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ARTIFICIAL INTELLIGENCE IN DRUG DESIGN:APPLICATION, CHALLENGES AND FUTURE PROSPECTS

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ABSTRACT

Artificial Intelligence (AI) has become a game-changer in drug discovery and development by speeding up the design, testing, and optimization of new medicines. Using machine learning, deep learning, and generative models, AI can analyze large and complex biological, chemical, and clinical datasets with high accuracy. This not only lowers research costs but also reduces the time needed to develop new drugs. Major applications include target identification, virtual screening of compounds, lead optimization, ADMET prediction, drug repurposing, and personalized medicine. Popular AI-based platforms such as AlphaFold, Atomwise, BenevolentAI, and Insilico Medicine have shown real-world benefits, like rapid protein structure prediction, virtual screening, and identifying potential drug candidates. AI is also contributing to precision medicine by predicting patient-specific responses and minimizing side effects.Despite its benefits, challenges such as poor data quality, limited interpretability of models, high computational needs, ethical concerns, and lack of generalizability still exist. Overcoming these issues is crucial for wider adoption.Looking forward, combining AI with quantum computing, multi-omics analysis, and advanced clinical trial simulations can make drug discovery even faster and more precise. Overall, AI is shifting from just a supportive tool to a core driver of pharmaceutical innovation, offering new opportunities for developing safer and more effective therapies.

KEYWORDS: *Artificial Intelligence, Drug Discovery, Drug Design, Machine Learning, Deep Learning, Drug Repurposing, Precision Medicine.*

INTRODUCTION

Drug discovery and development is a complex, time-consuming, and expensive process. On average, bringing a new drug to the market takes around 10–15 years and costs approximately 1–2 billion USD [1]. Despite these investments, the success rate of clinical trials remains extremely low, with only about 2% of candidate drugs ultimately reaching approval [2]. These challenges highlight the urgent need for innovative approaches to improve efficiency, reduce costs, and increase the probability of success in drug discovery.

In recent years, Artificial Intelligence (AI) has emerged as a powerful tool that promises to revolutionize drug design. AI refers to computational systems capable of learning patterns from data, making predictions, and performing tasks that usually require human intelligence [3]. By leveraging machine learning (ML), deep learning (DL), natural language processing (NLP), and generative models, AI can analyze massive biomedical datasets, identify potential drug targets, optimize lead molecules, and predict pharmacokinetics, toxicity, and efficacy with remarkable accuracy [4].

Background and Rationale: Traditional drug discovery faces several obstacles. The vast chemical space, estimated at nearly 10^60 possible molecules, is impossible to explore exhaustively using experimental methods [5]. AI enables researchers to efficiently navigate this space, identify promising candidates, and prioritize molecules for experimental testing. Additionally, AI shortens the timeline of discovery. For instance, AI-based platforms have reduced the time required to advance drug candidates into clinical trials to 18 months, compared to the industry average of 42 months [6].Another key driver is the increasing availability of large biomedical datasets, such as genomic, proteomic, and chemical structure databases. AI can integrate and analyze these diverse datasets to uncover hidden patterns and correlations, leading to more informed decision-making [7]. Furthermore, pharmaceutical giants like Eli Lilly have launched AI-enabled platforms (e.g., TuneLab) that democratize access to sophisticated tools, enabling even smaller biotech firms to leverage AI in drug discovery [8].

Growth of AI in Drug Discovery: The application of AI in drug design has grown exponentially in the past decade. A bibliometric analysis of publications between 1990 and 2023 identified over 4000 research papers on AI in drug discovery, with a rapid surge observed after 2014 [9]. This growth is attributed to the advancement of deep learning techniques and the increasing availability of high-quality biomedical data.Several reviews and studies highlight the role of AI across the drug discovery pipeline. For example, Paul et al. (2020) emphasized AI's impact on virtual screening and target identification [10], while Dhudum et al. (2024) discussed challenges related to data quality and interpretability [11]. More recent analyses, such as Bhat et al. (2025), have outlined AI's future role in precision medicine and personalized drug development [12].

Core AI Techniques in Drug Design
AI encompasses a broad range of computational approaches
1. Machine Learning (ML): Algorithms trained on large datasets can predict biological activity, optimize quantitative structure–activity relationships (QSAR), and assist in ADMET profiling [13].
2. Deep Learning (DL): Neural networks such as convolutional and recurrent architectures capture complex molecular representations and are especially useful in image-based screening and protein–ligand binding prediction [14].
3. Generative Models: Variational autoencoders (VAEs), generative adversarial networks (GANs), and reinforcement learning models are applied for de novo molecule generation, producing entirely new compounds with desired pharmacological properties [15].
4. Graph Neural Networks (GNNs): These models represent molecular structures as graphs, capturing atom-bond relationships for accurate property prediction and activity estimation [16].
5. Federated Learning: Initiatives like the MELLODDY project use privacy-preserving collaborative learning, enabling multiple pharma companies to train shared models without exposing proprietary data [17].

Why AI Matters Now
Several factors make AI particularly valuable in today's context
Data Explosion: With the growth of genomics, proteomics, and electronic health records, biomedical research is producing unprecedented amounts of data that traditional methods cannot fully utilize [18].
High Failure Rates: AI can improve prediction accuracy in early stages, reducing costly late-stage clinical failures [19].
Cost and Time Pressure: Pharma companies are under increasing pressure to develop safer drugs quickly. AI shortens cycles and reduces redundant experiments [20].
Precision Medicine: AI facilitates the design of drugs tailored to individual genetic profiles, supporting the shift toward personalized therapy [21].

2. Artificial Intelligence in Drug Design: An Overview

Artificial Intelligence (AI) has become a transformative force in modern drug design, providing new ways to analyze biomedical data, identify drug targets, and accelerate the development process. Traditional drug discovery is expensive, lengthy, and uncertain, whereas AI tools bring efficiency, accuracy, and predictive power to each stage of the pipeline.

2.1 Historical Perspective: Early computational methods such as QSAR modeling and molecular docking provided the first steps toward predictive chemistry, but limited datasets and computational power restricted their accuracy. The rise of machine learning (ML) and deep learning (DL) in the last decade changed this landscape, allowing researchers to process massive biological datasets and identify non-linear relationships [22]. Startups like Atomwise and BenevolentAI pioneered AI-based screening and target discovery, demonstrating real-world impact [23].

2.2 Importance of AI in Drug Discovery: The drug discovery pipeline traditionally requires 10–15 years and billions of dollars to bring a single drug to market [24]. AI reduces this burden in several ways:
Target Identification: Integration of genomic, proteomic, and clinical data enables better understanding of disease biology [25].
Virtual Screening: Millions of compounds can be tested in silico, lowering experimental costs [26].
ADMET Prediction: Early modeling of safety and pharmacokinetics prevents late-stage failures [27].
Drug Repurposing & Precision Medicine: AI helps find new uses for existing drugs and tailor treatments for individual patients [28].

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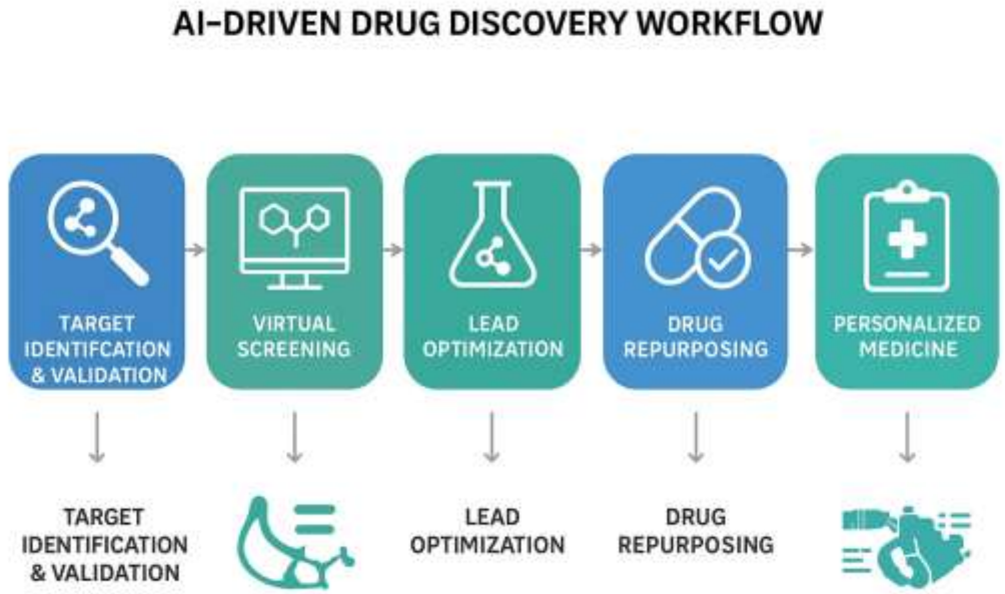
2.3 Core AI Techniques
AI employs several computational strategies
Machine Learning (ML): Tools like random forests and SVMs for bioactivity prediction [29].
Deep Learning (DL): CNNs and RNNs for protein–ligand binding and image-based assays [30].
Generative Models: VAEs and GANs for de novo molecular design [31].
Graph Neural Networks (GNNs): Representation of molecules as atom–bond graphs for property prediction [32].
Natural Language Processing (NLP): Mining biomedical literature to extract drug–disease relationships [33].
Federated Learning: Collaborative learning across institutions while protecting sensitive data, e.g., the MELLODDY project [34].

2.4 Industrial Adoption: Pharma giants like Pfizer, Novartis, and Roche have invested heavily in AI-driven collaborations [35]. A landmark example is AlphaFold, which solved protein structure prediction with unprecedented accuracy [36]. Building on this, Isomorphic Labs extended AI into drug design, while the Nobel Prize in Chemistry (2024) recognized AI's role in protein prediction and its potential in medicine [37].

3. Applications of AI in Drug Discovery and Development:
Artificial Intelligence (AI) has transformed various stages of drug discovery and development, making processes faster, cheaper, and more accurate. AI applications range from identifying novel drug targets to optimizing clinical outcomes, thereby enhancing overall efficiency in pharmaceutical research.



3.1 Target Identification and Validation: Identifying molecular targets is a crucial first step in drug discovery. AI algorithms analyze large-scale genomic, proteomic, and transcriptomic datasets to uncover disease-associated proteins and pathways. Machine learning models, including neural networks, can predict functional roles of these targets and prioritize them for further validation. Natural language processing (NLP) also extracts relevant target-disease associations from biomedical literature, enabling faster and more reliable identification of druggable proteins (38,39).

3.2 Virtual Screening and Hit Identification: Virtual screening evaluates large chemical libraries in silico to identify potential drug candidates. AI-powered models, especially deep learning architectures, predict protein–ligand interactions with high accuracy, reducing the need for expensive high-throughput screening. Start-ups like Atomwise leverage AI to virtually screen billions of compounds in days, significantly accelerating the discovery of potential hits (40,41).

3.3 Lead Optimization: After identifying initial hits, lead optimization improves molecular properties such as potency, selectivity, and safety. AI models predict structure–activity relationships and propose chemical modifications. Generative models, including variational autoencoders (VAEs) and generative adversarial networks (GANs), design novel molecules with optimized pharmacological profiles, reducing experimental iterations (42,43).

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3.4 ADMET Prediction: Early prediction of Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) properties is critical for drug safety. AI classifiers, including support vector machines and random forests, effectively predict hepatotoxicity, cardiotoxicity, and blood–brain barrier permeability. Such predictions minimize late-stage failures and enhance the likelihood of clinical success (44,45).

3.5 Drug Repurposing: Drug repurposing identifies new therapeutic uses for approved drugs. AI integrates chemical–protein interaction data, clinical records, and literature to discover candidates for novel indications. During the COVID-19 pandemic, AI platforms facilitated rapid identification of drugs like remdesivir and baricitinib for potential antiviral activity, demonstrating the utility of AI in urgent drug repositioning scenarios (46,47).

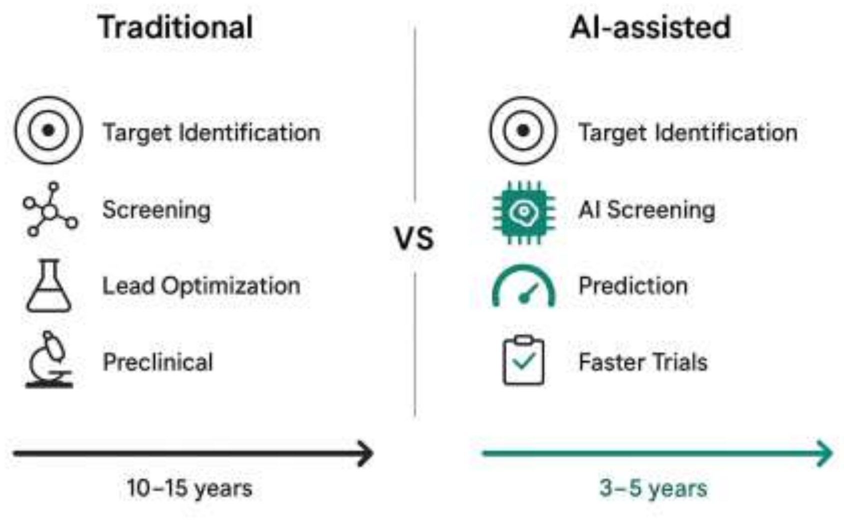
3.6 Precision and Personalized Medicine: AI enables personalized therapy by analyzing patient-specific genomic and clinical data. Predictive models can anticipate drug responses and potential adverse effects, allowing optimization of treatment regimens. In oncology, AI-assisted stratification of patients based on genetic mutations supports precision-targeted therapy, improving efficacy while reducing side effects (48,49).

3.7 Protein Structure Prediction: Knowledge of protein structures is vital for rational drug design. Deep learning tools like AlphaFold accurately predict 3D protein structures, facilitating design of inhibitors and modulators with precise binding characteristics. This approach accelerates discovery of drugs for previously challenging targets (50,51,52).

4. Case Studies and Industry Examples: Artificial Intelligence (AI) has already demonstrated significant impact in real-world drug discovery, with several successful case studies highlighting its potential in accelerating research and reducing costs. These examples showcase how AI-driven strategies are applied in industry to solve complex pharmaceutical challenges.

4.1 AlphaFold (DeepMind): Protein structure prediction is a fundamental step in rational drug design. DeepMind's AlphaFold leveraged deep learning to predict 3D structures of proteins with remarkable accuracy. Traditional experimental methods, such as X-ray crystallography and NMR spectroscopy, require months to years to determine structures, whereas AlphaFold predicts them within hours to days. This advancement has enabled pharmaceutical researchers to identify binding sites more efficiently and design inhibitors for previously undruggable targets. AlphaFold's database now includes millions of protein structures, transforming structural biology and facilitating the design of novel therapeutics (53,54).

4.2 Atomwise: Atomwise utilizes AI-driven convolutional neural networks for virtual screening of chemical compounds. By predicting ligand–target interactions, Atomwise screens billions of compounds in silico, drastically reducing the time and cost of experimental high-throughput screening. The platform has identified promising drug candidates for diseases including Ebola, multiple cancers, and neurodegenerative disorders. For example, Atomwise's AI model rapidly pinpointed potential antiviral compounds during emerging outbreaks, demonstrating the real-world utility of AI in urgent scenarios (55,56).



4.3 BenevolentAI: BenevolentAI applies AI to integrate biomedical knowledge, chemical data, and clinical information for drug repurposing and discovery. A notable success was during the COVID-19 pandemic, where BenevolentAI identified baricitinib, originally developed for rheumatoid arthritis, as a candidate to mitigate severe inflammatory responses in COVID-19 patients. By combining network analysis and predictive algorithms, the company shortened the timeline from hypothesis to clinical evaluation, exemplifying the value of AI in urgent drug repositioning (57,58).

4.4 Insilico Medicine: Insilico Medicine leverages AI-based generative models for de novo drug design. Using deep learning and reinforcement learning, the company designs novel molecules with optimized pharmacological properties, such as high potency, selectivity, and reduced toxicity. Insilico has successfully produced candidate compounds for fibrosis, cancer, and neurodegenerative diseases. Its AI platform demonstrates how machine intelligence can create entirely new drug candidates, significantly reducing the time from target identification to preclinical testing (59,60).

5. Challenges and Limitations

While AI has shown significant potential in drug discovery, several challenges and limitations hinder its widespread adoption.

5.1 Data Quality and Availability: AI relies heavily on large, high-quality datasets for training. In drug discovery, relevant data such as molecular interactions, omics profiles, and clinical records are often incomplete, noisy, or inconsistent. Poor data quality can lead to inaccurate predictions and reduce model reliability. Moreover, proprietary data held by pharmaceutical companies limits access for academic research, creating gaps in model generalization (61,62).

5.2 Interpretability and the "Black-box" Problem: Many AI models, especially deep learning networks, function as "black boxes," making it difficult to understand how decisions are made. Regulatory authorities require transparency for clinical applications, and lack of interpretability can slow approval processes. Efforts are ongoing to develop explainable AI (XAI) approaches that balance predictive accuracy with interpretability (63).

5.3 Computational Cost: Training and deploying advanced AI models demands significant computational resources, including GPUs and cloud infrastructure. Smaller research labs or companies may face financial and technical constraints, limiting the scalability of AI-based solutions. Efficient algorithms and optimized hardware are needed to make AI accessible across the industry (64).

5.4 Ethical, Legal, and Regulatory Issues: The use of patient data in AI-driven research raises ethical and legal concerns. Ensuring data privacy, avoiding biases in training datasets, and complying with regulations like GDPR or FDA guidelines are major challenges. AI models must be validated rigorously to prevent harm, particularly in personalized medicine applications (65).

5.5 Generalization and Reproducibility: AI models trained on one dataset may not perform well on another due to differences in population, experimental conditions, or data collection methods. This limits the reproducibility and generalization of findings. Developing standardized protocols and cross-institutional collaborations is essential to overcome these limitations (66).

6. Future Prospects

Artificial Intelligence (AI) continues to evolve rapidly, offering promising avenues for the future of drug discovery and development. With increasing computational power and expanding biomedical datasets, AI is expected to further accelerate the design of safer and more effective therapeutics.

6.1 Integration with Quantum Computing: Quantum computing holds the potential to revolutionize drug design by solving complex molecular simulations that classical computers struggle with. Combining AI with quantum algorithms could enable accurate prediction of molecular interactions, conformational dynamics, and binding affinities, drastically reducing lead optimization time (67,68). This synergy may allow pharmaceutical companies to explore chemical space far beyond current capabilities.

6.2 Multi-omics and Personalized Medicine: Future AI applications are likely to leverage multi-omics data, integrating genomics, proteomics, metabolomics, and transcriptomics. This will enable highly personalized drug design tailored to individual patient profiles. AI-driven analysis of multi-omics datasets can predict disease progression, drug response, and adverse reactions, thus supporting precision medicine initiatives and optimizing therapeutic efficacy (69,70).

6.3 Accelerated Clinical Trials: AI is expected to play a critical role in transforming clinical trials. Predictive models can identify suitable patient cohorts, anticipate dropout risks, and simulate trial outcomes. Virtual clinical trials powered by AI may reduce trial duration, costs, and failures, while improving regulatory compliance and decision-making (71). Real-world data integration will further enhance trial design and patient stratification.

6.4 AI-Driven Combination Therapies: Emerging AI platforms aim to design rational combination therapies by analyzing synergistic drug interactions. AI can predict optimal drug pairs or combinations for complex diseases like cancer, autoimmune disorders, and infectious diseases. This approach can improve therapeutic outcomes, reduce side effects, and address resistance mechanisms more efficiently than traditional trial-and-error methods (72).

6.5 Expansion in Global Pharmaceutical Industry: The adoption of AI is expected to increase globally, with integration in both large pharmaceutical companies and start-ups. Cloud-based AI platforms and collaborative initiatives will democratize access to AI tools, enabling smaller research organizations to contribute to drug discovery. Additionally, AI may facilitate rapid responses to emerging health threats, as seen during the COVID-19 pandemic (73).

7. Conclusion: Artificial Intelligence (AI) has become a game-changer in drug discovery and development. Over the last decade, AI has streamlined traditional processes by enabling rapid target identification, virtual screening, lead optimization, ADMET prediction, and drug repurposing. With tools like deep learning, generative models, and big data analytics, researchers can now manage complex biological and chemical datasets, improving decision-making and accelerating the pipeline.Industry platforms such as AlphaFold, Atomwise, BenevolentAI, and Insilico Medicine showcase AI's success in protein structure prediction, novel molecule design, and faster drug development, as seen during the COVID-19 pandemic. AI also plays a vital role in precision medicine by predicting patient-specific drug responses and reducing adverse effects.However, challenges like data quality, interpretability, computational demands, and ethical issues remain. Addressing these through explainable AI, better data sharing, and regulatory frameworks is crucial.Looking ahead, combining AI with quantum computing, multi-omics, and clinical trial simulations will further speed up therapeutic development and global access. In conclusion, AI is now a central driver of pharmaceutical innovation, promising faster, safer, and more effective treatments**.**

REFERENCES

1. *DiMasi JA, Grabowski HG, Hansen RW. Innovation in the pharmaceutical industry: New estimates of R&D costs. J Health Econ. 2016;47:20-33. DOI: 10.1016/j.jhealeco.2016.01.012*
2. *Hay M, Thomas DW, Craighead JL, Economides C, Rosenthal J. Clinical development success rates for investigational drugs. Nat Biotechnol. 2014;32:40-51.DOI: 10.1038/nbt.2786*
3. *Esteva A, Robicquet A, Ramsundar B, et al. A guide to deep learning in healthcare. Nat Med. 2019;25:24-29. DOI: 10.1038/s41591-018-0316-z*
4. *Vamathevan J, et al. Applications of machine learning in drug discovery and development. Nat Rev Drug Discov. 2019;18:463-477.DOI: 10.1038/s41573-019-0024-5*
5. *Polishchuk PG, et al. Estimation of the size of drug-like chemical space. J Comput Aided Mol Des. 2013;27:675-679. DOI: 10.1007/s10822-013-9672-4*
6. *Mullard A. Machine learning brings drug discovery to the clinic. Nat Rev Drug Discov. 2021;20:92-94. DOI: 10.1038/d41573-020-00253-y*
7. *Chen H, Engkvist O, Wang Y, Olivecrona M, Blaschke T. The rise of deep learning in drug discovery. Drug Discov Today. 2018;23(6):1241-1250. DOI: 10.1016/j.drudis.2018.01.039*
8. *Reuters. Eli Lilly launches platform for AI-enabled drug discovery. 2025. (news article, no DOI)*
9. *Koçak H, et al. Bibliometric analysis of artificial intelligence in drug discovery. J Cheminform. 2025;17:45. DOI: 10.1186/s13321-025-00988-4*
10. *Paul D, Sanap G, Shenoy S, et al. Artificial intelligence in drug discovery and development. Drug Discov Today. 2020;25(10):1788-1801. DOI: 10.1016/j.drudis.2020.07.014*
11. *Dhudum A, et al. Artificial intelligence in drug discovery: challenges and opportunities. Front Pharmacol. 2024;15:1389002. DOI: 10.3389/fphar.2024.1389002*
12. *Bhat M, et al. Future of AI in personalized medicine. Biomed Pharmacother. 2025;174:116512. DOI: 10.1016/j.biopha.2025.116512*
13. *Mitchell TM. Machine learning applications in molecular biology. Annu Rev Biochem. 2020;89:487-510. DOI: 10.1146/annurev-biochem-062917-012756*
14. *Jiménez J, Skalic M, Martinez-Rosell G, De Fabritiis G. KDEEP: Protein–ligand binding prediction using deep convolutional neural networks. J Chem Inf Model. 2018;58(2):287-296.DOI: 10.1021/acs.jcim.7b00650*
15. *Sanchez-Lengeling B, Aspuru-Guzik A. Inverse molecular design using machine learning. Science. 2018;361(6400):360-365. DOI: 10.1126/science.aat2663*
16. *Gilmer J, Schoenholz SS, Riley PF, Vinyals O, Dahl GE. Neural message passing for quantum chemistry. ICML. 2017;70:1263-1272. DOI: 10.48550/arXiv.1704.01212*
17. *Owkin. MELLODDY: Machine learning ledger orchestration for drug discovery. 2020. (project description, no DOI)*
18. *Topol EJ. High-performance medicine: the convergence of human and artificial intelligence. Nat Med. 2019;25:44-56. DOI: 10.1038/s41591-018-0300-7*
19. *Reddy AS, Zhang S. Polypharmacology: drug discovery for the future. Nat Rev Drug Discov. 2013;12:58-71. DOI: 10.1038/nrd3853*
20. *Schneider G. Automating drug discovery. Nat Rev Drug Discov. 2018;17:97-113. DOI: 10.1038/nrd.2017.232*
21. *Collins FS, Varmus H. A new initiative on precision medicine. N Engl J Med. 2015;372:793-795. DOI: 10.1056/NEJMp150052*
22. *Chen H, Engkvist O, Wang Y, Olivecrona M, Blaschke T. The rise of deep learning in drug discovery. Drug Discov Today. 2018;23(6):1241-1250.*
23. *Vamathevan J, Clark D, Czodrowski P, et al. Applications of machine learning in drug discovery and development. Nat Rev Drug Discov. 2019;18(6):463-477.*
24. *DiMasi JA, Grabowski HG, Hansen RW. Innovation in the pharmaceutical industry: New estimates of R&D costs. J Health Econ. 2016;47:20-33.*

25. Stokes JM, Yang K, Swanson K, et al. A deep learning approach to antibiotic discovery. Cell. 2020;180(4):688-702.
26. Zhavoronkov A, Ivanenkov YA, Aliper A, et al. Deep learning enables rapid identification of potent DDR1 kinase inhibitors. Nat Biotechnol. 2019;37(9):1038-1040.
27. Ursu O, Holmes J, Knockel J, et al. DrugCentral 2021: drug discovery knowledge base. Nucleic Acids Res. 2021;49(D1):D1160-D1169.
28. Pushpakom S, Iorio F, Eyers PA, et al. Drug repurposing: progress, challenges and recommendations. Nat Rev Drug Discov. 2019;18(1):41-58.
29. Zhang Q, Muegge I. Scaffold hopping through virtual screening using 2D and 3D similarity descriptors: a case study with kinase inhibitors. J Med Chem. 2006;49(23):7221-7234.
30. Jiménez J, Skalic M, Martínez-Rosell G, De Fabritiis G. KDEEP: Protein–ligand absolute binding affinity prediction via 3D-convolutional neural networks. J Chem Inf Model. 2018;58(2):287-296.
31. Sanchez-Lengeling B, Aspuru-Guzik A. Inverse molecular design using machine learning: Generative models for matter engineering. Science. 2018;361(6400):360-365.
32. Wu Z, Pan S, Chen F, Long G, Zhang C, Yu PS. A comprehensive survey on graph neural networks. IEEE Trans Neural Netw Learn Syst. 2021;32(1):4-24.
33. Lee K, Kim D, Lee D. Building a drug–disease knowledge base by extracting information from biomedical literature. J Biomed Inform. 2017;68:63-72.
34. Melnikov A, Vovk V, Smirnov P, et al. Federated learning for drug discovery. Front Pharmacol. 2022;13:834556.
35. Schneider P, Walters WP, Plowright AT, et al. Rethinking drug design in the artificial intelligence era. Nat Rev Drug Discov. 2020;19(5):353-364.
36. Jumper J, Evans R, Pritzel A, et al. Highly accurate protein structure prediction with AlphaFold. Nature. 2021;596(7873):583-589.
37. Apweiler R, Bairoch A. The impact of AlphaFold and AI-driven research on structural biology and
38. Chen H, Engkvist O, Wang Y, Olivecrona M, Blaschke T. The rise of deep learning in drug discovery. Drug Discov Today. 2018;23(6):1241-1250.
39. Vamathevan J, Clark D, Czodrowski P, et al. Applications of machine learning in drug discovery and development. Nat Rev Drug Discov. 2019;18(6):463-477.
40. Zhavoronkov A, Ivanenkov YA, Aliper A, et al. Deep learning enables rapid identification of potent DDR1 kinase inhibitors. Nat Biotechnol. 2019;37(9):1038-1040.
41. Stokes JM, Yang K, Swanson K, et al. A deep learning approach to antibiotic discovery. Cell. 2020;180(4):688-702.
42. Sanchez-Lengeling B, Aspuru-Guzik A. Inverse molecular design using machine learning: Generative models for matter engineering. Science. 2018;361(6400):360-365.
43. Jiménez J, Skalic M, Martínez-Rosell G, De Fabritiis G. KDEEP: Protein–ligand absolute binding affinity prediction via 3D-convolutional neural networks. J Chem Inf Model. 2018;58(2):287-296.
44. Wu Z, Pan S, Chen F, Long G, Zhang C, Yu PS. A comprehensive survey on graph neural networks. IEEE Trans Neural Netw Learn Syst. 2021;32(1):4-24.
45. Ursu O, Holmes J, Knockel J, et al. DrugCentral 2021: drug discovery knowledge base. Nucleic Acids Res. 2021;49(D1):D1160-D1169.
46. Pushpakom S, Iorio F, Eyers PA, et al. Drug repurposing: progress, challenges and recommendations. Nat Rev Drug Discov. 2019;18(1):41-58.
47. BenevolentAI. AI-powered drug repurposing for COVID-19. BenevolentAI Reports. 2020.
48. Lee K, Kim D, Lee D. Building a drug–disease knowledge base by extracting information from biomedical literature. J Biomed Inform. 2017;68:63-72.
49. Jiménez-Luna J, Grisoni F, Schneider G. Drug discovery with explainable AI. Nat Mach Intell. 2020;2:573-584.
50. Jumper J, Evans R, Pritzel A, et al. Highly accurate protein structure prediction with AlphaFold. Nature. 2021;596(7873):583-589.
51. Tunyasuvunakool K, Adler J, Wu Z, et al. AlphaFold predicts the human proteome. Nature. 2021;596(7873):590-596.
52. Apweiler R, Bairoch A. The impact of AlphaFold and AI-driven research on structural biology and drug discovery. FEBS Lett. 2024;598(15):2132-2144.
53. Jumper J, Evans R, Pritzel A, et al. Highly accurate protein structure prediction with AlphaFold. Nature. 2021;596(7873):583-589.
54. Tunyasuvunakool K, Adler J, Wu Z, et al. AlphaFold predicts the human proteome. Nature. 2021;596(7873):590-596.
55. Wallach I, Dzamba M, Heifets A. AtomNet: A deep convolutional neural network for bioactivity prediction in structure-based drug discovery. arXiv preprint arXiv:1510.02855. 2015.
56. Vamathevan J, Clark D, Czodrowski P, et al. Applications of machine learning in drug discovery and development. Nat Rev Drug Discov. 2019;18(6):463-477.
57. BenevolentAI Reports. AI-powered drug repurposing for COVID-19. 2020.
58. Richardson P, Griffin I, Tucker C, et al. Baricitinib as potential treatment for COVID-19 acute respiratory disease. Lancet. 2020;395:939-943.
59. Zhavoronkov A, Ivanenkov YA, Aliper A, et al. Deep learning enables rapid identification of potent DDR1 kinase inhibitors. Nat Biotechnol. 2019;37(9):1038-1040.
60. Insilico Medicine. AI-driven generative models for drug discovery. Insilico Reports. 2020.
61. Vamathevan J, Clark D, Czodrowski P, et al. Applications of machine learning in drug discovery and development. Nat Rev Drug Discov. 2019;18(6):463-477.
62. Chen H, Engkvist O, Wang Y, et al. The rise of deep learning in drug discovery. Drug Discov Today. 2018;23(6):1241-1250.
63. Jiménez-Luna J, Grisoni F, Schneider G. Drug discovery with explainable AI. Nat Mach Intell. 2020;2:573-584.

64. *Wu Z, Pan S, Chen F, et al. A comprehensive survey on graph neural networks. IEEE Trans Neural Netw Learn Syst. 2021;32(1):4-24.*
65. *Liu X, Faes L, Kale AU, et al. A comparison of deep learning performance against health-care professionals in detecting diseases from medical imaging: a systematic review and meta-analysis. Lancet Digital Health. 2019;1(6):e271–e297.*
66. *Pushpakom S, Iorio F, Eyers PA, et al. Drug repurposing: progress, challenges and recommendations. Nat Rev Drug Discov. 2019;18(1):41-58.*
67. *Cao Y, Romero J, Olson JK, Degroote M, Johnson PW, Kieferová M, et al. Quantum chemistry in the age of quantum computing. Chem Rev. 2019;119(19):10856-10915.*
68. *Biamonte J, Wittek P, Pancotti N, Rebentrost P, Wiebe N, Lloyd S. Quantum machine learning. Nature. 2017;549:195-202.*
69. *Li X, Li Q, Cheng S, et al. Multi-omics integration in precision medicine: applications and challenges. Brief Bioinform. 2021;22(6):bbab298.*
70. *Subramanian I, Verma S, Kumar S, et al. Multi-omics data integration, interpretation, and its application. Bioinformatics. 2020;36(7):2343–2350.*
71. *He Z, Xie L, Li J, et al. Artificial intelligence in clinical trials: opportunities and challenges. Contemp Clin Trials. 2021;109:106537.*
72. *Preuer K, Lewis R, Hochreiter S, et al. DeepSynergy: predicting anti-cancer drug synergy with deep learning. Bioinformatics. 2018;34(9):1538–1546.*
73. *Zhavoronkov A, Vanhaelen Q, O'Reilly T. Artificial intelligence for drug discovery, biomarker development, and generation of novel chemistry. Mol Pharm. 2019;16(6):2291–2302.*