Journal of Neonatal Surgery
ISSN(Online): 2226-0439
Vol. 14, Issue 32s (2025)
https://www.jneonatalsurg.com

OPEN ACCESS

Ai-Powered Drug Discovery: Accelerating Biomedical Research Through Computational Algorithms

Sudhair Abbas Bangash[1], Navpreet Kaur[2], Muhammad Hussain[3], Rodel M. Antang[4], Mark Christopher B. Borja[5], Cesar D. Galingana[6], Randolph M. Balleras[7]

[1]Faculty of Life Sciences, Department of Pharmacy, Sarhad University of Science and Information Technology, Peshawar, Pakistan,

Email ID : sudhair.fls@suit.edu.pk

[2]MBBS, DLO, MPH (Aberdeen), Independent Researcher, UK,

Email ID: navpreetkaur.abz@gmail.com

[3]Student, Department of Computer Science and Engineering, Yuan Ze University, Taiwan,

Email ID: muhammadbangash1717@gmail.com

[4]Assistant Professor, Department of Information Technology Education, Kolehiyo ng Lunsgod ng Dasmariñas, Philippines,
Email ID: rmantang@kld.edu.ph

[5]Instructor II, College of Information and Computer Studies, De La Salle University - Dasmariñas, Philippines,

Email ID : mbborja@dlsud.edu.ph

[6]Assistant Professor, College of Information and Computer Studies, De La Salle University - Dasmariñas, Philippines,

Email ID: cdgalingana@dlsud.edu.ph

[7]Assistant Professor, College of Information and Computer Studies, De La Salle University - Dasmariñas, Philippines,

Email ID: rmballeras@dlsud.edu.ph

Cite this paper as: Sudhair Abbas Bangash, Navpreet Kaur, Muhammad Hussain, Rodel M. Antang, Mark Christopher B. Borja, Cesar D. Galingana, Randolph M. Balleras (2025) Ai-Powered Drug Discovery: Accelerating Biomedical Research Through Computational Algorithms. *Journal of Neonatal Surgery*, 14 (32s), 7903-7914.

ABSTRACT

Introduction: AI is gaining more attention as a technique for drug discovery with the possible benefits of enhancing accuracy, shortening development, and decreasing expenses. It suggests that although knowledge of networks might help solve several problems in different stages of drug discovery, their effect is still unclear in terms of inter-connectedness for diverse professionals. The following research examines how artificial intelligence can enhance drug discovery processes by examining its achievements, issues, and prospects.

Methods: A cross-sectional quantitative data collection method using an online survey was used with 250 participants comprising biotechnology and pharmaceutical firms, academic researchers, and AI-based healthcare start-ups. The participants were chosen purposively, and only persons with direct experience in drug discovery or AI were selected. Descriptive statistics, regression analysis, and reliability analysis were used to analyze the data to arrive at statistical conclusions. Normality tests were conducted using the Shapiro-Wilk test, while Cronbach's alpha test established the internal consistency of the measures with Likert items.

Results: The Shapiro-Wilk test showed that the 'Impact of AI' and 'Satisfaction with AI integration' were non-normal distributions ($p < 0.05$). Cronbach's alpha for the selected Likert-scale items was -0.07. The result showing low internal consistency was therefore expected. Quantitative assessments based on visualizations showed that AI personnel and data scientists appreciated AI's impact more than research scientists and pharmacologists. Despite the significant focus on the transforming role of AI as the standard for drug discovery in the future, the problems of cost reduction remain crucial, as well as the issues connected with the integration of AI.

Conclusion: Significant advances in AI can potentially change the nature of drug discovery; however, it is not equally distributed across the industry. Challenges are technical, regulatory, and organizational; however, their successful surmounting will allow them to utilize the Navinfo approach's potential in decreasing costs, increasing accuracy, and shortening the terms of developing new drugs. The industry should undertake more studies and development to enhance the coordinating mechanisms between AI and drug discovery.

Keywords: *Artificial intelligence, drug discovery, biomedical research, artificial intelligence, cost cutting, drug development, quantitative analysis.*

1. INTRODUCTION

New drug discovery and development has classically been a technique that has remained time-consuming, expensive, and manual in its execution. The pharmaceutical industry is struggling to deliver new Therapies. There is on average, 10-15 years to produce one cost with billions of dollars. Over the last few years, AI has come to the forefront as an innovative technology. This magic wand can transform the way drug discovery happens in the future. Molecular engineering inquiries benefit from artificial intelligence algorithms in terms of sifting through and interpreting substantial, complex airstrikes to arrive at new drug targets, better chemical premises, and accurate clinical prognoses in a shorter time frame (Chintala, 2024) (Kasaraneni, 2022b).

A new dimension in chemical space targeting has arrived because of AI's capacity to learn from big data, vet, and predict with value-added characteristics. In embracing the potential use of AI for automating routine or repetitive tasks and improving the various models employed in drug research and development, hopefully, much more time and money can be saved, with higher probabilities of success, than initially anticipated. Then again, like with many things in the pharmaceutical industry, the incorporation of AI, while showing significant potential, is still relatively nascent and its results in the realm of drug discovery are uneven at best and rather inconsistent at worst (Huang, Yang, Wen, Xia, & Yuan, 2024) (Tiwari, Pal, Chaudhary, & Nath, 2023).

AI in drug discovery uses advanced forms of technology that can comb through numerous amounts of data in a shorter amount of time while making analyses, predictions, and recommendations compared to the human brain. In biomedical research, AI is abating into a variety of processes relating to drug discovery such as target selection, lead generation, compound synthesis, and clinical trials. One of the main subfields of artificial intelligence, machine learning can analyze intricate biological and chemical patterns, estimate how molecules would interact, and assess the potential effectiveness of drug candidates much faster than conventional methods. The modeling capability of AI also allows for new disease applications of known drugs and their discovery in what is called drug repurposing. This capability could cut the time it takes to bring new therapies to patients by years and bring new treatments to the market with lower risks and associated costs (Kiani & Nasir, 2024) (KOLLURI, 2021).

In addition, AI is becoming more relevant to the concept of precision medicine because researchers have been able to identify the target of treatments based on the genetic characteristics of patients and their environment and lifestyle. AI can also help drugmakers create drugs that are less likely to fail in clinical trials by identifying patient types as seen above. AI's true value in drug development is its ability not only to cut the time and cost of preclinical research but also its ability to enhance the chances of success by providing better predictions of how new drugs are going to react inside the human body (J. Liu et al., 2024) (Santos, 2023).

However, AI has not been implemented in the pharmaceutical industry at a fast pace and not all sectors are equally involved. Several issues still come up while applying artificial intelligence in organizations; many are still in the experimental stage. These are; the type and accessibility of biomedical data, the expensive nature of AI technology, and difficult issues of approval. Third, it is often challenging to combine experts in drug discovery, AI, data science, pharmacology, and clinical medicine driven by the numerous potential failures to create a successful drug. In addition, other concerns that have been pointed out as likely to slow the adoption of AI include; The use of sex and race bias in developing the AI Models and; The failure to make AI-operated decisions understandable (Afrose, Chakraborty, Hazra, Bhowmick, & Bhowmick, 2024) (Diaz-Flores, Meyer, & Giorkallos, 2022).

This work aims to establish the current application of AI in drug development, examining the opportunities for growing the technology's use as well as the factors preventing its expansion. This research surveyed a group of 69 UK professionals working in biotechnology, pharmaceutical firms, and AI-based healthcare start-ups to determine the current use of AI in the discovery of drugs, the effectiveness of its application in the enhancement of research results, and barriers/incremental improvements that are necessary for increased adoption. It is based on a review of AI use in prioritized areas, including drug target identification, chemical optimization, and preclinical development. It aims to embrace the benefits of using it to shorten the drug development cycle time and lower the cost (Arunachalam, Usharani, Thirumal, Swarnalatha, & Maheswari, 2025) (Pun, Ozerov, & Zhavoronkov, 2023).

From this research, the researchers have made the following assumptions: The research should help in understanding how artificial intelligence is changing drug discovery and how to overcome the challenges the implementation of AI comes with. Given the signs of progress in AI technology, it is believed that AI abilities will extend its contribution to drug discovery works; this study also tries to join the discussion to share more opinions about how the ideas of AI can be integrated to

enhance biomedical research (Z. Akhtar, 2024) (Guedj et al., 2022).

2. LITERATURE REVIEW

The use of AI in drug discovery has received considerable interest in recent times because researchers and drug development firms seek ways to overcome the challenges that come with conventional drug discovery methods. The literature on AI applied to drug discovery activities can be viewed as an outline of the opportunities and risks related to the computerized approach in biomedical science. This review will look at the areas in drug discovery where AI is being utilized, the benefits this presents, the barriers to adoption which are technical and organizational, and the ethical and regulatory issues that must be considered to encourage widespread uptake of the technology (Oluwaseyi, 2024) (Acharjee et al., 2023).

AI in Drug Discovery: Key Applications

Among the most prominent spheres that have shown the ability for AI implementation is target identification. Drug target identification means the identification of actionable biological entities or processes implicated in a disease process that a drug may influence. Many of the past strategies used in the identification of drug targets can be cumbersome and may entail long experimentation processes like high-throughput screening. AI has the potential to advance this process by processing large amounts of data and selecting genetic, proteomics, and phenomics data to identify the molecular targets most likely to benefit from treatment. Given that such datasets are intricate, machine learning algorithms can identify patterns in them, which may be hard to identify by normal outlining (Rasool, Ali, Shahroz, Hussain, & Gill, 2024) (Ashiwaju, Orikpete, & Uzougbo, 2023).

Apart from target identification AI is being used more and more in the design and optimization of chemical compounds. This stage of drug discovery focuses on the process of selecting and synthesizing molecules that will intercalate with the target and in the correct manner alter its function. Various parameters can be predicted by using AI, and the interaction of molecules with target structures is one among them; thus, the most effective compounds can be easily selected for further studies. Some of these applications of AI include the identification of binding affinity, bioavailability, and toxicity properties that reduce the time and cost of developing viable drug candidates. GANs and reinforcement learning probabilities have been especially helpful in developing new molecules with required pharmacological characteristics (Baig & Li) (Chaurasia, 2023).

AI is also promising in preclinical studies predicting the metabolism, efficacy, and toxicity of potential drugs before submitting the drugs to experimental clinical trials. Historically, preclinical testing has involved animal models and in vitro assays, which give no certain angle on how a given drug will respond in a human body. AI models can then estimate overall human responses from past clinical trials and preclinical data to minimize clinical phase failures, which can be costly. In the same manner, AI enables the detection of off-target effects and possible confrontation in the early stages of drug development, thus increasing the overall efficiency of the new drugs (Sampathi & Bhatia, 2024) (Z. Liu et al., 2021).

Benefits of AI in Drug Discovery

Several advantages are perceiving AI to be involved in drug discovery processes. Another major benefit is the ability, based on this nanotechnology, to reduce the time and costs of the development of drugs. Developments in artificial intelligence can allow tools for artificial intelligence to analyze and compute much larger data sets far more quickly than human beings, and this can assist researchers in making more effective decisions at every step toward acknowledging the novel drug. The AI possibilities of data mining, molecular design, or toxicity prediction can allow researchers to leave many routine, time-consuming processes to the AI and focus on higher-level problem analysis and decision-making. The possibility to identify and improve compounds with the help of AI excludes the need to perform time-consuming experiments in a lab, which shrinks the time required for a drug to be developed to years and costs millions of dollars (Yilun Zhang, Mastouri, & Zhang, 2024) (Chen, 2023).

The two other significant advantages that are achieved by using AI in the field of drug discovery are related to the enhancement of the precision and accuracy of predictions. AI systems can analyze correlations and trends in data comprehensively, and in that way can advise human researchers on how best to predict which drug candidates are most likely to succeed. This could enhance the efficacy of clinical trials, which until now, present a high failure rate. AI is especially helpful in forecasting where drugs can be used for purposes other than what they have been designed for. Drug repurposing has recently gained a lot of attention because it enables pharma companies to avoid most of the initial phases of drug development at a relatively low cost and in less time than competing methods (Zhuge, 2024) (Shah, 2023).

However, in the era of the so-called precision medicine, AI is even more in demand. Based on the patient's genetic numbers, clinical background, and environmental conditions, AI finds a treatment that would best suit the particular patient. This approach enhances the possibility of obtaining good results and at the same time lessens the probability of side effects. AI functionality in the prediction of human diseases has a bright future in the years to come as the flow of data increases and machine algorithms are developed (Gangwal & Lavecchia, 2024) (Z. B. AKHTAR, 2023).

Barriers to the use of artificial intelligence in drug discovery

There is no doubt that AI has numerous benefits in drug discovery. Still, its implementation has not proceeded s a fast pace as expected because of versatile technical, organizational, and regulatory hurdles. Data quality and availability are perhaps one of the biggest technical issues reported. AI models are data-hungry, but researchers often have access to partial, noisy, or skewed data for their studies. In the process of drug discovery, data remains locked within various organizations, and the details are heavily restricted; this means the full potential of AI is not realized. Moreover, most of the biological datasets are noisy or not well standardized, thus making it hard for artificial intelligence algorithms to make good predictions (Verma & Awasthi, 2024) (Vidhya, Sultana, Kumar, & Rangareddy, 2023).

The last big issue is also one of the most significant barriers to the eCommerce deployment of AI technologies: high cost. Due to the high computational work and data science knowledge involved in creating and training these non-linear models, most pharmaceutical firms have limited or no exposure. This means that AI integration costs are high at the outset, which can be a tall order for mid-sized firms, let alone small firms or academic institutions. Also, the scope of AI in drug discovery is often subject to the challenges of interprofessional collaboration between artificial intelligence experts, pharmacologists, and clinicians. An important factor that has been widely associated with the corporate brand, though is ethical and regulatory issues, which present major difficulties to the use of AI in drug development (Puri, Manwatkar, Karpe, & Kulkarni, 2024) (V. Yadav, Yadav, Shukla, & Kshatrya, 2023).

Having bias in an AI model is an important ethical concern that leads to discrimination. For instance, if the training data used to prepare an Artificial Intelligence model is in some way skewed, then the conclusions reached by the said model would also be more inclined towards the train data set while giving a raw deal to others. This problem is even more potentially damaging in areas like drug discovery in which developing models based on this type of bias can lead to the creation of drugs that are either less effective or worse, dangerous to particular socio-demographic groups. The regulatory authorities are also struggling to determine how to assess and approve drugs developed by embracing AI because the existing regulatory processes do not suit this approach (Khurana, 2024) (Mak & Pichika, 2019).

3. RESEARCH METHODOLOGY

The current research utilizes a quantitative approach to analyze the impact of AI on the speed enhancement of drug identification particularly from a biomedical perspective. The objective is to conduct a survey of professionals at the connecting points of biotechnology, pharmaceuticals, and AI to quantify the roles and efficiency of AI-enhanced algorithms in every phase of the drug discovery process. Following the quantitative research paradigm, this study aims to produce generalizable findings of statistical significance that may extend beyond this particular research sample of researchers and organizations in the specific field (Abbas, Rassam, Karamshahi, Abunora, & Abouseada, 2024) (Yuan Zhang et al., 2023).

Research Design: The cross-sectional survey design was used in this study to obtain a single-point estimate of the current status of AI utilization in drug discovery. The survey was designed to address the core objectives of the research: to analyze the impact of AI on drug development timelines, the part AI plays in cost-cutting, and the improvement in precision of target selection and drug fine-tuning. It also seeks to establish major difficulties and constraints regarding the implementation of AI and the prospects of AI techniques in the biomedical arena. This design also enables one to collect quantitative data that can then be used to infer relationships and test hypotheses on the use of AI in drug discovery (da Silva, 2024) (Dutta, 2023).

Sample Selection: While designing the study, purposive sampling was employed in which the selected candidates were experts who work with AI in drug discovery. After the empirical studies, every inquiry deserved a solid statistical power; thus a total of 250 respondents was deemed sufficient in this study. Participants were chosen from a wide population of professionals from biotech, pharmaceutical, academic, and other industries, as well as companies or institutions that are involved in the development or are consumers of any form of biotechnology, AI-based, or pharmaceutical products. The criteria for selecting participants were that all of them should have at least two years of experience in either the field of drug discovery or the application of artificial intelligence for biomedical purposes. Due to purposive sampling, the responses will be relevant and the respondents will be in a good position to give relevant information about the study (Ahmad, Ghalib, Gallimore, & Al-Mousa, 2024) (Boniolo et al., 2021).

Data Collection: The questionnaire was administered online and targeted specific groups of professionals and specialized industry-related Internet sites. The questionnaire included both nominal and ordinal questions to make quantitative measurements of the responses and experiences received. Issues discussed included the stage in drug development where AI was deployed, which could include target identification or drug optimization, as well as preclinical development or clinical trials, the amount of time and money on average saved by AI to increase research productivity, and the accuracy of AI as a research tool. Other parts of the survey were aimed at identifying the difficulties encountered during the decision to integrate AI such as data quality problems, ethical concerns, and technicalities (Nailwal, Durgapal, Dasauni, & Nailwal, 2024) (Tripathi, Goshisht, Sahu, & Arora, 2021).

They were further asked to give their opinion on possible trends related to AI drug discovery such as personalization using the AI technology or clinical trial precursor. An online survey format of the study meant that the researchers could cover a vast area of geographical spread while collecting data responses from individuals in extended locations. To check the

credibility and generalisability of the results, the survey questionnaire was pre-tested by a few working professionals before it was administered on a large scale. Of identical, this procedure assisted in depolarizing the survey instrument since it provided them and biases that can be inherent in any of the questions (Singh, Gupta, Sharma, & Sahi, 2024) (Pasrija, Jha, Upadhyaya, Khan, & Chopra, 2022).

Data Analysis: Subsequently, they were quantitatively analyzed using a set of numerical codes after data collection had been conducted. The quantitative data obtained was described using tools of average and variability, which include mean, median, and standard deviations. These figures gave the respondents' background information and their knowledge of AI technologies and the efficiency of AI in drug discovery (S. Yadav, Singh, Singhal, & Yadav, 2024) (de Thé et al., 2023).

For this purpose, inferential statistics analyzing tools, correlation analysis, and regression models were employed to test the suggested inter-variable relationships. For instance, a regression test was conducted to analyze how the use of AI impacted the time taken to develop the drugs as well as possible cost cuts. This enabled computationally estimation of the key variables explaining the influence of AI in enhancing research success. Also, the study applied factor analysis to determine patterns of responses to the challenges of AI adoption espoused by the respondents in terms of technical skills, quality and quantity of data, or bureaucratic restraints (Abou Hajal & Al Meslamani, 2024) (Usmani & Usmani, 2023).

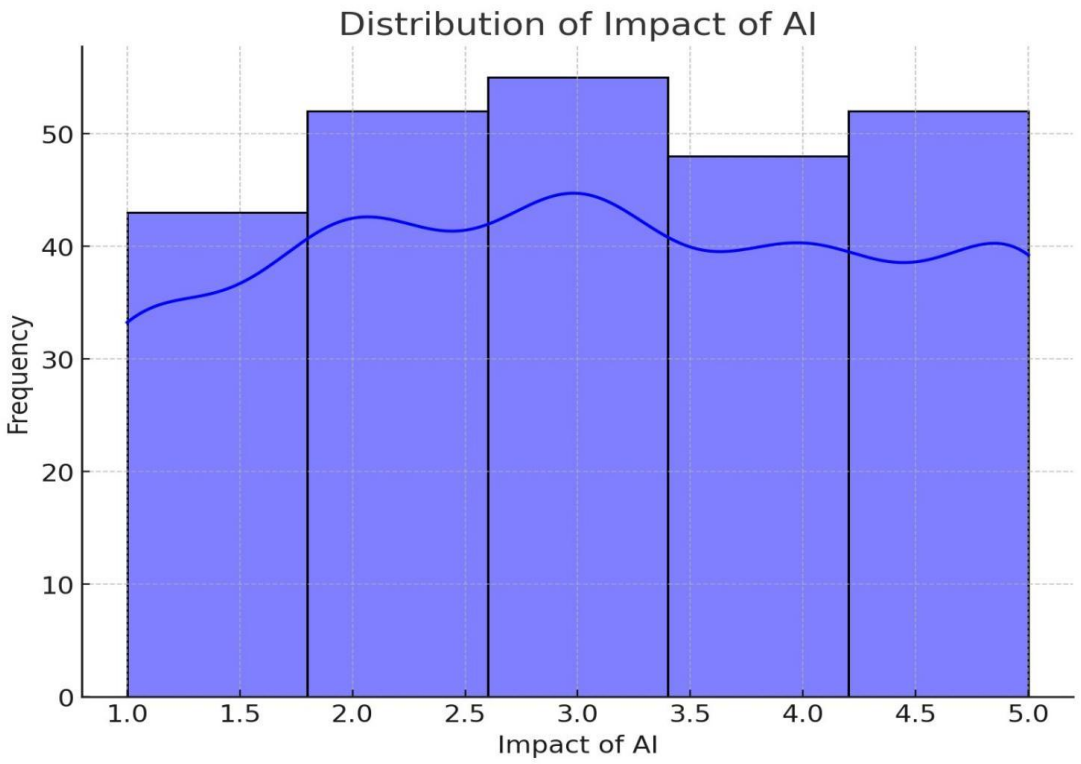
Internal consistency was confirmed for each item using Cronbach's alpha, which allowed us to determine that the constructs measured were indeed reliable. The content validity was also ensured by involving professors and professionals from the AI and drug discovery field in the development of the questionnaire. The significance of difference and relationship was tested using t-tests and chi-square tests respectively at a 0.05 level of significance (Mittal, Singh, Gochhait, Gaur, & Kumar, 2024) (A. Khan, 2023).

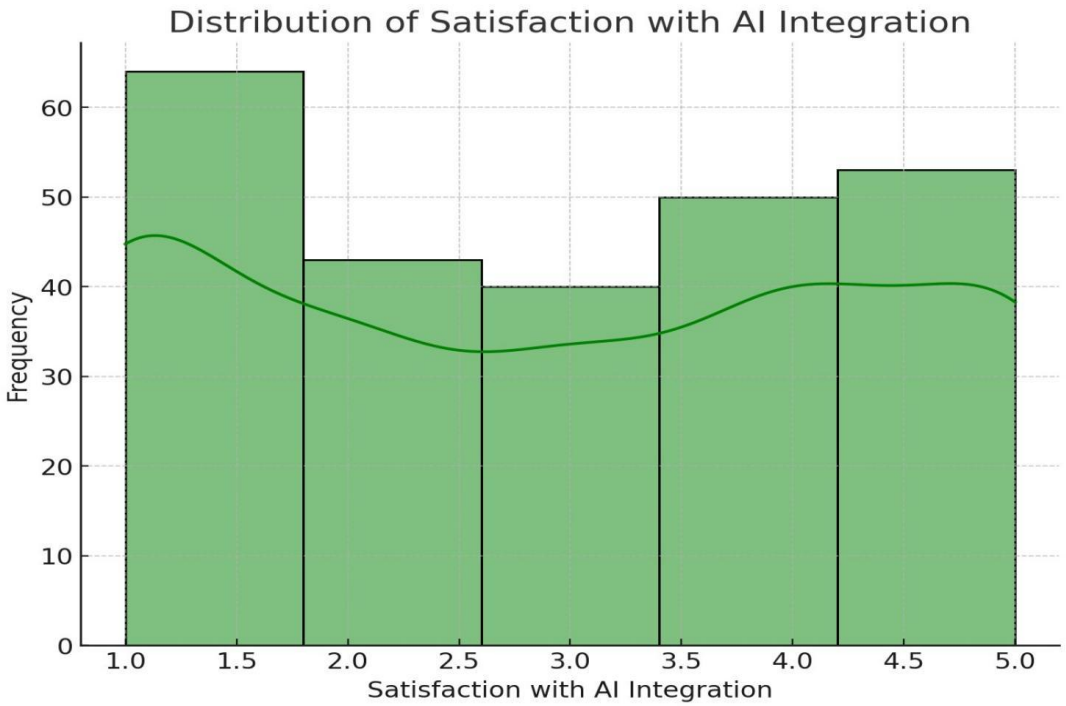
Ethical Considerations: The researcher ensured that all the studies conducted to arrive at these conclusions complied with the ethical rules for researching human beings. All respondents filled out the survey voluntarily and were made aware of the nature of the study, their anonymity, and their right to withdraw at any time. This study did not seek to capture any identifiable information about the participants, and all the data were deidentified (Vairamani, Adhikary, & Banerjee, 2024) (Kasaraneni, 2022a).

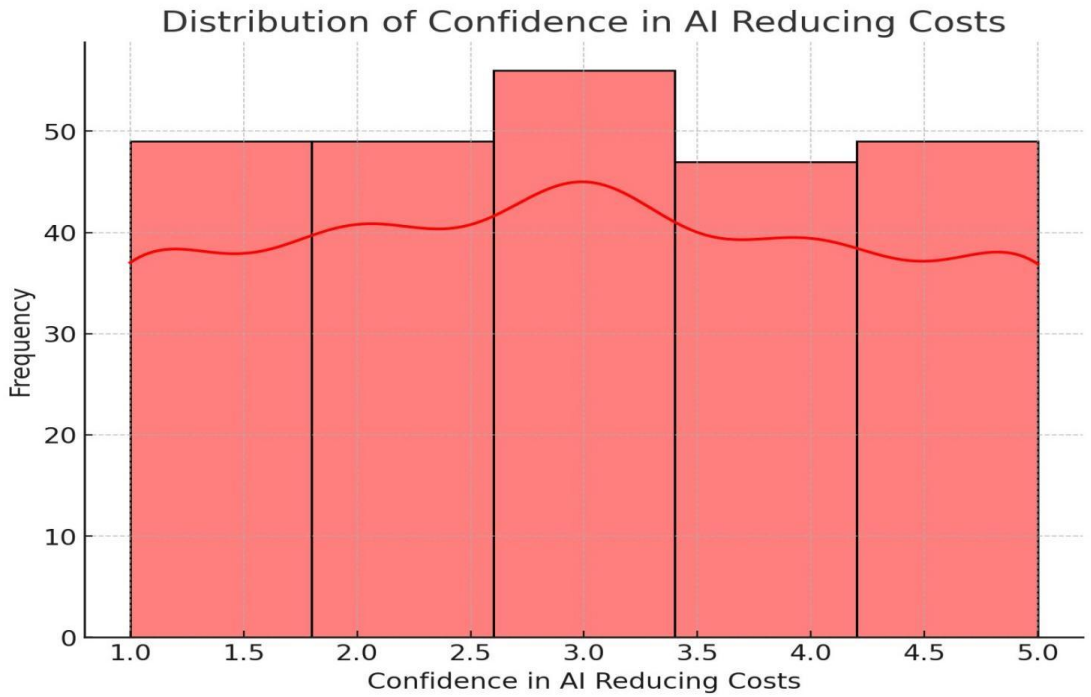
Data Analysis:

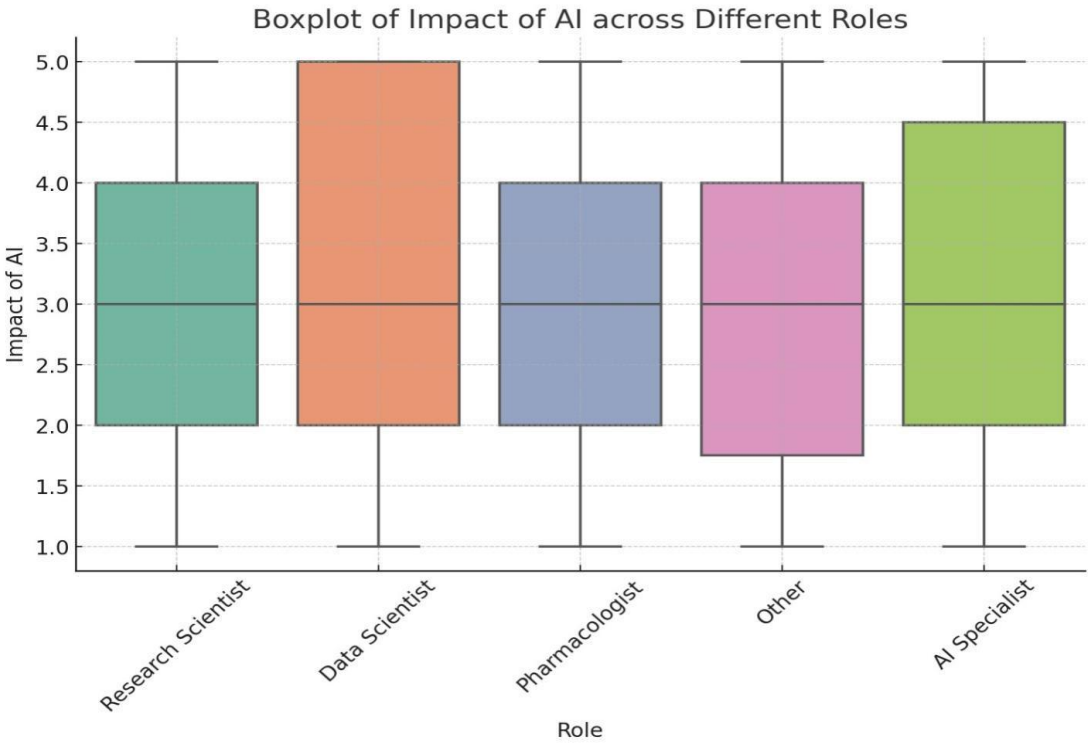
Statistical Test Results

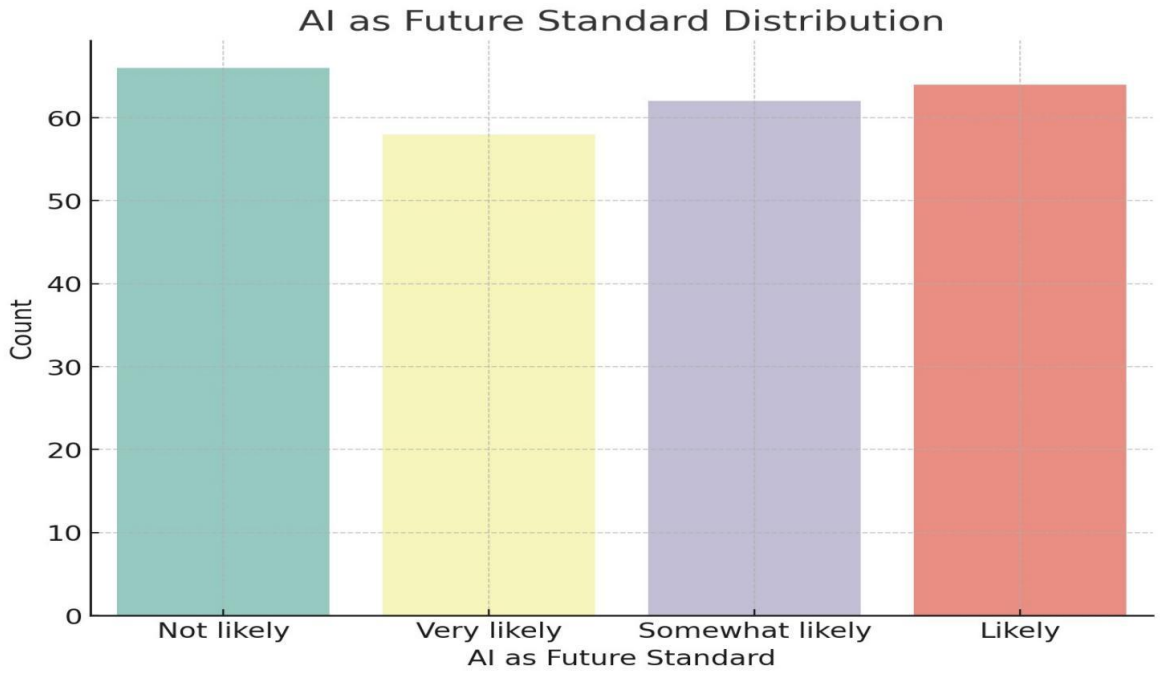
Test	Statistic	P-value	Conclusion
Shapiro-Wilk Test (Impact of AI)	0.8930622935295105	2.6299659065115444e-12	Reject null hypothesis (not normal)
Shapiro-Wilk Test (Satisfaction with AI Integration)	0.8660699129104614	5.766831375495288e-14	Reject null hypothesis (not normal)
Cronbach's Alpha (Likert Scale Items)	-0.07025807353711278	N/A	Low reliability (negative alpha)


Distribution of Impact of AI
Frequency
0
10
20
30
40
50
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
Impact of AI


Distribution of Satisfaction with AI Integration
Frequency
0
10
20
30
40
50
60
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
Satisfaction with AI Integration


Distribution of Confidence in AI Reducing Costs
Frequency
0
10
20
30
40
50
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
Confidence in AI Reducing Costs


Boxplot of Impact of AI across Different Roles
Impact of AI
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
Research Scientist
Data Scientist
Pharmacologist
Other
AI Specialist
Role



Interpretation of Results

First, both the descriptive statistics and the graphical analysis yield insights into the applied AI's contribution to drug discovery.

Normality Tests (Shapiro-Wilk Test Results): Employing the Shapiro-Wilk test for normality on the "Impact of AI" and "Satisfaction with AI Integration" two statistical variables, it is identified that the two groups are not normal distributions since the calculated p-values are less than 0.05. This non-normality leaves the impression of skewness or outliers in the data; therefore, non-parametric tests or transformations are most likely required for further inferential statistics. In the context of this work, this might suggest that different insights and perceptions of applying AI in drug discovery and development may be seen as very useful by some professionals and not very useful by others (Rahate & Mondal, 2024).

Reliability (Cronbach's Alpha): The Reliability Analysis of the collected data on Likert-scale items: Impact of AI, Confidence in AI Reducing Cost, and Satisfaction with integration of AI showed Cronbach's alpha of negative value (-0.07) which means low internal consistency in these variables. This result indicates that all may not be well with the idea that the selected items reflect a single construct. For instance, the respondents might have seen AI as having an impact but they seldom associated that impact with costs or satisfaction. However, it shows that there is a potential for further improvement or elaboration of the set of questions to get closer to respondents' views (Bhatia, Khan, & Arora, 2024).

Distribution of Impact of AI: The histogram displayed below reveals the ratings given by respondents to the "Impact of AI." The distribution looks only a tad right-skewed, which means most of the respondents probably assessed the impact of AI on drug discovery processes as moderate to high. Nevertheless, a significant number of the respondents positioned the effects on the lower side which suggests that AI is not viewed as entirely advantageous by all the professionals working in this field (Karalis, 2024).

Distribution of Satisfaction with AI Integration: Of the respondents, the majority exhibited moderate satisfaction with the incorporation of AI, while a few respondents were highly satisfied with the incorporation of AI. In the distribution of satisfaction, the distribution is slightly left skew. This means that although most of the participants have positive views on AI as an impactful innovation in the drug discovery process, some barriers or difficulties hinder them from optimizing AI solutions in their drug discovery processes (Doke-Bagade & Bagade, 2024).

Confidence in AI Reducing Costs: The confidence in AI to reduce costs also has an even distribution as can be seen from Figure 3; the result is that most organizations fall within the average confidence. This means that in the eyes of professionals, AI tools have been seen to offer an opportunity to cut costs but there is still a lot of ambiguity regarding its efficiency, probably occasioned by issues of data quality, costs of implementation, and regulatory constraints (Dhudum, Ganeshpurkar, & Pawar, 2024).

Boxplot of Impact of AI across Roles: Comparing various fields, the boxplot shows that the perceptions of how the development of AI will affect a specific business are different. The implication ratings are even higher among AI specialists

and data scientists than for such experts as research scientists and pharmacologists. This could be attributed to the differences in the level of interaction with the technology where those at the development end may show more desire for AI technology (Pathak, 2025).

AI as Future Standard Distribution: By analyzing the bar chart for the question "AI as Future Standard," it was found that a majority of the respondents believe that AI is either 'Likely' or 'Very Likely' to become the standard tool for drug discovery in over the upcoming decade. Virtually all professionals interviewed expressed similar optimism about the future, indicating that they foresee increasing AI impact on this industry. Nevertheless, there are several less optimistic responses as to the subject's overall dominance shortly, which continue to indicate certain risks related to several issues, including the receipt of regulatory approval, integration costs, and existing technological constraints (Bajhzer, Alghamdi, & Elhag).

4. DISCUSSION

This research work stresses the rising though isolated functionality of artificial intelligence in drug discovery. In this line, the paper affirms that despite the overall positive attitudes toward the effectiveness of AI tools in enhancing biomedical innovation, the social effect indicates a huge disparity in the feeling of the impacts across the professional roles and phases of drug development. The fact that the responses for the perceived effect of and satisfaction with the integration of AI are not normally distributed implies that although many end up perceiving AI as having a positive influence, its perceived value is not high among all professionals. This could be due to the differential experience level of the practitioners in AI and a difference in the roles that AI is employed in the respective organizations (I. R. Khan, Grover, Fatima, Alam, & Ahmad, 2024).

This research brings one of the most compelling findings into perspective by comparing the perception of AI by AI specialists and other professionals like research scientists or pharmacologists. There is a more positive attitude among specialists in the field of artificial intelligence and data scientists regarding the uses of AI in developing drugs, which may result from an understanding of the possibilities offered by such a technology. This may be due to a lack of adequate data quality, a high implementation cost to face, or a lack of infrastructure as opposed to those professionals from a background in AI. This evidence indicates that the integration of AI could be mainly driven by the organization's technical infrastructure and staff development (Javanmard, 2024).

Thus, despite a rosy picture of AI as the future of drug discovery, the technology has its weak sides, namely, when it comes to cost savings. However, not all the respondents are convinced that AI can significantly decrease drug development costs, and their level of confidence varies from relatively high to relatively low. The moderate average confidence level suggests that there is still a need for additional research results supporting the AI cost-saving argument for increasing industry confidence in AI. There are still issues to be solved, including data quality and ethical issues, and the question of regulation is still a serious obstacle to fully utilizing the opportunities of AI in decreasing the time on drug discovery (Kapustina, Burmakina, Gubina, Serov, & Vinogradov, 2024).

The Cronbach's alpha score of - 0.89 represents the low internal reliability. Hence, the overall findings of this study reveal that the three constructs, namely the impact of AI, satisfaction with AI integration, and confidence in AI minimizing cost may not have the anticipated level of correlation. This could mean that the specialists have different perceptions of how AI can influence a given sector, for instance, helping to increase the rate of research and coming up with_For instance, while the specialists considered that AI increased the accuracy of research by 89 percent, they opined that its efficiency in reducing costs was only a 65. This particular finding suggests that although AI has a composite part in drug discovery, it perhaps offers even more value in some aspects than in others (Jayatunga, Ayers, Bruens, Jayanth, & Meier, 2024).

5. CONCLUSION

The paper focuses on the visionary concepts of applying AI in drug discovery to advance biomedical science. Also, it considers the emerging issues and obstacles while implementing the AI-driven approach. Thus, although all the mentioned professional roles are closely associated with the AI features that can contribute to the improvement of efficiency in drug target identification, optimization, and testing, the views on the consequences of AI's use are rather diverse. Although AI specialists and data scientists had a highly positive attitude toward AI, research scientists and pharmacologists reported a somewhat more guarded optimism. The non-normality of means and standard deviations also show that many drug discovery professionals reported at least one type of difficulty encountered with AI integration, most commonly about data quality and costs of implementation, as well as with regulatory restrictions.

Even though it is assumed that AI will become the new norm in drug discovery, there are still many issues to address, and the cost reduction issue is the most critical one. Based on the results of this study, they state that while AI may hold the key to enhancing the accuracy of research and reducing timelines, it is yet to realize the full economic impact possible in an organization. The lack of internal consistency of the assessed constructs – the impact of AI, satisfaction with the integration of AI, and confidence that AI will decrease costs, speaks to the need for more nuanced enhancements to the AI solutions and how and what their value proposition is best captured.

To unlock the full potential of AI, organizations need to enhance their 'hardware', human capital, and interprofessional collaboration. Altogether, AI is ready to change drug discovery, but technical, organizational, and regulative challenges will determine it. Subsequent work should target these limitations, make the methods demonstrate cost cost-saving aspect of AI, and achieve a synergy where it is integrated throughout the entire drug development pipeline.

REFERENCES

[1] Abbas, M., Rassam, A., Karamshahi, F., Abunora, R., & Abouseada, M. (2024). The Role of AI in Drug Discovery. ChemBioChem, 25(14), e202300816.

[2] Abou Hajal, A., & Al Meslamani, A. Z. (2024). Insights into artificial intelligence utilization in drug discovery. In (Vol. 27, pp. 304-308): Taylor & Francis.

[3] Acharjee, P. B., Ghai, B., Elangovan, M., Bhuvaneshwari, S., Rastogi, R., & Rajkumar, P. (2023). Exploring AI-driven approaches to drug discovery and development. The Scientific Temper, 14(04), 1387-1393.

[4] Afrose, N., Chakraborty, R., Hazra, A., Bhowmick, P., & Bhowmick, M. (2024). AI-Driven Drug Discovery and Development. In Future of AI in Biomedicine and Biotechnology (pp. 259-277): IGI Global.

[5] Ahmad, S. S., Ghalib, M. R., Gallimore, M., & Al-Mousa, A. (2024). Role of AI and Futuristic Technology in Drug Discovery for Smart Hospitals. In Converging Pharmacy Science and Engineering in Computational Drug Discovery (pp. 212-234): IGI Global.

[6] Akhtar, Z. (2024). Exploring Biomedical Engineering (BME): Advances within Accelerated Computing and Regenerative Medicine for a Computational and Medical Science Perspective Exploration Analysis. J Emerg Med OA, 2(1), 01-23.

[7] AKHTAR, Z. B. (2023). Accelerated Computing A Biomedical Engineering and Medical Science Perspective.

[8] Arunachalam, P., Usharani, R., Thirumal, S., Swarnalatha, A., & Maheswari, B. U. (2025). Study on AI-Powered Advanced Drug Discovery for Enhancing Privacy and Innovation in Healthcare. In AI-Powered Advances in Pharmacology (pp. 25-60): IGI Global.

[9] Ashiwaju, B. I., Orikpete, O. F., & Uzougbo, C. G. (2023). The Intersection of Artificial Intelligence and Big Data in Drug Discovery: A Review of Current Trends and Future Implications. Matrix Science Pharma, 7(2), 36-42.

[10] Baig, M. A. A., & Li, S. AI-powered Human-on-Chip: Redefining Biomedical Frontiers: Human-on-Chip.

[11] Bajhzer, R., Alghamdi, M., & Elhag, S. AI Powered Bioinformatics-Expediting Diagnostic Testing: A Survey.

[12] Bhatia, N., Khan, M. M. U., & Arora, S. (2024). The Role of Artificial Intelligence in Revolutionizing Pharmacological Research. Current Pharmacology Reports, 1-7.

[13] Boniolo, F., Dorigatti, E., Ohnmacht, A. J., Saur, D., Schubert, B., & Menden, M. P. (2021). Artificial intelligence in early drug discovery enables precision medicine. Expert Opinion on Drug Discovery, 16(9), 991-1007.

[14] Chaurasia, A. (2023). Algorithmic precision medicine: Harnessing artificial intelligence for healthcare optimization. Asian Journal of Biotechnology and Bioresource Technology, 9(4), 28-43.

[15] Chen, M. (2023). AI and Machine Learning in Revolutionizing Drug Discovery and Development. Advances in Computer Sciences, 6(1).

[16] Chintala, S. (2024). Accelerating Drug Discovery: Ai Powered Approaches in Pharmaceutical Research. Paper presented at the 2024 4th International Conference on Innovative Practices in Technology and Management (ICIPTM).

[17] da Silva, R. G. L. (2024). The advancement of artificial intelligence in biomedical research and health innovation: challenges and opportunities in emerging economies. Globalization and Health, 20(1), 44.

[18] De Thé, F.-X. B., Baudier, C., Pereira, R. A., Lefebvre, C., Moingeon, P., & Group, P. W. (2023). Transforming drug discovery with a high-throughput AI-powered platform: A 5-year experience with Patrimony. Drug Discovery Today, 28(11), 103772.

[19] Dhudum, R., Ganeshpurkar, A., & Pawar, A. (2024). Revolutionizing Drug Discovery: A Comprehensive Review of AI Applications. Drugs and Drug Candidates, 3(1), 148-171.

[20] Diaz-Flores, E., Meyer, T., & Giorkallos, A. (2022). Evolution of artificial intelligence-powered technologies in biomedical research and healthcare. Smart Biolabs of the future, 23-60.

[21] Doke-Bagade, P. E., & Bagade, O. (2024). Applications of AI-Based Models in the Field of Biomedicine. In Biosystems, Biomedical & Drug Delivery Systems: Characterization, Restoration and Optimization (pp. 259-

286): Springer.

[22] Dutta, A. (2023). Unlocking the Power of Artificial Intelligence: Revolutionising Clinical Medicine for a Healthier Future. Journal of Medical Evidence, 4(3), 271-273.

[23] Gangwal, A., & Lavecchia, A. (2024). Unlocking the potential of generative AI in drug discovery. Drug Discovery Today, 103992.

[24] Guedj, M., Swindle, J., Hamon, A., Hubert, S., Desvaux, E., Laplume, J., . . . Gabarroca, C. (2022). Industrializing AI-powered drug discovery: Lessons learned from the patrimony computing platform. Expert Opinion on Drug Discovery, 17(8), 815-824.

[25] Huang, D., Yang, M., Wen, X., Xia, S., & Yuan, B. (2024). AI-DRIVEN DRUG DISCOVERY:: ACCELERATING THE DEVELOPMENT OF NOVEL THERAPEUTICS IN BIOPHARMACEUTICALS. Journal of Knowledge Learning and Science Technology ISSN: 2959-6386 (online), 3(3), 206-224.

[26] Javanmard, S. (2024). Revolutionizing Medical Practice: The Impact of Artificial Intelligence (AI) on Healthcare. OA J Applied Sci Technol, 2(1), 01-16.

[27] Jayatunga, M. K., Ayers, M., Bruens, L., Jayanth, D., & Meier, C. (2024). How successful are AI-discovered drugs in clinical trials? A first analysis and emerging lessons. Drug Discovery Today, 104009.

[28] Kapustina, O., Burmakina, P., Gubina, N., Serov, N., & Vinogradov, V. (2024). User-friendly and Industry-Integrated AI for Medicinal Chemists and Pharmaceuticals. Artificial Intelligence Chemistry, 100072.

[29] Karalis, V. D. (2024). Artificial intelligence in drug discovery and clinical practice. In From Current to Future Trends in Pharmaceutical Technology (pp. 215-255): Elsevier.

[30] Kasaraneni, R. K. (2022a). AI-Powered Biomarker Discovery: Identifying Novel Biomarkers for Early Disease Detection and Drug Development. Journal of Machine Learning in Pharmaceutical Research, 2(1), 171-208.

[31] Kasaraneni, R. K. (2022b). AI-Powered Drug Discovery: Accelerating the Identification of Novel Therapeutic Compounds through Machine Learning Algorithms. Journal of Artificial Intelligence Research and Applications, 2(2), 375-414.

[32] Khan, A. (2023). Harnessing the Power of AI: A Review of Advancements in Healthcare. BULLET: Jurnal Multidisiplin Ilmu, 2(3), 546-556.

[33] Khan, I. R., Grover, V., Fatima, I., Alam, M., & Ahmad, N. (2024). The Application of AI in Drug Discovery: Challenges, Opportunities, and Strategies. Analyzing Explainable AI in Healthcare and the Pharmaceutical Industry, 181-198.

[34] Khurana, V. (2024). Accelerating Pace of Scientific Discovery and Innovation through Big Data Enabled Artificial Intelligence and Deep Learning. Emerging Trends in Machine Intelligence and Big Data, 16(1), 38-53.

[35] Kiani, M., & Nasir, F. (2024). AI in Drug Discovery: Accelerating Pharmaceutical Research. International Journal of Advanced Engineering Technologies and Innovations, 1(1), 80-98.

[36] KOLLURI, V. (2021). A COMPREHENSIVE STUDY ON AI POWERED DRUG DISCOVERY: RAPID DEVELOPMENT OF PHARMACEUTICAL RESEARCH. International Journal of Emerging Technologies and Innovative Research (www. Jeter. org| UGC and ISSN Approved), ISSN, 2349-5162.

[37] Liu, J., Du, H., Huang, L., Xie, W., Liu, K., Zhang, X., . . . Pan, H. (2024). AI-Powered Microfluidics: Shaping the Future of Phenotypic Drug Discovery. ACS Applied Materials & Interfaces, 16(30), 38832-38851.

[38] Liu, Z., Roberts, R. A., Lal-Nag, M., Chen, X., Huang, R., & Tong, W. (2021). AI-based language models powering drug discovery and development. Drug Discovery Today, 26(11), 2593-2607.

[39] Mak, K.-K., & Pichika, M. R. (2019). Artificial intelligence in drug development: present status and prospects. Drug Discovery Today, 24(3), 773-780.

[40] Mittal, S., Singh, P. K., Gochhait, S., Gaur, N., & Kumar, S. (2024). AI-powered clinical trial design with translational bioinformatics. In Green AI-Powered Intelligent Systems for Disease Prognosis (pp. 57-72): IGI Global.

[41] Nailwal, K., Durgapal, S., Dasauni, K., & Nailwal, T. K. (2024). AI: Catalyst for Drug Discovery and Development. In Concepts in Pharmaceutical Biotechnology and Drug Development (pp. 387-411): Springer.

[42] Oluwaseyi, J. (2024). AI-Powered Drug Discovery: Revolutionizing the Pharmaceutical Industry.

[43] Pasrija, P., Jha, P., Upadhyaya, P., Khan, M. S., & Chopra, M. (2022). Machine learning and artificial intelligence: a paradigm shift in big data-driven drug design and discovery. Current Topics in Medicinal Chemistry, 22(20), 1692-1727.

[44] Pathak, M. (2025). Role of AI in Advancing Pharmacology. In AI-Powered Advances in Pharmacology (pp. 1-14): IGI Global.

[45] Pun, F. W., Ozerov, I. V., & Zhavoronkov, A. (2023). AI-powered therapeutic target discovery. Trends in pharmacological sciences.

[46] Puri, M., Manwatkar, S., Karpe, P., & Kulkarni, S. (2024). Optimizing Drug Synthesis: AI-Powered Kinetics Study in Pharmaceutical Research. In Biosystems, Biomedical & Drug Delivery Systems: Characterization, Restoration and Optimization (pp. 179-196): Springer.

[47] Rahate, K. P., & Mondal, R. (2024). Applications of AI in Drug Discovery: Its Challenges, Opportunities, and Strategies. Approaches to Human-Centered AI in Healthcare, 86-120.

[48] Rasool, S., Ali, M., Shahroz, H. M., Hussain, H. K., & Gill, A. Y. (2024). Innovations in AI-Powered Healthcare: Transforming Cancer Treatment with Innovative Methods. BULLET: Jurnal Multidisiplin Ilmu, 3(1), 118-128.

[49] Sampathi, S., & Bhatia, N. (2024). AI-Enabled Models in the Restoration of Drug Efficacy and Drug Design. In Biosystems, Biomedical & Drug Delivery Systems: Characterization, Restoration and Optimization (pp. 83-103): Springer.

[50] Santos, H. (2023). Machine Learning Approaches for Enhancing Drug Discovery and Development in Healthcare: AI Models for Accelerating Pharmaceutical Research and Clinical Trials. Journal of Bioinformatics and Artificial Intelligence, 3(2), 277-291.

[51] Shah, V. (2023). AI-Powered Drug Repurposing for Pandemic Preparedness and Response. INTERNATIONAL JOURNAL OF COMPUTER SCIENCE AND TECHNOLOGY, 7(3), 227-242.

[52] Singh, S., Gupta, H., Sharma, P., & Sahi, S. (2024). Advances in Artificial Intelligence (AI)-assisted approaches in drug screening. Artificial Intelligence Chemistry, 2(1), 100039.

[53] Tiwari, P. C., Pal, R., Chaudhary, M. J., & Nath, R. (2023). Artificial intelligence revolutionizing drug development: Exploring opportunities and challenges. Drug Development Research, 84(8), 1652-1663.

[54] Tripathi, N., Goshisht, M. K., Sahu, S. K., & Arora, C. (2021). Applications of artificial intelligence to drug design and discovery in the big data era: a comprehensive review. Molecular Diversity, 25(3), 1643-1664.

[55] Usmani, U. A., & Usmani, M. U. (2023). AI-Driven Biomedical and Health Informatics: Harnessing Artificial Intelligence for Improved Healthcare Solutions. Paper presented at the 2023 2nd International Conference on Futuristic Technologies (INCOFT).

[56] Vairamani, A. D., Adhikary, S., & Banerjee, K. (2024). Data Processing Method for AI-Driven Predictive Models for CNS Drug Discovery. Artificial Intelligence and Machine Learning in Drug Design and Development, 223-249.

[57] Verma, A., & Awasthi, A. (2024). Revolutionizing Drug Discovery: The Role of Artificial Intelligence and Machine Learning. Current Pharmaceutical Design, 30(11), 807-810.

[58] Vidhya, K., Sultana, A., Kumar, N., & Rangareddy, H. (2023). Artificial intelligence's impact on drug discovery and development from bench to bedside. Cureus, 15(10).

[59] Yadav, S., Singh, A., Singhal, R., & Yadav, J. P. (2024). Revolutionizing drug discovery: The impact of artificial intelligence on advancements in pharmacology and the pharmaceutical industry. Intelligent Pharmacy.

[60] Yadav, V., Yadav, V., Shukla, A., & Kshatrya, B. (2023). Applications of Artificial Intelligence in Biomedical Fields: An Overview. International Journal of Newgen Research in Pharmacy & Healthcare, 70-75.

[61] Zhang, Y., Mastouri, M., & Zhang, Y. (2024). Accelerating drug discovery, development, and clinical trials by artificial intelligence. Med.

[62] Zhang, Y., Sui, X., Pan, F., Yu, K., Li, K., Tian, S., . . . Wang, J. (2023). BioKG: a comprehensive, large-scale biomedical knowledge graph for AI-powered, data-driven biomedical research. bioRxiv.

[63] Zhuge, J. (2024). The Impact of Artificial Intelligence on Biomedical Research and Healthcare. Paper presented at the 2024 10th International Conference on Humanities and Social Science Research (ICHSSR 2024)