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Role of Artificial Intelligence and Machine Learning in Pharmaceutical Formulation: Recent Advances Existing Challenges and Future Prospectus

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The spur growth of the pharmaceutical industry took a digital transformation face with help of artificial intelligence (AI) machine learning (ML). These technology is not only taken keen role in analytical tool but also help in developing drug formulation manufacturing aspects. A tremendous shift was observed between 2020 and 2025 AI and ML have taken rapid role in application enabling in developing predictive model right from the primary physical chemical properties optimization of pharmaceutical parameters and technology driver of automation of process control. This review article put emphasis on recent existing advances alongside highlighting the technology in making more neural connections in network and support the vectors system in machines. The generated models were helped in redefining the design and quality. These technologies help in innovation in predicting excipient compatibility developed a simulator resolution profile finally helping to develop robust formulation part improving overall reproducibility and efficacy. The other technology such as Quantum machine learning federal learning and twin technology have made their own place in creating a new era of collaborative and autonomous formulation development.

Keywords: Artificial Intelligence (AI); Drug Development; Formulation; Machine Learning; Technology.

Now one can assume AI and ml are no more futuristic approach rather can see recent trends realistic approach for formulation cycle. Right from the solubility to stability study parameters, the role of AI and ml in optimization of excipient ratio process condition has inside lesson the burden of experimentation and rather increased precision. Their ability to learn from historical data has opened new frontiers in formulation informatics, where AI algorithms such as neural networks, random forests, and support vector machines enable scientists to simulate, optimize, and validate formulations virtually well before they reach the bench.[1]

Over the last five years, there has been a growing trend of research work associated with formulating through the use of AI and ML. many review articles explained the research work conducted using AI and ML. these formulations not only described the accuracy of predicting outcome enhance, but also physical testing can be sometimes reduced by 50%.[2]

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Data integration computation automation have created transformative era of pharmaceutical science. The traditional empirical methods such as extends you experimentation trial and error method more human intuition. These old methods constrained, un-sustained in the present time expectations of quicker smarter development cycle design therapies and faster production. The dramatically change was found with integration of AI and ML which solved complex based assets discovered hidden pattern and made more predictive decision hence improved overall formulation outcomes.[3]

The paradigm shifts in pharmaceutical product design using data has marked the onset of the 'digital renaissance in formulation science. The current compute capabilities, in addition to the accessibility of quality datasets, have ensured that the principles of Quality by Design (QbD) become more attainable than before. Formulation scientists are able to predict key parameters such as the rate of dissolution, compaction, and polymorphism using the capabilities of predictive modeling powered by machine learning capabilities.[4]

However, this shift is not without challenges. Questions and concerns surrounding the quality and explainability of the models, as well as their acceptance among regulators, are still being debated.[23] The phenomenon known as the "black box" effect, brought about by the nature of certain AI algorithms, makes it difficult to test and accredit these models and algorithms. These technologies have reached a new milestone and received much attention still facing many challenges such as data scarcity model integration and universal acceptance. The other aspects include such as data transparency intellectual property and algorithm mismatch. In upcoming time, the AI will be integrated with Pharma 5.0 a paradigm – a theoretical and practical approach pertained by sustainability collaboration of human with artificial intelligence and agile manufacturing. That will take a new face of adaptive predictive completely reliable and ethical driven.

In contrast to existing literature, which to a very large extent tends to focus on Drug Discovery, the present paper will focus on formulation and production, which represent the domains of practical implementation of AI contributions.

The current review focus on innovations in analysis of current methodology development process applications imitations future directions with the emphasis on integrating AI with formulation science.

The goals of this review are to:

1. Highlight contemporary progress being achieved in AI/ML in the field of formulation science.
2. Discuss the ways in which these technologies enhance design, optimization, and efficiency in
3. Describe challenges and ethical issues posed for implementation.
4. Determine the emerging technologies that will influence the upcoming decade in AI-formulation.
5. Describe a vision for the integration of AI in sustainable patient-centric pharmaceutical systems.

At its core, the integration of AI and ML is revolutionizing formulation science from an art to an intelligent and predictive science that is able to precisely predict and develop safer, more effective, and personalized therapies.

Literature survey

There has been a major integration of AI and ML that has significantly altered the early development process of pharmaceuticals, especially the design and preformulation development of drugs. This was a traditional process that required a lot of experimentation in order to test the solubility, stability, and compatibility of excipients through a process that was labor-intensive.

AI and ML in Drug Design and Preformulation

AI and ML have significantly altered this process. Supervised learning methods and neural network models have been found extremely successful in detecting nonlinear interrelations in formulation variables. Recently, researchers used the structure-property relation and structure-activity relation concepts and applied them for predicting key formulation properties. The other research described that neural networks can successfully predict the interactions of excipients for complicated molecules for researchers to avoid compatibility problems in the early stages of development.[1]

Similarly, another research was able to successfully predict the dissolution rate in solid dispersions by applying Random Forest and Gradient Boosting methods, which gave better results than regression methods. Recent breakthroughs in deep learning have further improved the predictability of these systems.[2]

One of article demonstrated the potential of Convolutional Neural Networks in predicting polymorphic transformations and particle size distributions from limited datasets, making their applicability highly desirable in the early stages of formulation screening.[3, 26] Taken together, it is apparent that there has been a paradigm shift in the use of simulation tools in the area of preformulation towards the adoption of Quality by Design.

Machine Learning in Formulation Optimization

Once preformulation data are determined, ML-driven models are very instrumental in the optimization of formulation parameters for various dosage forms, including tablets, capsules, emulsions, and nanoparticle systems. Traditional methods, such as design of experiments, are still helpful but can rarely tackle nonlinear interactions that happen with multi-variant problems in modern formulations. In such cases, ML models can be trained on complex relationships between input variables, like excipient ratios or process temperatures, and output properties, such as dissolution rate, hardness, and bioavailability. Research have reported that Support Vector Machine models, Artificial Neural Network models, and other Support Vector Machine models were more accurate than DoE-based models for predicting tablet disintegration time and mechanical strength [4]. Similarly, another review have emphasized that Bayesian optimization methods can be considered an effective approach for optimizing model parameters with a low number of experiments, especially in cases involving expensive or hard-to-find materials.[5,40] On the other hand, with the increasing use of Nano medicine, techniques like GA, Particle Swarm Optimization, among other design techniques, are being widely used. The research showed how a combination of ANN and GA can be used to optimize lipid nanoparticle formulations, achieving a stable mRNA delivery system, which marked a significant step in the development of the COVID-19 vaccine. Most remarkably, AI enables multi-objective optimization, which means achieving several aims related to the target formulation in one go.[6,24,34]

AI-Driven Manufacturing and Process Modeling

According to Joshi & Sheth, deep learning algorithms integrated within Process Analytical Technology (PAT) enable the continuous observation of key process parameters like blend uniformity, granule moisture, or tablet weight. Such technologies automatically make corrections for any anomalies as soon as they are detected to minimize operator mistakes.[8,27]

There is also the idea of Digital Twins, which describes the digital replication of real manufacturing systems. The application of Digital Twins with the use of Machine Learning was one of the first mentioned by one of authors in 2021, which can be used to model manufacturing processes, test control concepts, and eliminate deviations from the desired process even before they occur.[10] This is the basis of the idea of continuous manufacturing. Also, several reinforcement learning-based algorithms have been promising in dynamic process condition control. The Reinforcement Learning (RL) agents will "learn" the best actions from the real-time feedback to improve coating uniformity, reduce variability, and increase the yield of production. Put together, these works show how artificial intelligence has been changing pharmaceutical manufacturing from a static operation into an intelligent self-optimizing system that aligns with GMP and Industry 4.0 principles.

AI in Quality Control and Regulatory Compliance

The implementation of AI technology in QA processes in the pharmaceutical industry is transforming the manner in which pharmaceutical quality is tracked, validated, and sustained. computer vision, based on deep learning, is now capable of detecting even microscopic imperfections on tablets, capsules, or packaging with accuracy not humanly possible.[7,28]

According to Fitzgerald et al. "Explainable AI (XAI) will play a pivotal role in winning the trust of the regulatory environment, particularly with the adoption of MIR by the FDA, the EMA, and other organizations." Regulator bodies are finally beginning to acknowledge the importance of AI, although they stress the importance of transparency, transparency, and traceability.[22] Nonetheless, transparency, according to one of article, is a crucial consideration in obtaining approval of any AI solution. Finally, the establishment of Good Machine Learning Practice (GMLP) guidelines is a significant step toward the integration of AI into the release process of active pharmaceutical ingredients.[23] These systems could finally make the process of batch release, quality auditing, and, finally, real-time release testing (RTRT) possible without any manual intervention.

Emerging Trends and Innovative Applications

Between 2023 and 2025, a new generation of innovations has further increased the role of AI in pharmacy formulation, now including generative, collaborative, and quantum innovations.

1. Generative Artificial Intelligence (GenAI): Through the use of Generative Adversarial Networks (GANs) and/or Variation Auto encanners (VAEs), a GenAI can self-generate novel formulation suggestions. It was shown in a paper given by Chinnaiyan & Mugundhan in 2025 that a generative approach was better, faster, and more accurate.[12, 38]

2. Federated Learning (FL): Federated Learning allows for shared AI model development among various organizations without transferring their personal data. This model helps in collaborative research for proprietary formulation studies in privacy-preserving manners, as pointed out by one of the review.[11, 37]

3. Quantum Machine Learning: Quantum computing combined with AI allows for the exploration of massive formulation spaces simultaneously. These research suggested that QML could perform optimizations that have high-dimensional solution spaces, such as excipient selection and molecular packing, a task that pushes classical computing to the limits.[13, 39]

4. Digital Twins and Pharma 5.0: AI-powered digital twins, with the integration of the Internet of T 3.

Applications of AI and ML in pharmaceutical formulation design

AI in Preformulation: Predicting Physicochemical Properties and Excipient Compatibility

In the old process, this would entail conducting laboratory tests. However, with the aid of AI, computational customs can be utilized to make remarkably accurate predictions. Quantitative Structure-Property Relationship studies, also known as Quantitative Structure-Activity Relationship studies, are the cornerstones of AI-aided preformulation. These studies describe relationships between the chemical structure of a molecule, as reflected by a series of numerical chemical descriptors, and performance-related chemical attributes like solubility, dissolution rate, or hygroscopicity. The research proved that using a neural network modelled on a Quantitative Structure Property Relationship data-set, the compatibility of excipients in poorly soluble substances can be predicted.[1]

Similarly, in another research employed the Random Forest (RF) algorithm and the Gradient Boosting (GB) algorithm to make predictions related to the rate of dissolution for Solid Dispersions. These models allowed for the prediction of nonlinear relationships between variables more accurately compared to standard regression models. Further advancements in this area have been induced by deep learning.[2]

The research described the use of Convolutional Neural Networks in the analysis of spectral and microscopy datasets to predict the morphology of particles, polymorphic transformations, which are two influential stability-drivers.[3, 26]

Machine Learning in Formulation Design and Optimization

The effective use of ML algorithms enables the determination of optimal formulation variables with minimum experimental trials.

Bayesian Optimization (BO), has received special attention in adaptive experimentation. The research demonstrated that Bayesian Optimization algorithms can optimize formulation variables such as binder material, lubricant content, and granulation time iteratively to near-optimal levels in a few trials. The method takes into account experimental data in a dynamic manner by adapting next trials based on past outcomes.[5,40]

In more sophisticated delivery methods, as seen in nanoparticles, liposomes, and emulsions, the problem becomes even more complicated due to the complex multiple-dimensional effects of particle size, charge, and entrapment efficiency. In these applications, Genetic Algorithms and Particle Swarm Optimization have been shown to be very beneficial. According to one of research work, a combined ANN-GA approach enabled a successful optimization of lipid nanoparticle formulations for mRNA delivery applications.[6,24,34]

The optimized formulation process utilizing AI tools increased the efficiency of the formulation and improved the reproducibility of the results in scaled-up productions. The capability of the AI to process a massive multidimensional dataset opens the possibility of considering more than one goal at a given point in time, thus allowing a comprehensive optimization approach to be achieved in a multidimensional space. This is highly useful in the scenario of Quality by Design (QbD), in which the quality of the product is built into the formulation and not tested at the end point of the process through the traditional quality testing.

Process Modeling and Scale-Up: Toward Intelligent Manufacturing

Although the application of AI in the field of formulation design is well understood, its effect on process modeling and manufacturing optimization is more revolutionary. A classical process control system is based on deterministic models with fixed parameters. However, AI brings with it the concept of self-adjusting and data-driven feedback channels for process control. Process Analytical Technology (PAT) tools have been integrated with machine learning algorithms that enable the simultaneous tracking and adjustment of crucial process variables, including particle size, moisture, and homogeneity. Joshi and Sheth observed a 35% improvement in the stability of processes that employed deep learning-based PAT tools in a continuous tablet manufacturing process, which greatly influenced the variability between batches.[8, 27]

One of the most promising applications in this domain is working out Digital Twins-discrete virtual models of physical processes that gain knowledge continuously with the help of sensor data. These twins simulate manufacturing conditions, predict deviations, and recommend corrective actions in advance to prevent the occurrence of an issue. Djuris et al. were among the first to demonstrate ML-enabled process validation using digital twins that could provide real time feedback loops for blending and granulation.

Besides, a class of ML, which uses iteration and feedback for learning, has been successfully employed in dynamic processes such as coating and drying. RL agents automatically adjust the variables in the process to achieve an optimum in uniformity and minimize waste in coating, thus making self-regulating manufacturing environments. AI integrated into CM represents a big step to achieve Pharma 4.0, which is described as a framework of automation, traceability, and predictive quality assurance. These pave the way for smart manufacturing plants, where every component of the production line in a plant works in an integrated digital environment.

AI in Quality Control and Regulatory Compliance

The impact of AI is not confined to the structuring and production processes, extending to quality control (QC), and regulatory matters, where accuracy and reliability are essential. In this respect, the adoption of XAI tools, such as LIME and SHAP, will help meet these standards by providing interpretable and auditable AI decision-making. What AI is doing, in effect, is to help close the loop between formulation design, process execution, and regulatory assurance-to create one continuum of quality and compliance right across the product lifecycle.

Advanced and Emerging Applications

• Recent breakthroughs within the period of 2023-2025 have unveiled a new frontier that AIenabled formulation science enters into, farther from optimization and control

• Generative AI GenAI can now itself propose a new hypothesis in formulation through GAN and VAE. Chinnaiyan and Mugundhan 2025 showed that the GenAI systems can design nanoparticle formulations optimized for controlled drug release and stands as an example for autonomous formulation discovery.[12, 38]

• Federated Learning: FL would further cross-sector innovation by having institutions share their training processes for AI models across organizations without necessarily sharing the raw data itself. As documented in one of research 2025, FL enhanced model robustness by incorporating datasets from varied organizations.[11, 37]

• Quantum Machine Learning (QML): Owing to the potential of quantum computation in dealing with high-dimensional data, the use of QML in excipient screening and prediction of molecular packing has vast potential. The potential of QML in optimizing problems, which are otherwise hard for classical systems.[13, 39]

• Internet of Things (IoT)-Enabled Intelligent Systems: Integration of IoT sensors with AI makes it possible to monitor the environment continuously by tracking variables such as humidity, vibration, and temperature, which ensures the stability of the formulation being stored or transported.[14, 35]

Challenges and limitations

Several challenges and limitations observed while deploying AI and ML in pharmaceutical formulation that obstruct its full fledge utilization in formulation sciences. These hurdles, ranging from data quality, interpretability, government preparedness, and technological constraints, are the growing pains of an industry which is changing its face from an empirical past to a future of digital intelligence.

Data Scarcity and Quality Limitations

One of the most problematic aspects of AI-formulation is the issue of data. In contrast to genomics or imaging, for example, where large quantities of standardized data in centralized databases support scientific inquiry, the typical dataset in formulation science may consist of a few studies with small, disjoint, and often proprietary datasets. Moreover, the existing data, especially the legacy data, in the field of formulation science remains physical, in the sense that the data is stored in lab books, PDFs, or incompatible data management systems [13, 39]. The research work also highlighted that over 60% of the existing studies on formulation using AI utilize hand-curated data, which leads to some inconsistency and human biases.[11,37]

Model Interpretability and the "Black Box" Problem

If the algorithm identifies an optimal combination of excipients, formulation experts must be able to understand why the identified parameters are optimal; for example, through solubility, molecular interaction, or their stability relationships. Unless this occurs, the predictions made by the algorithm are difficult to verify from the perspectives of QbD or regulations. Recent trends in the area of Explainable Artificial Intelligence (XAI), like the use of Shapley Additive exPlanations (SHAP) techniques, along with Local Interpretable Model-Agnostic Explanations (LIME), have the potential to fill this gap. However, number of studies publishing the formulation of the Artificial Intelligence work, focusing specifically on metrics for interpretability, is less than 10%. The application of black-box models, therefore, faces limitations unless the practice of interpretability gains widespread acceptance.[13, 39]

Regulatory and Compliance Challenges

The regulatory environment regarding AI applications in the pharmaceutical sector is still in its infancy. Even though there is some material that has been produced in the form of position papers about AI applications in the healthcare domain, such as those produced by the FDA and the EMA, there is no overarching framework that addresses AI-driven formulation and manufacturing. [16, 30]The lack of traceability, validation, and replicability is a challenge for continuously learning models. The subject validation approach was intended for traditional static models, making it a challenge for the AD systems that need to automatically update the parameters periodically. Additionally, the idea of complying with the standards of "Good Manufacturing Practice" (GMP) within "Good Automated Manufacturing Practice" (GAMP 5) also carries the risk of violating the opaque nature of deep models.[20, 33] "There is a tension between the need for flexibility in regulation, particularly in the context of technologies, and the requirements for regulation, specifically the need for a closed, prevalidated model."

Technical Barriers and Infrastructure Gaps

Realization of AI in pharmaceuticals requires extensive technological support in terms of computing power and sensor-enabled manufacturing facilities. Still, most pharmaceutical institutions have been unable to access this technological support in academic institutions and small to medium enterprises (SMEs). This is because of the technological divide between more well-funded industries and smaller institutions.[18,32] Additionally, there are some problems that come with legacy systems. These Traditional Laboratory Information Management Systems and associated processes controlled by software that were not meant to work in conjunction with some of the currently available artificial intelligence software, which makes interoperability difficult. Additionally, most artificial intelligence software requires a continuous flow of data for learning and monitoring. However, most factory environments are batch mode. The past research also pointed out the possibility of model overfitting, which is a common problem in small-sample studies. Many models work perfectly well during the validation process but collapse during application or execution in reality.[6,24,34]

Ethical, Privacy, and Security Concerns

In formulation data, information can be

proprietary or relate to patients, requiring robust data governance. Fed learn and differential privacy provide a way around this problem to train models distantly with security, not sharing data.[17, 31]

Bias is another area that requires immediate attention. Incompletion and biases in the dataset pose risks in developing biased models, which in turn generate biased outputs and contribute to inequitable formulation development. For example, models that are mainly developed for small molecules but not for biologics and nano-carriers may show poor performance in biologics and nano-carriers because of biases in the data that existed in the past. [15, 29] Issues related to intellectual property (IP) are also gaining prominence.[21]

Finally, there's also the increased risk of cybersecurity threats. AI models and datasets are digital assets that can be hacked or misused. A hacked AI model may render predictions or data provided incorrect or even forge information, leading to risks concerning both safety and compliance. Therefore, adopting ethical AI also needs a rounded approach that addresses innovation and accountability together.

Reproducibility and Cross-Platform Validation

Reproducibility has always remained a hallmark of scientific integrity, but still, it remains a problem in AI-based formulation studies. There are numerous studies which do not report enough detail regarding the process, therefore making the task of reproducing them a difficult job. According to review work have shown, only fewer than 20% of the literature could provide open-source data sets or source codes. The differences in the process of data preprocessing and feature choice, combined with the algorithms being adjusted in each case, make cross-platform validation even more difficult.[13, 39]

In addition to this, the AI solutions provided by the pharmaceutical industry are often provided in closed frameworks that can be neither inspected nor verified by academic factors. This can lead to the onset of the "AI knowledge divide." To address this challenge, there is a need to prioritize projects that focus on open-source AI frameworks and data. This will aid in the creation of common standards regarding data curation and model reporting. This will, in turn, improve model reproduction and comparability.

Future directions

The integration of AI and Machine Learning ML in pharmaceutical formulation is no longer a 'future possibility', but it's becoming a 'norm'. As we move ahead in this domain, we are bound to witness emerging 'new normals', which would have the power to shatter the thinking horizon with which we 'design' medicine. The coming era would witness 'AI moving ahead from being a 'Decision Support System' to 'Scientific Collaboration'. The following section would highlight areas that are 'heading to become a 'new normal' in 2025 and onwards', which would shape this upcoming landscape: Federated Learning, Quantum Machine Learning, Generative AI, Smart Manufacturing in IoT, and 'Regulatory/ethical frameworks.

Federated Learning and Collaborative Intelligence

Among the most revolutionary future applications of AI in pharmaceutical formulation is Federated Learning, which is a decentralized model that enables several corporations to jointly train AI systems without sharing their confidential information. The use of AI in pharmaceutical formulation is significantly hampered by the fact that there is a lack of larger joint datasets owing to the issue of confidentiality. A federated system allows the data to reside within their boundaries and for algorithms to learn from distributed data sources. This allows pharmaceutical companies, research institutions, and regulators to work together to develop predictive models without having to share their proprietary information. Many research mentioned that FL frameworks improve model generalizability by capturing data distributions from various institutions to develop more robust and unbiased predictive models.[11, 37]

Quantum Machine Learning (QML) and Computational Acceleration

The research explained that utilizing the strengths of quantum-boosted neural networks could potentially assess millions of formulation variants in milliseconds, shortening preformulation screening from months to mere hours.[19] The combination of QML with generative models should therefore unlock the potential for modeling complex physico-chemical interactions, which remain impossible with traditional algorithms. Although quantum hardware is not yet mature, joint initiatives between pharmaceutical companies and quantum computer companies, including the collaboration between Pfizer and IBM, are promising. During the coming decade, it is likely that QML theory will enter the implementation phase, thereby revolutionizing the pace of formulation science computation.[36]

Generative AI for Autonomous Formulation Design

Of all emerging trends, one of the most revolutionary and innovative technologies is Generative AI (GenAI) because it stands out among all other technologies as one of the most innovative technologies which can be used for research purposes in the pharmaceutical field. As opposed to general ML, which relies on general hypotheses based on available information, Generative AI can come up with new hypotheses on their own. This can be achieved by using Generative Adversarial Networks (GANs) or Variational Autoencoders (VAEs). One of research showed the capability of the GenAI "to design nanoparticle formulations on its own with optimal release properties and bioavailability, outdoing the process in terms of efficiency, efficacy, performance, and speed by a wide margin." These "co-scientists" can examine an infinite number of permutations of nanoparticle formulation on the computer, thereby reducing the need for physical experiments by a massive number. The next step in this evolution will be the integration of Gen AI with Reinforcement Learning and digital twin technology.[12, 38]

CONCLUSION

Redefining pharmaceutical formulation from form of 4 to form of 5 with integration of artificial intelligence and machine learning. As Pharma 4 completely based on extensive fermentation these technologies transformed empirical practice into predictive and data driven fields. Air powered tools help with the formal letter to imitate complex formulation optimize excipients ratios or excipient combination and keep track on manufacturing process into real time hence creating a new era of intelligent formulation design.

At the same time A I needs to overcome the other key barrier that are abstracting its potential you say it including data scarcity model transparency regulatory alignments and ethical account ability.

The near future of pharmaceutical formulation will be an AI driver with collaboration of human expertise such as academia industry regulatory authorities to develop a standard framework and ethical practices.

Anticipating future and searching Paradise such as Quantum computing federal learning generative AI guarantees the advance formulation science with greater autonomy adaptability and sustainability full stop this industrial transition from AI assistant to AI driver innovation with human expertise will shape future medicine that are more safe more precise and designed to patient needs making if perfect genuine paradigm shifts towards pharma 5.0

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This research does not involve any clinical trials.

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Author Contributions

Shanti Sagar and Mukthinutalapati Sowjanya: conceptualized the study and proposed the initial topic, focusing on the importance and emerging trends of artificial intelligence and Machine Learning in pharmaceutical formulation research; Maheshwari Reddy: conducted the comprehensive literature survey and was responsible for collecting and organizing relevant published studies; Rajeshwar Vodeti: contributed to the analysis and compilation of current applications of artificial intelligence and machine learning in pharmaceutical formulation and development; Basavraj Nanjwade: critically contributed to drafting the sections on existing challenges, regulatory considerations, and future directions of AI-driven pharmaceutical research. All authors reviewed, revised, and approved the final manuscript.

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