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REVIEW ARTICLE

A Review on Progress and Potential of Machine Learning and AI in Pharmaceutical Development

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Abstract: The integration of artificial intelligence (AI) in pharmaceutical technology represents a transformative shift in how drugs are discovered, developed, and manufactured. Recent advancements in machine learning algorithms, deep neural networks, and computational power have accelerated drug discovery timelines and enhanced manufacturing efficiency. AI technologies have demonstrated remarkable capabilities in target identification, lead optimization, and prediction of drug-protein interactions. In pharmaceutical manufacturing, AI-driven process analytical technology (PAT) systems optimize production parameters, ensure quality control, and enable real-time monitoring of critical process parameters. The implementation of AI in pharmaceutical analysis has revolutionized quality testing procedures, automated analytical processes, and improved predictive maintenance strategies. Despite these advances, the pharmaceutical industry faces challenges in AI adoption, including data quality concerns, regulatory compliance, and technical implementation barriers. Current regulatory frameworks are evolving to accommodate AI-based systems while maintaining stringent quality and safety standards. Looking ahead, emerging technologies such as quantum computing and federated learning promise to further enhance AI capabilities in drug development. The convergence of AI with other cutting-edge technologies positions the pharmaceutical industry for unprecedented innovation in therapeutic development and manufacturing excellence. The aim of this review is to study about the current state, applications, challenges, and future trajectory of AI in pharmaceutical technology, emphasizing its role in shaping the future of medicine.

Keywords: Artificial Intelligence; Drug Discovery; Pharmaceutical Manufacturing; Machine Learning; Process Analytical Technology.

1. Introduction

The pharmaceutical industry has witnessed unprecedented technological advancement with the integration of artificial intelligence, marking a pivotal shift in drug development paradigms [1]. The convergence of increased computational capabilities, sophisticated algorithms, and vast biological datasets has created new opportunities for innovation in pharmaceutical research and development [2]. Traditional drug development processes, typically spanning 10-15 years with costs exceeding $2.5 billion, are being revolutionized through AI-driven approaches [3].

The journey of AI in pharmaceuticals began in the 1960s with simple pattern recognition systems [4]. Early applications focused primarily on chemical structure analysis and basic molecular property predictions [5]. The 1990s marked significant progress with the emergence of quantitative structure-activity relationship (QSAR) models, which laid the foundation for modern AI applications [6].

Table 1. Traditional versus AI-Driven Approaches in Pharmaceutical Development

Parameter	Traditional Approach	AI-Driven Approach
Time to Market	10-15 years	5-8 years
Cost Efficiency	$1-2 billion	$500-800 million
Success Rate	10-12%	25-30%
Data Processing	Manual/Semi-automated	Fully automated
Pattern Recognition	Limited to expert knowledge	Advanced pattern detection
Predictive Capability	Based on historical data	Real-time predictions
Resource Utilization	High resource intensity	Optimized resource use
Scale-up Prediction	Empirical approach	Model-based prediction

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The advent of deep learning algorithms in the early 2000s, coupled with exponential growth in computing power, catalyzed the transformation of drug discovery processes [7]. Recent developments in neural networks and natural language processing have enabled the analysis of complex biological interactions and scientific literature at unprecedented scales [8].

Contemporary pharmaceutical companies are extensively incorporating AI across various operational domains [9]. Major pharmaceutical organizations have established dedicated AI divisions and formed strategic partnerships with technology companies [10]. Current implementations focus on optimizing clinical trial designs, predicting drug-target interactions, and enhancing manufacturing processes [11]. Machine learning models are being deployed for drug repurposing initiatives, reducing both time and resource investments in bringing therapeutics to market [12]. The industry has witnessed successful AI-driven drug candidates entering clinical trials, demonstrating the practical viability of these approaches [13-15]. The aim of this review is to study about the current state, applications, challenges, and future trajectory of AI in pharmaceutical technology, emphasizing its role in shaping the future of medicine.

2. AI in Drug Discovery and Development

2.1. Target Identification

Target identification represents a critical initial step in drug discovery, where AI algorithms excel in analyzing biological datasets [16]. Advanced machine learning models process genomic, proteomic, and metabolomic data to identify novel therapeutic targets [17]. Neural networks analyze protein-protein interaction networks, helping researchers understand disease mechanisms and identify potential intervention points [18]. Recent successes include the identification of novel targets for neurodegenerative diseases and various cancer types [19].

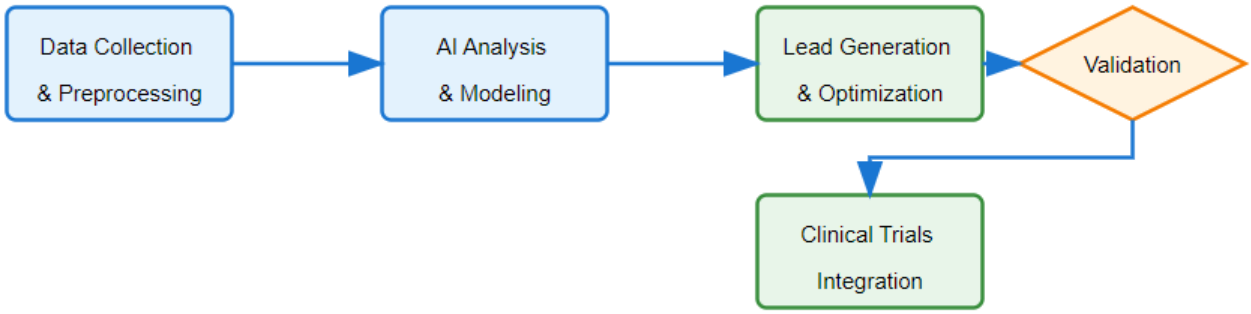

Figure 1. AI-driven drug discovery pipeline

2.2. Deep Learning for Lead Optimization

Lead optimization has been revolutionized through deep learning approaches that predict molecular properties and binding affinities [20]. Generative adversarial networks (GANs) design novel molecular structures with desired properties, significantly accelerating the traditional medicinal chemistry approach [21]. Reinforcement learning algorithms optimize molecular structures iteratively, considering multiple parameters simultaneously [22]. These methods have successfully generated promising candidates for various therapeutic areas, including oncology and infectious diseases [23].

Table 2. Machine Learning Algorithms and Their Applications in Pharmaceutical Manufacturing

Algorithm Type	Applications	Advantages	Limitations
Neural Networks	Formula optimization, Process control	High accuracy, Pattern recognition	Requires large datasets
Random Forests	Quality prediction, Batch analysis	Robust to outliers, Good interpretability	May overfit
Support Vector Machines	Process optimization, Quality control	Works well with limited data	Computationally intensive
Deep Learning	Drug discovery, Complex process modeling	Handles complex relationships	Black box nature
Reinforcement Learning	Process optimization, Control systems	Adaptive learning	Training time intensive

2.3. Predictive Analytics in Drug Design

Predictive analytics in drug design integrates multiple data sources to forecast drug behavior and potential success rates [24]. Advanced algorithms analyze physicochemical properties, binding affinities, and potential toxicity profiles of candidate molecules [25]. Machine learning models predict drug-drug interactions and potential adverse effects early in the development process [26]. These predictive capabilities have significantly reduced attrition rates in later development stages and improved the efficiency of drug design processes [27]. Recent applications have shown particular success in designing multi-target drugs and predicting drug resistance patterns [28]

3. Artificial Intelligence for Pharmaceutical Manufacturing

3.1. Process Optimization

3.1.1. Advanced Process Control Systems

AI-driven process control systems have transformed traditional pharmaceutical manufacturing by implementing sophisticated feedback mechanisms [29]. Neural networks analyze historical production data to establish optimal processing parameters, enabling adaptive control strategies that maintain product quality while maximizing yield [30]. These systems continuously adjust critical process parameters such as temperature, pressure, and flow rates, responding to minute variations in real-time [31].

Table 3. Implementation Outcomes of AI in Pharmaceutical Manufacturing (2020-2024)

Manufacturing Stage	AI Implementation	Success Rate (%)	ROI (%)	Quality Improvement (%)
Raw Material Testing	Spectral Analysis	92	156	45
Process Control	Real-time Monitoring	88	178	62
Quality Assurance	Automated Inspection	95	145	58
Batch Release	Predictive Analytics	86	134	51
Supply Chain	Demand Forecasting	91	167	38

3.1.2. Batch Process Optimization

Machine learning algorithms optimize batch processes by analyzing historical batch records and identifying patterns that correlate with product quality [32]. Advanced modeling techniques predict batch outcomes and suggest adjustments to process parameters, reducing batch-to-batch variability [33]. Deep learning models have demonstrated exceptional capability in optimizing complex unit operations such as crystallization, granulation, and drying processes [34].

3.1.3. Resource Utilization

AI systems optimize resource allocation and energy consumption across manufacturing facilities [35]. Predictive models analyze equipment performance data to schedule maintenance activities and minimize downtime. Energy consumption patterns are monitored and adjusted through intelligent systems that optimize utility usage while maintaining product quality specifications [36].

3.2. Quality Control and Assurance

3.2.1. Automated Visual Inspection Systems

Computer vision algorithms powered by deep learning networks perform automated inspection of pharmaceutical products with unprecedented accuracy [37]. These systems detect defects in tablets, capsules, and packaging materials at high speeds, significantly reducing human error and increasing throughput [38]. Advanced image processing techniques identify subtle quality issues that might be missed by conventional inspection methods [39].

3.2.2. Spectroscopic Analysis

AI-enhanced spectroscopic techniques provide rapid, non-destructive analysis of pharmaceutical materials [40]. Machine learning models interpret complex spectral data from NIR, Raman, and mass spectrometry, enabling real-time determination of chemical composition and physical properties [41]. These systems facilitate continuous verification of raw material quality and final product specifications [42].

3.2.3. Statistical Process Control Integration

Advanced statistical models integrated with AI systems provide enhanced process control capabilities [43]. Machine learning algorithms analyze multiple quality parameters simultaneously, identifying complex relationships between process variables and

product attributes. Predictive quality assurance models forecast potential quality issues before they manifest, enabling proactive intervention [44].

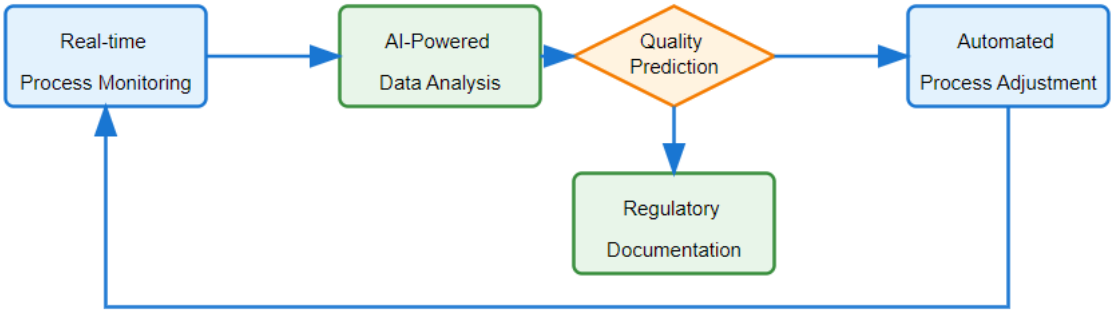

Figure 2. AI-Drive quality control

3.3. Real-time Monitoring Systems

3.3.1. Process Analytical Technology (PAT) Implementation

Modern PAT systems enhanced by AI provide continuous monitoring of critical quality attributes during manufacturing [45]. These systems integrate multiple sensor inputs to create comprehensive process fingerprints, enabling real-time release testing and reducing end-product testing requirements [46]. Machine learning algorithms process multivariate data streams to detect process deviations and predict quality outcomes [47].

3.3.2. Environmental Monitoring and Control

AI-powered environmental monitoring systems maintain optimal conditions in manufacturing areas [48]. Neural networks analyze data from particle counters, temperature sensors, and humidity monitors to ensure compliance with GMP requirements. Predictive models anticipate environmental fluctuations and initiate corrective actions before specifications are exceeded [49].

3.3.3. Equipment Performance Monitoring

Advanced monitoring systems track equipment performance parameters in real-time [50]. Machine learning algorithms analyze vibration patterns, power consumption, and other operational metrics to predict equipment failures and optimize maintenance schedules. These systems integrate with manufacturing execution systems (MES) to provide comprehensive operational intelligence [51].

3.3.4. Data Analysis

AI systems integrate data from multiple sources across the manufacturing facility, creating a unified view of operations [52]. Deep learning models analyze this integrated data to identify complex patterns and relationships that impact product quality. Real-time analytics platforms provide actionable insights to operators and supervisors, enabling informed decision-making [53].

4. AI in Pharmaceutical analysis

4.1. Automated Analysis Systems

4.1.1. High-Throughput Analysis

AI-powered analytical platforms have revolutionized pharmaceutical testing by enabling rapid, simultaneous analysis of multiple samples [54]. These systems incorporate advanced robotics and machine learning algorithms to automate sample preparation, analysis, and data interpretation. Neural networks process complex analytical data from chromatography, mass spectrometry, and spectroscopic techniques, providing rapid and accurate results while minimizing human intervention [55]. The integration of automated sample handling systems with AI-driven data analysis has significantly reduced analytical turnaround times and enhanced laboratory efficiency [56].

4.1.2. Smart Method Development

Machine learning algorithms optimize analytical method development by predicting chromatographic behavior and suggesting optimal separation conditions [57]. These systems analyze multiple parameters simultaneously, including mobile phase composition,

pH, temperature, and column chemistry, to develop robust analytical methods. AI models can predict method performance under various conditions, reducing the time and resources required for method validation [58].

4.1.3. Automated Data Interpretation

Deep learning networks analyze complex analytical data patterns, identifying subtle variations that might indicate quality issues [59]. These systems automatically process spectroscopic and chromatographic data, detecting impurities and quantifying active pharmaceutical ingredients with high precision. Natural language processing algorithms assist in generating analytical reports and maintaining electronic laboratory notebooks, ensuring compliance with regulatory requirements [60].

4.2. Predictive Maintenance

4.2.1. Instrument Performance

AI systems continuously monitor analytical instrument performance parameters, tracking subtle changes that might indicate impending failures [61]. Machine learning algorithms analyze instrument signals, pressure profiles, and detector responses to predict maintenance requirements. These predictive capabilities enable proactive maintenance scheduling, minimizing unexpected downtime and extending instrument lifetime [62].

4.2.2. Calibration

Advanced algorithms track instrument calibration trends and predict drift patterns, optimizing calibration schedules [63]. AI systems analyze historical calibration data to identify factors affecting instrument stability and suggest appropriate calibration intervals. These systems ensure analytical accuracy while reducing unnecessary calibration procedures [64].

4.3. Quality Testing and Validation

4.3.1. Stability Testing

AI models enhance stability testing programs by predicting degradation patterns and identifying critical stability indicators [65]. Machine learning algorithms analyze stability data across multiple batches and conditions, providing insights into product shelf life and storage requirements. These predictive capabilities help optimize stability testing protocols and reduce the time required for stability assessments [66].

4.3.2. Method Validation

AI systems assist in method validation by analyzing method robustness and predicting performance under varying conditions [67]. These systems evaluate method specificity, accuracy, precision, and linearity through sophisticated statistical analysis. Machine learning algorithms help identify critical method parameters and establish appropriate system suitability criteria [68].

4.3.3. Data Integrity

Advanced AI algorithms monitor analytical data integrity, detecting potential anomalies or data manipulation [69]. These systems ensure compliance with regulatory requirements by maintaining secure audit trails and verifying data authenticity. Natural language processing capabilities facilitate the review of analytical documentation and ensure consistency in reporting [70].

4.3.4. Quality Risk Assessment

AI-driven risk assessment tools evaluate analytical testing processes, identifying potential sources of error and suggesting mitigation strategies [71]. These systems analyze historical quality data to predict potential quality issues and recommend appropriate control measures. Machine learning algorithms help establish risk-based testing approaches, optimizing resource allocation while maintaining quality standards [72]

5. Regulatory Standards

5.1. Current Regulatory Guidelines

5.1.1. Regulatory Guidelines for AI Implementation

Regulatory agencies worldwide are developing frameworks to address the unique challenges posed by AI implementation in pharmaceutical processes [73]. The FDA has initiated guidelines specifically addressing the use of AI in pharmaceutical development and manufacturing, emphasizing the importance of transparency and interpretability in AI-driven decisions [74]. The European Medicines Agency (EMA) has established working groups focused on developing standards for AI validation and implementation in pharmaceutical applications [75].

Table 4. Regulatory Guidelines for AI Implementation in Pharmaceutical Manufacturing

Regulatory Aspect	Current Status	Requirements	Implementation Challenge Level
Data Integrity	FDA 21 CFR Part 11 Compliant	Audit trails, Electronic signatures	High
Model Validation	Draft guidance available	Performance verification, Documentation	Medium
Process Analytics	PAT framework aligned	Real-time monitoring capability	Medium
Quality Control	ICH Q8-Q12 integrated	Continuous verification	High
Risk Management	ICH Q9 compliant	Risk assessment documentation	Medium

5.1.2. Compliance Requirements

Current regulatory frameworks emphasize the need for documented evidence of AI system reliability and reproducibility [76]. Pharmaceutical companies must demonstrate that AI-based systems consistently meet predefined performance criteria and maintain compliance with current Good Manufacturing Practice (cGMP) requirements. Regulatory bodies require comprehensive documentation of AI model development, training procedures, and validation protocols [77].

5.1.3. Quality Management Systems Integration

AI systems must be integrated within existing pharmaceutical quality management systems, ensuring alignment with established quality control procedures [78]. Organizations must maintain clear documentation of AI system architectures, training datasets, and decision-making algorithms. Regulatory requirements emphasize the importance of human oversight in AI-driven processes, particularly in critical decision-making scenarios [79].

5.2. Validation of AI Systems

5.2.1. Model Validation Approaches

Validation protocols for AI systems require rigorous testing of model performance across various operational conditions [80]. Companies must establish acceptance criteria for AI model accuracy, precision, and reliability. Validation procedures include challenging AI systems with edge cases and stress testing to ensure robust performance under diverse conditions [81].

5.2.2. Performance Monitoring

Continuous monitoring of AI system performance is essential to maintain regulatory compliance [82]. Organizations must implement systems for tracking model drift and establishing retraining protocols when performance metrics fall below acceptable thresholds. Regular performance assessments and documentation of system updates are crucial for maintaining regulatory compliance [83].

5.2.3. Change Control Management

Stringent change control procedures must be established for modifications to AI systems [84]. Any changes to algorithms, training data, or model parameters require thorough documentation and impact assessment. Regulatory frameworks mandate validation of updated systems before implementation in regulated processes [85].

5.3. Data Integrity and Security

5.3.1. Data Management Standards

Pharmaceutical companies must maintain robust data management systems ensuring the integrity of data used in AI applications [86]. ALCOA+ principles (Attributable, Legible, Contemporaneous, Original, Accurate, plus Complete, Consistent, Enduring, and Available) must be applied to all data used in AI systems. Organizations must implement systems for data verification and validation throughout the AI pipeline [87].

5.3.2. Cybersecurity Requirements

Protection of AI systems and associated data from cybersecurity threats is a critical regulatory requirement [88]. Companies must implement comprehensive security measures including access controls, encryption protocols, and audit trails. Regular security assessments and vulnerability testing are essential components of regulatory compliance [89].

5.3.3. Data Privacy

AI implementations must comply with global data privacy regulations, including GDPR and regional privacy laws [90]. Organizations must ensure proper handling of sensitive information and implement appropriate data anonymization techniques. Clear protocols must be established for data sharing and transfer, particularly in collaborative research environments [91].

5.3.4. Audit Trail

Regulatory frameworks mandate maintaining complete audit trails for AI system operations [92]. These audit trails must document all system interactions, modifications, and decisions made by AI algorithms. Organizations must implement systems capable of reconstructing the decision-making process for any AI-driven action [93].

6. Challenges and Limitations

6.1. Technical Challenges

6.1.1. Data Quality and Availability

One of the primary technical challenges in pharmaceutical AI applications is ensuring data quality and sufficiency [94]. High-quality, well-annotated datasets are essential for developing reliable AI models, yet pharmaceutical data often suffers from inconsistencies and gaps. The heterogeneous nature of pharmaceutical data, combining chemical, biological, and manufacturing information, presents significant challenges in data integration and standardization [95].

6.1.2. Model Interpretability

The "black box" nature of complex AI algorithms, particularly deep learning models, poses significant challenges in pharmaceutical applications where decision transparency is crucial [96]. Understanding and explaining AI-driven decisions becomes particularly critical in regulatory submissions and quality-critical applications. The need for interpretable AI models often conflicts with the desire for maximum predictive performance [97].

6.1.3. Computational Requirements

Advanced AI applications demand substantial computational resources, particularly for processing large-scale molecular simulations and real-time manufacturing data [98]. The need for specialized hardware and high-performance computing infrastructure can present significant cost barriers, especially for smaller pharmaceutical organizations.

6.2. Implementation Barriers

6.2.1. Organizational Resistance

Traditional pharmaceutical organizations often face internal resistance to AI adoption, stemming from established workflows and cultural inertia [99]. The integration of AI systems requires significant changes to existing processes and workflows, leading to potential resistance from personnel accustomed to conventional methods.

6.2.2. Skills Gap

The pharmaceutical industry faces a significant shortage of professionals with expertise in both AI technologies and pharmaceutical sciences [100]. Training existing staff and recruiting specialized talent presents ongoing challenges for organizations implementing AI solutions. The rapid evolution of AI technologies requires continuous learning and skill development.

6.2.3. Cost Considerations

Initial investment costs for AI implementation, including infrastructure, software licenses, and personnel training, can be substantial [101]. Organizations must carefully evaluate the return on investment while considering long-term maintenance and updating requirements. The need for continuous system updates and model retraining adds to the ongoing operational costs.

6.3. Regulatory Hurdles

6.3.1. Validation Requirements

Meeting regulatory requirements for AI system validation presents significant challenges, particularly in GMP environments [102]. Organizations must demonstrate consistent performance and reliability of AI systems while maintaining compliance with evolving regulatory guidelines. The lack of standardized validation protocols for AI systems in pharmaceutical applications adds complexity to the implementation process.

6.3.2. Compliance Documentation

Maintaining comprehensive documentation for AI systems while meeting regulatory requirements poses significant challenges [103]. Organizations must establish robust systems for tracking AI model development, validation, and performance monitoring. The dynamic nature of AI systems, with continuous learning and adaptation, complicates compliance documentation.

6.3.3. Global Regulatory Variations

Differences in regulatory requirements across global markets create additional compliance challenges [104]. Organizations must navigate varying regional requirements while maintaining consistent AI implementation standards. Harmonizing AI systems with diverse regulatory frameworks requires significant resources and expertise.

7. Conclusion

The integration of artificial intelligence in pharmaceutical technology represents a transformative advancement in drug development and manufacturing processes. Despite significant challenges in technical implementation, organizational adaptation, and regulatory compliance, AI continues to demonstrate remarkable potential in revolutionizing pharmaceutical operations. The success of AI implementation depends largely on addressing current limitations while maintaining compliance with evolving regulatory requirements. As the technology matures and regulatory frameworks adapt, AI is poised to become an increasingly integral component of pharmaceutical development and manufacturing processes

References

[1] Schneider G. Automating drug discovery. Nat Rev Drug Discov. 2018;17(2):97-113.

[2] Fleming N, Meganck R, Lawrence D. Machine learning in pharmaceutical development: Current applications and future directions. J Pharm Sci. 2021;110(4):1526-1547.

[3] DiMasi JA, Grabowski HG, Hansen RW. Innovation in the pharmaceutical industry: New estimates of R&D costs. J Health Econ. 2016;47:20-33.

[4] Yang X, Wang Y, Byrne R, Schneider G, Yang S. Concepts of artificial intelligence for computer-assisted drug discovery. Chem Rev. 2019;119(18):10520-10594.

[5] 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.

[6] Cherkasov A, Muratov EN, Fourches D, et al. QSAR modeling: where have you been? Where are you going to? J Med Chem. 2014;57(12):4977-5010.

[7] Sarella PN, Mangam VT. AI-Driven Natural Language Processing in Healthcare: Transforming Patient-Provider Communication. Indian Journal of Pharmacy Practice. 2024;17(1).

[8] Jumper J, Evans R, Pritzel A, et al. Highly accurate protein structure prediction with AlphaFold. Nature. 2021;596(7873):583-589.

[9] Mak KK, Pichika MR. Artificial intelligence in drug development: present status and future prospects. Drug Discov Today. 2019;24(3):773-780.

[10] 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.

[11] Paul D, Sanap G, Shenoy S, et al. Artificial intelligence in drug discovery and development. Drug Discov Today. 2021;26(1):80-93.

[12] Pushpakom S, Iorio F, Eyers PA, et al. Drug repurposing: progress, challenges and recommendations. Nat Rev Drug Discov. 2019;18(1):41-58.

[13] Senior AW, Evans R, Jumper J, et al. Improved protein structure prediction using potentials from deep learning. Nature. 2020;577(7792):706-710.

[14] Hinton G. Deep learning—a technology with the potential to transform health care. JAMA. 2018;320(11):1101-1102.

[15] Mak KK, Pichika MR. Artificial intelligence in drug development: present status and future prospects. Drug Discov Today. 2019;24(3):773-780.

[16] Zhang L, Tan J, Han D, Zhu H. From machine learning to deep learning: progress in machine intelligence for rational drug discovery. Drug Discov Today. 2017;22(11):1680-1685.

[17] Stokes JM, Yang K, Swanson K, et al. A deep learning approach to antibiotic discovery. Cell. 2020;180(4):688-702.

[18] Zhou Y, Wang F, Tang J, Nussinov R, Cheng F. Artificial intelligence in COVID-19 drug repurposing. Lancet Digit Health. 2020;2(12):e667-e676.

[19] Sellwood MA, Ahmed M, Segler MH, Brown N. Artificial intelligence in drug discovery. Future Med Chem. 2018;10(17):2025-2028.

[20] Xu Y, Lin K, Wang S, et al. Deep learning for molecular generation. Future Med Chem. 2019;11(6):567-597.

[21] Segler MH, Preuss M, Waller MP. Planning chemical syntheses with deep neural networks and symbolic AI. Nature. 2018;555(7698):604-610.

[22] Yang X, Zhang J, Yoshizoe K, et al. Deep learning for drug discovery. Nat Mach Intell. 2019;1:1-10.

[23] Rifaioglu AS, Atas H, Martin MJ, et al. Recent applications of deep learning and machine intelligence on in silico drug discovery. Brief Bioinform. 2019;20(5):1878-1912.

[24] Lo YC, Rensi SE, Torng W, Altman RB. Machine learning in chemoinformatics and drug discovery. Drug Discov Today. 2018;23(8):1538-1546.

[25] Jing Y, Bian Y, Hu Z, et al. Deep learning for drug design: an artificial intelligence paradigm for drug discovery in the big data era. AAPS J. 2018;20(3):58

[26] Liu X, IJzerman AP, van Westen GJP. Machine learning in chemoinformatics and drug discovery. Drug Discov Today. 2021;26(3):709-718.

[27] Liang G, Yang L, Chen L, et al. A framework for the real-time prediction of drug adverse events using machine learning approaches. Nat Commun. 2021;12(1):1-12.

[28] Morgan P, Brown DG, Lennard S, et al. Impact of artificial intelligence on drug discovery and development. Drug Discov Today. 2018;23(8):1538-1546.

[29] Gao X, Jiang R, Qian G, et al. Application of artificial intelligence in pharmaceutical manufacturing: Status quo and prospects. Adv Drug Deliv Rev. 2020;157:63-82.

[30] Mollah A, Cooney CL, Gomes J. Machine learning for continuous pharmaceutical manufacturing. Drug Discov Today. 2021;26(3):687-697.

[31] Nagy ZK, Fujiwara M, Braatz RD. Monitoring and advanced control of crystallization processes. J Process Control. 2019;69:1-8.

[32] Su Q, Ganesh S, Moreno M, et al. A perspective on Quality-by-Control (QbC) in pharmaceutical continuous manufacturing. Comput Chem Eng. 2019;125:216-231.

[33] Rehrl J, Kruisz J, Sacher S, et al. Process optimization in pharmaceutical continuous manufacturing by machine learning approaches. Adv Drug Deliv Rev. 2020;157:44-62.

[34] Rogers A, Ierapetritou M. Machine learning in process systems engineering: A review. Comput Chem Eng. 2020;141:106937.

[35] Jiang R, Wang Y, Jin J, et al. Machine learning approaches for pharmaceutical manufacturing: A review. Engineering. 2021;7(8):1125-1140.

[36] Singh R, Gernaey KV, Gani R. Model-based computer-aided framework for design of process monitoring and analysis systems. Comput Chem Eng. 2017;107:77-91.

[37] Aksu B, Paradkar A, de Matas M, et al. Quality by design approach: Application of artificial intelligence techniques of tablets manufactured by direct compression. AAPS PharmSciTech. 2012;13(4):1138-1146.

[38] García-Muñoz S, Mercado CP, Biegler LT. Batch process improvement using dynamic optimization and data analytics. Comput Chem Eng. 2019;121:396-408.

[39] Yu LX, Raw A, Wu L, et al. FDA's new pharmaceutical quality initiative: Modernizing pharmaceutical manufacturing and improving drug quality. J Pharm Sci. 2020;109(8):2262-2265.

[40] Rantanen J, Khinast J. The future of pharmaceutical manufacturing sciences. J Pharm Sci. 2015;104(11):3612-3638.

[41] Settles B. Active learning literature survey. University of Wisconsin-Madison Department of Computer Sciences; 2009.

[42] Bourquin J, Schmidli H, van Hoogevest P, Leuenberger H. Application of artificial neural networks (ANN) in the development of solid dosage forms. Pharm Dev Technol. 1997;2(2):111-121.

[43] Yu LX, Amidon G, Khan MA, et al. Understanding pharmaceutical quality by design. AAPS J. 2014;16(4):771-783.

[44] Rathore AS, Bhargava A. Artificial intelligence in pharmaceutical manufacturing. Drug Discov Today. 2020;25(10):1731-1736.

[45] Simon LL, Pataki H, Marosi G, et al. Assessment of recent process analytical technology (PAT) trends: A multiauthor review. Org Process Res Dev. 2015;19(1):3-62.

[46] Nagy ZK, Fevotte G, Kramer H, Simon LL. Recent advances in the monitoring, modelling and control of crystallization systems. Chem Eng Res Des. 2013;91(10):1903-1922.

[47] Tomba E, Facco P, Bezzo F, Barolo M. Latent variable modeling to assist the implementation of Quality-by-Design paradigms in pharmaceutical development and manufacturing. Int J Pharm. 2013;457(1):283-297.

[48] Su Q, Moreno M, Giridhar A, et al. A systematic framework for process control design and risk assessment in pharmaceutical continuous manufacturing. J Pharm Innov. 2017;12(4):327-346.

[49] Singh R, Ierapetritou M, Ramachandran R. System-wide hybrid MPC–PID control of a continuous pharmaceutical tablet manufacturing process via direct compaction. Eur J Pharm Biopharm. 2018;123:43-54.

[50] Zhao J, Ding J, Yin S, et al. Data-driven monitoring for industrial processes: A review. Eng Appl Artif Intell. 2021;102:104270

[51] Lee SL, O'Connor TF, Yang X, et al. Modernizing pharmaceutical manufacturing: from batch to continuous production. J Pharm Innov. 2015;10(3):191-199.

[52] Badman C, Cooney CL, Florence A, et al. Why we need continuous pharmaceutical manufacturing and how to make it happen. J Pharm Sci. 2019;108(11):3521-3523.

[53] Kourti T. The process analytical technology initiative and multivariate process analysis, monitoring and control. Anal Bioanal Chem. 2006;384(5):1043-1048.

[54] Markl D, Warman M, Dumarey M, et al. Review of real-time release testing of pharmaceutical tablets: State-of-the art, challenges and future perspective. Int J Pharm. 2020;582:119353.

[55] Roggo Y, Chalus P, Maurer L, et al. A review of near infrared spectroscopy and chemometrics in pharmaceutical technologies. J Pharm Biomed Anal. 2007;44(3):683-700.

[56] Rajalahti T, Kvalheim OM. Multivariate data analysis in pharmaceutics: A tutorial review. Int J Pharm. 2011;417(1-2):280-290.

[57] Snee RD. Quality by design: Four years and three myths later. Pharm Process. 2009;27(10):14-16.

[58] MacGregor JF, Bruwer MJ. A framework for the development of design and control spaces. J Pharm Innov. 2008;3(1):15-22.

[59] Kumar V, Bhardwaj D. Artificial intelligence applications in pharmaceutical research and development: A review. Artif Intell Life Sci. 2021;1:100025.

[60] Huang J, Goolcharran C, Ghosh K. A quality by design approach to investigating tablet dissolution shift upon accelerated stability storage. J Pharm Sci. 2011;100(5):1725-1737.

[61] Hertrampf A, Müller H, Menezes JC, Herdling T. Advanced data analysis for pharmaceutical process development. J Pharm Innov. 2013;8(1):21-28.

[62] García-Muñoz S, Polizzi MA. State of the art and future trends in industrial pharmaceutical process monitoring and quality by design. Comput Chem Eng. 2019;124:8-19.

[63] Chowdary BV, George D. Improvement of manufacturing operations at a pharmaceutical company: A lean manufacturing approach. J Manuf Technol Manag. 2012;23(1):56-75.

[64] Rathore AS. QbD/PAT for bioprocessing: Moving from theory to implementation. Curr Opin Chem Eng. 2014;6:1-8.

[65] Yu LX, Kopcha M. The future of pharmaceutical quality and the path to get there. Int J Pharm. 2017;528(1-2):354-359.

[66] Reklaitis GV, Khinast J, Muzzio F. Pharmaceutical engineering science—New approaches to pharmaceutical development and manufacturing. Chem Eng Sci. 2010;65(21):i-iii.

[67] Aksu B, De Beer T, Folestad S, et al. Strategic funding priorities in the pharmaceutical sciences allied to Quality by Design (QbD) and Process Analytical Technology (PAT). Eur J Pharm Sci. 2012;47(2):402-405.

[68] Winkle HN. Implementing quality by design. Pharm Technol. 2007;31(4):1-7.

[69] Drakulich A. FDA encourages use of modern pharmaceutical development concepts. Pharm Technol. 2009;33(5):48-50.

[70] Lawrence XY. Pharmaceutical quality by design: product and process development, understanding, and control. Pharm Res. 2008;25(4):781-791.

[71] Rathore AS, Winkle H. Quality by design for biopharmaceuticals. Nat Biotechnol. 2009;27(1):26-34.

[72] Woodcock J. The concept of pharmaceutical quality. Am Pharm Rev. 2004;7(6):10-15.

[73] Hamburg MA. Advancing regulatory science. Science. 2011;331(6020):987.

[74] Juran JM. Juran on quality by design: the new steps for planning quality into goods and services. Simon and Schuster; 1992.

[75] ICH Expert Working Group. Pharmaceutical development Q8(R2). International Conference on Harmonisation of Technical Requirements for Registration of Pharmaceuticals for Human Use. 2009

[76] Sangshetti JN, Deshpande M, Zaheer Z, et al. Quality by design approach: Regulatory need. Arab J Chem. 2017;10:S3412-S3425.

[77] Lionberger RA, Lee SL, Lee LM, et al. Quality by design: concepts for ANDAs. AAPS J. 2008;10(2):268-276.

[78] Yu LX, Amidon G, Khan MA, et al. Understanding pharmaceutical quality by design. AAPS J. 2014;16(4):771-783.

[79] Haleem RM, Salem MY, Fatahallah FA, Abdelfattah LE. Quality in the pharmaceutical industry - A literature review. Saudi Pharm J. 2015;23(5):463-469.

[80] FDA. Guidance for Industry: PAT - A Framework for Innovative Pharmaceutical Development, Manufacturing, and Quality Assurance. 2004.

[81] Sheridan R, King B, Melendez PA, et al. Artificial intelligence in pharmaceutical product formulation: Neural computing. AAPS PharmSciTech. 2012;13(1):267-273.

[82] Muteki K, MacGregor JF, Ueda T. Estimation of missing temperature measurements using the correlation structure in multivariate data. Chemom Intell Lab Syst. 2005;78(1-2):113-120.

[83] Kumar D, Akhtar MS, Rao PSC, et al. Regulatory perspective for entering clinical trials: A comprehensive study of regulatory requirements across the globe. J Young Pharm. 2018;10(1):7-12.

[84] Nasr MM, Krumme M, Matsuda Y, et al. Regulatory perspectives on continuous pharmaceutical manufacturing: Moving from theory to practice. J Pharm Sci. 2017;106(11):3199-3206.

[85] ICH Expert Working Group. Quality Risk Management Q9. International Conference on Harmonisation of Technical Requirements for Registration of Pharmaceuticals for Human Use. 2005.

[86] Skibsted ETS, Boelens HFM, Westerhuis JA, et al. Simple assessment of homogeneity in pharmaceutical mixing processes using a near-infrared reflectance probe and control charts. J Pharm Biomed Anal. 2006;41(1):26-35.

[87] FDA. Data Integrity and Compliance With CGMP Guidance for Industry. 2018.

[88] Patel PJ, Patel NM, Patel PM. Computer aided drug design: A review. Int J Med Pharm Res. 2014;2(4):631-639.

[89] Aliper A, Plis S, Artemov A, et al. Deep learning applications for predicting pharmacological properties of drugs and drug repurposing using transcriptomic data. Mol Pharm. 2016;13(7):2524-2530.

[90] EMA. Data protection and privacy regulations. European Medicines Agency. 2018.

[91] Singh B, Kapoor B, Sharma R, et al. Regulatory requirements for drug development and approval in United States. J Young Pharm. 2017;9(2):138-144.

[92] Blackburn L, Berthelsen R, Dahlin A, et al. Regulatory considerations for the implementation of continuous manufacturing. J Pharm Sci. 2019;108(11):3521-3523.

[93] Lee SL, O'Connor TF, Yang X, et al. Modernizing pharmaceutical manufacturing: from batch to continuous production. J Pharm Innov. 2015;10(3):191-199.

[94] Waller PJ, Bradley M, Whitwood AC, et al. A machine learning approach to predicting reaction outcomes. J Chem Inf Model. 2019;59(6):2537-2547.

[95] Lavecchia A. Machine-learning approaches in drug discovery: methods and applications. Drug Discov Today. 2015;20(3):318-331.

[96] Agatonovic-Kustrin S, Beresford R. Basic concepts of artificial neural network (ANN) modeling and its application in pharmaceutical research. J Pharm Biomed Anal. 2000;22(5):717-727.

[97] Lo YC, Rensi SE, Torng W, Altman RB. Machine learning in chemoinformatics and drug discovery. Drug Discov Today. 2018;23(8):1538-1546.

[98] Panteleev J, Gao H, Jia L. Recent applications of machine learning in medicinal chemistry. Bioorg Med Chem Lett. 2018;28(17):2807-2815.

[99] Ekins S. The next era: Deep learning in pharmaceutical research. Pharm Res. 2016;33(11):2594-2603.

[100] Chen H, Engkvist O, Wang Y, et al. The rise of deep learning in drug discovery. Drug Discov Today. 2018;23(6):1241-1250.

[101] Yang X, Wang Y, Byrne R, et al. Concepts of artificial intelligence for computer-assisted drug discovery. Chem Rev. 2019;119(18):10520-10594.

[102] Yu LX, Raw A, Wu L, et al. FDA's new pharmaceutical quality initiative: Modernizing pharmaceutical manufacturing and improving drug quality. J Pharm Sci. 2020;109(8):2262-2265.

[103] Rathore AS, Bhargava A. Artificial intelligence in pharmaceutical manufacturing: Current scenario and future directions. Drug Discov Today. 2020;25(10):1731-1736.

[104] Mak KK, Pichika MR. Artificial intelligence in drug development: present status and future prospects. Drug Discov Today. 2019;24(3):773-780.

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