molecules to move through several barriers and reach the intended location. Duration is the interval of time between a drug's pharmacological response and its entry. Their toxicity parameters, which show no adverse effects on the organism, are part of the safety regulations. Solubility, chemical stability, dissolution rate, and a reasonable synthetic pathway are all related to pharmaceutical action.

Traditional library screening, fragment-based screening, and virtual screening are the foundations of lead molecule discovery (Jain, 2004; Lavecchia & Di Giovanni, 2013). The goal of rapid drug discovery is to identify and validate targets. Hit identification and lead discovery phases are created for novel drug discovery after the target validation procedure. In order to create an efficient lead molecule for drug development, changes to the structural properties of compounds are determined by physical and biochemical parameters.

TYPES OF LEAD MOLECULES

Many natural leads that have some biological activity against a biological target and could be used as a drug after some chemical modification can be found in databases and the literature. The three types of lead molecules used in pharmaceutical sciences are natural, synthetic, and semisynthetic (Leisner, 2020).

1. Natural lead compounds
2. Synthetic lead compound.[9]

The prediction of the toxicity of any drug molecule is vital to avoid toxic effects. Cell-based in vitro assays are often used as preliminary studies, followed by animal studies to identify the toxicity of a compound, increasing the expense of drug discovery. Several web-based tools, such as LimTox, pkCSM, admetSAR, and Toxtree, are available to help reduce the cost. Advanced AI-based approaches look for similarities among compounds or project the toxicity of the compound based on input features. The US Food and Drug Administration (FDA), Environmental Protection Agency (EPA), and National Institutes of Health launched the Tox21 Data Challenge as a way to assess a number of computer methods to predict the toxicity of 12 707 medications and environmental substances; an ML algorithm named DeepTox performed better than any other technique by detecting static as well as dynamic elements in the chemical descriptors of the molecules, including Van der Waals and

molecular weight (MW) volume, and could effectively forecast a molecule's toxicity. according to predetermined 2500 toxicophore characteristics.[6]

PRE-CLINICAL CHARECTERIZATION

New drug development is seen as a very complicated process that may be explained from a variety of angles; the business case and scientific evidence for a new medicine's introduction do not always align. More than 90% of medication leads fail to reach the market, therefore a quick scientific discovery could result in clinical study failure or even withdrawal after debut.[7] A crucial phase in the drug design process is forecasting potential reactions to a medication. By using binding affinity or free energy of binding, machine learning techniques based on similarity or features can be used to anticipate how a drug will react to specific cells and how well a medicine will interact with its target. The premise of similarity techniques is that similar medications affect similar targets.[8]

Specific Ai Techniques Used Machine Learning

AI innovation plays a crucial role in drug design by advancing machine learning techniques and gathering pharmacological data. Rather than depending on theoretical enhancements, AI is fundamentally focused on converting medical information into practical applications, such as reusable methodologies. Various machine learning approaches are employed in this context, including Random Forest, Naive Bayesian Classification (NBC), Multiple Linear Regression (MLR), Logistic Regression (LR), Linear Discriminant Analysis (LDA), Probabilistic Neural Networks (PNN), Multi-Layer Perceptron (MLP), and Support Vector Machine (SVM), among others (Lavecchia and Di Giovanni 2013).

In order to gain capability in feature extraction and feature generalization, AI advancements are specifically used as a deep learning technique towards drug design. Also, Fig. 3 shows respective applications which illustrate an outline of AI procedures utilized to respond to drug discovery queries in the review. A scope of classifier and regression strategies i.e. supervised learning techniques utilized to respond addresses desire expectations in continuous or categorical data factors, also unsupervised methods utilized in creating a model which empowers the clustering data.[12]

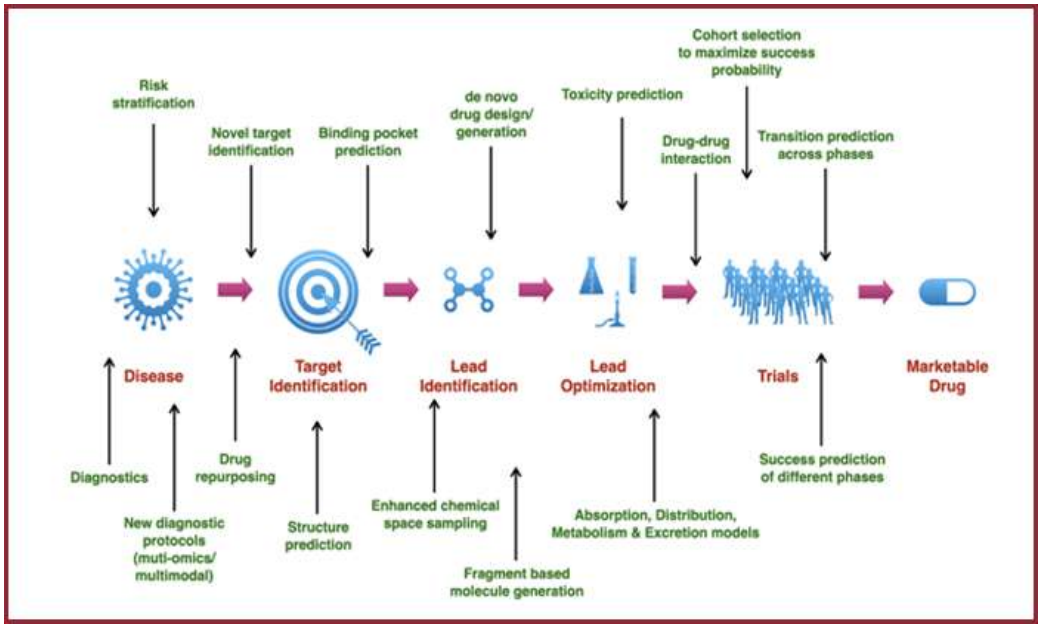

Fig. Drug Discovery by Machine Learning

DEEP LEARNING:

Machine-learning provides a theoretical framework for the discovery and prioritization of bioactive compounds with desired pharmacological effects and their optimization as drug-like leads. Biological target identification and protein design are emerging areas of application.[13] Recent advancements in research have highlighted various applications of machine learning (ML), including spam detection, video recommendations, image classification, and multimedia idea retrieval. Among the various ML techniques, deep learning (DL) has emerged as one of the most widely employed methods in these domains. The continuous emergence of new DL research can be attributed to the unpredictable nature of data acquisition and significant advancements in hardware technology. While DL is rooted in traditional neural networks, it demonstrates a marked superiority over them. Additionally, DL leverages transformations and graph technology to develop multi-layer learning models. With their ground-breaking invention, Machine Learning and Deep Learning have revolutionized the world's perspective. Deep learning approaches have revolutionized the way we tackle problems. Deep learning models come in various shapes and sizes, capable of effectively resolving problems that are too complex for standard approaches to tackle. We'll review the various deep learning models in this section.[14]

The rapid growth in computing power, amount of data, and advanced algorithms has led to breakthroughs in AI for drug discovery, especially in the application of deep generative models. The models have emerged as high potential tools to transform the design, optimization, and synthesis of small molecules, and macromolecules. Applications of deep generative models have already delivered new partially optimized candidate leads, in some cases in less time typically required by conventional sequential approaches. If applied on a large scale, deep generative modelling has the potential of boosting the development (R&D) process.

Deep generative models correspond to a theoretical framework for generating novel chemical and biological structures with desired properties using data structures, such as graphs and fingerprints, and operations, such as the flow of functional or experimental information. Creative deep generative models can significantly promote algorithm development and application in drug discovery.[15]

Application of Deep Learning in Compound Property and Activity Prediction

When compounds are presented by the same number of molecular descriptors, the straight forward method is to use fully connected DNNs to build models. Applied a DNN on the Merck Kaggle challenge dataset using a large number of 2D topological descriptors; and the DNN showed slightly better performance in 13 of the total 15 targets than the standard RF method.[16]

Some of the key learnings from the study are:	(i) DNNs can handle thousands of descriptors without the need of feature selection
	(ii) dropout can avoid the notorious overfitting problem faced by a traditional ANN
	(iii) hyper-parameter (number of layers, number of nodes per layer, type of activation functions, etc.) optimization can maximize the DNN performance;
	(iv) multitask DNN models perform better than single-task models.

Fig. Key learnings

CONCLUSION

The integration of artificial intelligence (AI) in drug discovery has revolutionized the field, transforming the way we identify, design, and optimize therapeutic candidates. AI powered approaches, such as machine learning (ML), deep learning (DL), have demonstrated remarkable potential in analyzing vast amounts of biological and chemical data, predicting molecular interactions, and streamlining the drug development process.

REFERENCES

1. Jiang Y, Li X, Luo H, Yin S, Kaynak O. Quo vadis artificial intelligence? Discover Artificial Intelligence. 2022 Mar 7;2(1):4.
2. Sellwood MA, Ahmed M, Segler MH, Brown N. Artificial intelligence in drug discovery. Future medicinal chemistry. 2018 Sep 1;10(17):2025-8.
3. Hamet P, Tremblay J. Artificial intelligence in medicine. metabolism. 2017 Apr 1;69: S36-40.
4. Deng J, Yang Z, Ojima I, Samaras D, Wang F. Artificial intelligence in drug discovery: applications and techniques. Briefings in Bioinformatics. 2022 Jan;23(1): bbab430.
5. Blanco-Gonzalez A, Cabezon A, Seco-Gonzalez A, Conde-Torres D, Antelo-Riveiro P, Pineiro A, GarciaFandino R. The role of AI in drug discovery: challenges, opportunities, and strategies. Pharmaceuticals. 2023 Jun 18;16(6):891.
6. Mak KK, Wong YH, Pichika MR. Artificial intelligence in drug discovery and development. Drug discovery and evaluation: safety and pharmacokinetic assays. 2024 Oct 22:1461-98.
7. Brodniewicz T, Grynkiewicz G. Preclinical drug development. Acta Pol Pharm. 2010 Dec;67(6):578-85.
8. Qureshi R, Irfan M, Gondal TM, Khan S, Wu J, Hadi MU, Heymach J, Le X, Yan H, Alam T. AI in drug discovery and its clinical relevance. Heliyon. 2023 Jul 1;9(7).
9. Huang D, Yang M, Zheng W. Integrating AI and Deep Learning for Efficient Drug Discovery and Target Identification.
10. Zhou G, Rusnac DV, Park H, Canzani D, Nguyen HM, Stewart L, Bush MF, Nguyen PT, Wulff H, YarovYarovoy V, Zheng N. An artificial intelligence accelerated virtual screening platform for drug discovery. Nature Communications. 2024 Sep 5;15(1):7761.
11. Verma S, Pathak RK. Discovery and optimization of lead molecules in drug designing. InBioinformatics 2022 Jan 1 (pp. 253-267). Academic Press.
12. Gupta R, Srivastava D, Sahu M, Tiwari S, Ambasta RK, Kumar P. Artificial intelligence

to deep learning: machine intelligence approach for drug discovery. Molecular diversity. 2021 Aug; 25:1315-60.

13. Gawehn E, Hiss JA, Schneider G. Deep learning in drug discovery. Molecular informatics. 2016 Jan;35(1):3-14.
14. Askr H, Elgeldawi E, Aboul Ella H, Elshaier YA, Gomaa MM, Hassanien AE. Deep learning in drug discovery: an integrative review and future challenges. Artificial Intelligence Review. 2023 Jul;56(7):5975-6037.
15. Zeng X, Wang F, Luo Y, Kang SG, Tang J, Lightstone FC, Fang EF, Cornell W, Nussinov R, Cheng F. Deep generative molecular design reshapes drug discovery. Cell Reports Medicine. 2022 Dec 20;3(12).
16. Chen H, Engkvist O, Wang Y, Olivecrona M, Blaschke T. The rise of deep learning in drug discovery. Drug discovery today. 2018 Jun 1;23(6):1241-50.

HOW TO CITE: Nilesh Savale*, Artificial Inteligence Used in Drug Discovery, Int. J. of Pharm. Sci., 2025, Vol 3, Issue 3, 138-147. https://doi.org/10.5281/zenodo.14961715