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ARTIFICIAL INTELLIGENCE (AI) & COMPUTER AIDED DRUG DESIGN (CADD) FOR UTILIZATION IN PHARMACEUTICAL FIELD: A CRITICAL REVIEW

Pawan Kumar Gupta*[1]
[1]Research Scholar, Department of Pharmacy, MJP Rohilkhand University, Bareilly, 243006, Uttar Pradesh, India

Shweta Gupta[1]
[1]Research Scholar, Department of Pharmacy, MJP Rohilkhand University, Bareilly, 243006, Uttar Pradesh, India

Prashant Kumar[1]
[1]Research Scholar, Department of Pharmacy, MJP Rohilkhand University, Bareilly, 243006, Uttar Pradesh, India

Yogendra Pal[1]
[1]Research Scholar, Department of Pharmacy, MJP Rohilkhand University, Bareilly, 243006, Uttar Pradesh, India

Shiv Dev Singh[2]
[2]Associate Professor, Department of Pharmacy, MJP Rohilkhand University, Bareilly, 243006, Uttar Pradesh, India

S B Tiwari[3*]
[3*]Associate Professor, Department of Pharmacy, MJP Rohilkhand University, Bareilly, 243006, Uttar Pradesh, India

***Corresponding author:** S B Tiwari
Associate Professor, Department of Pharmacy, MJP Rohilkhand University, Bareilly, 243006, Uttar Pradesh, India **Email id:** s.tiwari@mjpru.ac.in

Abstract:
Artificial Intelligence (AI) approaches have been widely used in pharmacy research to optimize the output of the drug discovery and development pipeline. To identify and design small molecules as clinically effective therapeutics, various computational methods have been evaluated as promising strategies, depending on the purpose and systems of interest. Ligand and structure-based drug design methods are effective technologies, which can be applied to virtual screening for lead identification and optimization. Here, we review the progress in this field and summarize the application of some new technologies which have already developed. These state-of-the-art tools have been used for the discovery and development of active agents for various diseases, and their application in different therapies. The described protocols are appropriate for all drug discovery

stages, but expertise is still needed to perform the studies based on the targets of interest. It focused to create awareness for AI as a component of pharmacy practice in the future, to encourage pharmacists to embrace this advancement, and as much as possible put in the effort to acquire the relevant skills, which will enable pharmacists and researchers to contribute towards the much-envisaged development.

Keywords: Artificial Intelligence, Computer Aided Drug Design, Pharmaceutical field, Tele-medicine

Introduction:

The roots of computer-aided drug design can be traced back to the mid-20th century when computers started becoming available for scientific research [1]. Early efforts were focused on using computers for structure-activity relationship (SAR) studies and simple quantitative structure-activity relationship (QSAR) models [2]. Emergence of Molecular Modeling: The advent of molecular modeling in the 1970s marked a significant development in CADD. Molecular mechanics and molecular dynamics simulations became popular for studying the behavior of molecules at the atomic level [3,4]. Structure-Based Drug Design (SBDD): SBDD became a cornerstone of CADD, emphasizing the importance of understanding the three-dimensional structures of biological macromolecules, such as proteins and nucleic acids. Advances in X-ray crystallography and NMR spectroscopy contributed to obtaining high-resolution structures [5]. QSAR and Chemo-informatics: Quantitative Structure-Activity Relationship (QSAR) models gained prominence in predicting the biological activity of compounds based on their chemical structure [6,7]. Chemo-informatics, involving the storage and analysis of chemical information, became integral to CADD. High-Throughput Screening (HTS): The rise of high-throughput screening in the late 20th century generated vast amounts of biological data. CADD methods were employed to process and analyze HTS data, aiding in the identification of potential drug candidates [8].

Integration of Computational Biology: The integration of computational biology techniques, such as bioinformatics and genomics, into CADD allowed for a more holistic approach to drug discovery. Understanding biological pathways and networks became crucial for target identification and validation. Virtual Screening Techniques: Virtual screening, including methods like molecular docking and pharmacophore modeling, gained popularity for the efficient screening of compound libraries. These techniques helped prioritize compounds for experimental testing, reducing time and costs. Quantum Mechanics and Molecular Dynamics: The incorporation of quantum mechanics and molecular dynamics simulations provided a more accurate representation of molecular interactions [9]. These methods allowed for the study of dynamic behavior, including protein-ligand interactions over time. Machine Learning and Artificial Intelligence: The 21st century witnessed a paradigm shift with the integration of machine learning and artificial intelligence in CADD. Advanced algorithms, including neural networks and deep learning models, were applied to predict bioactivity and optimize molecular structures. Personalized Medicine and

Targeted Therapies: CADD started contributing to the development of personalized medicine by considering individual patient characteristics and genetic information [10].

Targeted therapies, designed with precision, aimed to maximize therapeutic effects while minimizing side effects [11]. Ethical Considerations and Open Science. The ethical use of CADD technologies and the importance of transparency in algorithms gained attention [12,13]. Open-source initiatives and collaborative efforts became common, promoting the sharing of tools, databases, and knowledge. Current Challenges and Future Directions: Despite significant progress, challenges such as accurate prediction of off-target effects [14] and understanding complex biological systems persist. Future directions include more comprehensive integration of omics data, increased use of explainable AI, and advancements in quantum computing for complex simulations. In summary, the background of computer-aided drug design in pharmacy reflects a continuous evolution driven by technological advancements, interdisciplinary collaborations, and a relentless pursuit of more efficient and effective drug discovery processes [15-17].

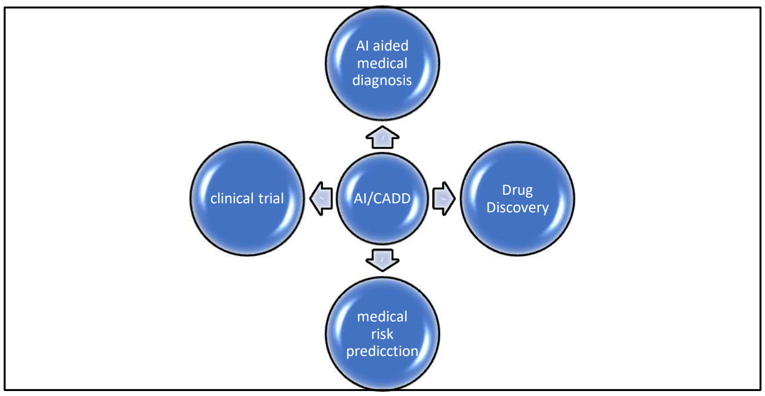

Fig. 1. Different Research network of AI/CADD in Pharmaceutical Field

Materials and Method:

The integration of Artificial Intelligence (AI) in pharmacy encompasses various materials and technologies aimed at improving pharmaceutical research, drug discovery, clinical care, and overall healthcare outcomes [18]. Here are some key aspects of AI in pharmacy: Machine Learning (ML) and Drug Discovery: Materials: High-performance computing systems, large datasets of chemical structures, and biological data [19,20]. ML algorithms analyze massive datasets to identify patterns and predict potential drug candidates. This involves the use of computational models for virtual screening, QSAR modeling, and predicting drug-target interactions [21]. Natural Language Processing (NLP) for Literature Mining: Materials: Text-mining tools, curated biomedical databases, and natural language processing algorithms. NLP is employed to extract information from a vast amount of scientific literature [22]. It helps researchers stay updated on the latest findings, drug interactions, and emerging trends in pharmaceutical research. Clinical Decision Support Systems (CDSS): Materials: Patient records, electronic health records (EHRs), and clinical databases [23]. CDSS, powered by AI, assists healthcare professionals in making informed decisions by analyzing patient data. It aids in personalized medicine, medication management, and treatment planning [24]. Robotics and Automation in Pharmacies: Materials: Robotic systems, AI-driven automation platforms. Robotics in pharmacies, managed by AI, can handle tasks such as medication dispensing, inventory management, and prescription filling, reducing errors and increasing efficiency [25,26]. Predictive Analytics for Inventory Management: Materials: Historical sales data, inventory records, and predictive analytics tools. AI-driven predictive analytics models help pharmacies optimize inventory levels, reduce wastage, and ensure that essential medications are always available. Personalized Medicine and Genomic Data: Materials: Genomic data, patient health records, and AI algorithms. AI analyzes genomic data to identify individual variations that may impact drug responses [26]. This contributes to the development of personalized medicine tailored to a patient's genetic makeup. Tele pharmacy and Remote Patient Monitoring: Materials: Telecommunication infrastructure, wearable devices, and AI algorithms [27-29]. AI facilitates remote patient monitoring by analyzing data from wearable and other connected devices. It enables pharmacists to provide timely interventions and support, especially for chronic disease management. Drug Repurposing and Computational Biology Materials: Biological databases, chemical databases, and computational biology tools [30]. AI is used to identify existing drugs that may have potential applications in new therapeutic areas. This accelerates drug development by repurposing existing compounds for different indications. Explainable AI (XAI) for Regulatory Compliance Materials: Regulatory guidelines, AI models with explainability features. In pharmaceuticals, where regulatory compliance is critical, Explainable AI ensures that AI-driven decisions are transparent and can be understood by regulatory authorities. Block-chain for Drug Traceability: - Materials: Block-chain technology, sensors, and AI algorithms. AI, in conjunction with block-chain, helps track the entire pharmaceutical supply chain, ensuring the authenticity of drugs and minimizing the risk of counterfeit medications [31]. Drug Safety Monitoring: - Materials: Pharmacovigilance databases, adverse event reports, and AI algorithms. AI aids in the continuous monitoring of drug safety by analyzing adverse event reports and identifying potential safety concerns associated with medications [32]. The integration of AI in pharmacy is a multi-faceted approach that leverages various materials and technologies to enhance different aspects of pharmaceutical research, drug development, and healthcare delivery. The combination of computational power, diverse datasets, and advanced algorithms is transforming the landscape of pharmacy and contributing to more personalized and efficient patient care.

METHOD: Artificial Intelligence (AI) is increasingly playing a pivotal role in various aspects of pharmacy, ranging from drug discovery and development to patient care and pharmacy operations. Here are some key methods of AI application in pharmacy: Drug Discovery and Design: Method: Machine Learning (ML) and Deep Learning. AI algorithms analyze large datasets of molecular structures, biological data, and chemical properties to predict potential drug candidates. Deep learning models, such as neural networks, are used for image analysis and pattern recognition in drug discovery. Virtual Screening: Method: Molecular Docking, Structure-Based Drug Design. AI is used to simulate and predict the binding of small molecules to target proteins [33]. This helps identify potential drug candidates by virtually screening large chemical libraries. Quantitative

Structure-Activity Relationship (QSAR) Modeling: Method: Machine Learning, Chemo-informatics. AI models predict the biological activity of compounds based on their chemical structure. QSAR models assist in understanding the relationship between molecular features and bioactivity.

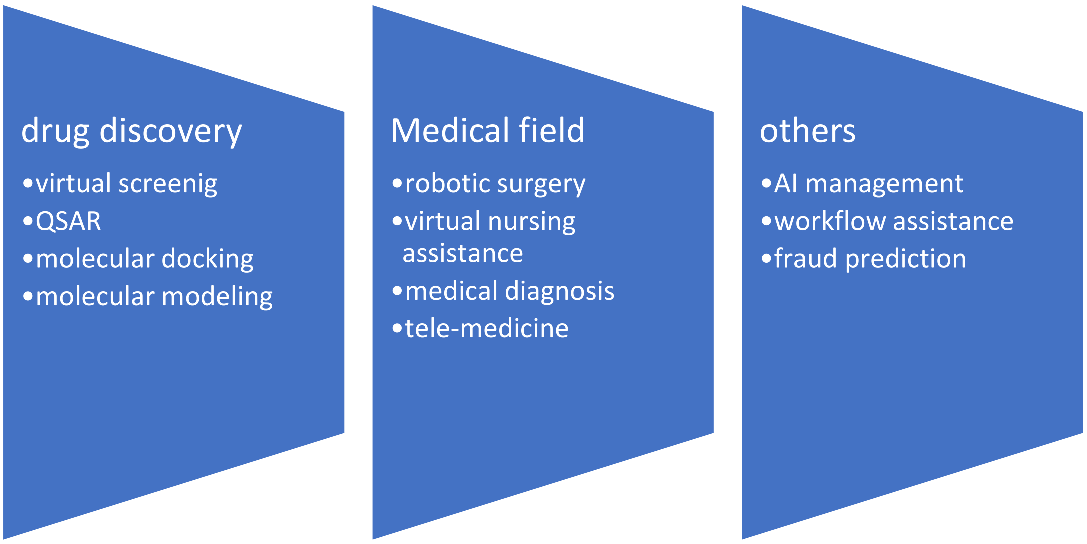

Fig. 2. Utilization of AI/CADD in Advancement of Pharmacy

Clinical Decision Support Systems (CDSS): Method: Rule-based Systems, Machine Learning. CDSS helps healthcare professionals make informed decisions by analyzing patient data and providing evidence-based recommendations for drug selection, dosing, and monitoring. Pharmacovigilance and Adverse Event Monitoring: Natural Language Processing (NLP), Machine Learning. AI is used to analyze textual information from electronic health records, social media, and other sources to identify and monitor adverse drug reactions and safety concerns [34]. Personalized Medicine: Genomic Data Analysis, Machine Learning. AI analyzes genomic data to identify genetic variations that influence drug responses. This information is used to tailor drug therapies to individual patients, maximizing efficacy and minimizing side effects [35]. Medication Adherence and Patient Monitoring: Predictive Analytics, Remote Patient Monitoring. AI algorithms analyze patient data, including medication adherence patterns and physiological parameters from wearable, to monitor and improve patient adherence to prescribed medications. Tele-pharmacy Services: Telecommunication Technology, AI Chat-bots. AI-powered chat-bots and virtual assistants support patient consultations, answer medication-related queries, and provide information on drug interactions in Tele-pharmacy services. Inventory Management and Supply Chain Optimization: Predictive Analytics, Machine Learning. AI analyzes historical data and predicts demand patterns to optimize inventory levels [36]. This ensures efficient supply chain management, reduces stock-outs, and minimizes excess inventory. Robotics and Automation: Robotic Process Automation (RPA), Machine Learning. AI-driven robotics automate repetitive tasks in pharmacy operations, such as medication dispensing and inventory management, improving efficiency and reducing errors. Block-chain for Drug Traceability: Block-chain Technology, Smart Contracts. AI can be integrated with block-chain to enhance drug traceability, ensuring the authenticity of pharmaceutical products throughout the supply chain [37,38]. These methods collectively contribute to the advancement of pharmacy practice by improving efficiency, accuracy, and patient outcomes. The interdisciplinary nature of AI in pharmacy involves collaboration between pharmacists, healthcare professionals, data scientists, and computer scientists to harness the full potential of these technologies.

Result and Discussion:

Artificial Intelligence (AI) applications in pharmacy are diverse, ranging from drug discovery and development to patient care and operational efficiency. Here are several key applications of AI in pharmacy: Drug Discovery and Development: AI is used to analyze biological data, chemical properties, and molecular structures to identify potential drug candidates. Machine learning models predict the efficacy and safety of new compounds, accelerating the drug development process [39]. Virtual Screening and Molecular Docking: AI-driven virtual screening methods help in identifying potential drug candidates by simulating the interaction between molecules and target proteins. Molecular docking predicts the binding affinity of drug candidates to specific targets [40]. Quantitative Structure-Activity Relationship (QSAR) Modeling: AI is employed to develop models that predict the biological activity of compounds based on their chemical structure. QSAR models assist in understanding the relationship between molecular features and pharmacological effects. Clinical Decision Support Systems (CDSS): AI-driven CDSS assists healthcare professionals in making informed decisions about drug selection, dosing, and patient monitoring. These systems integrate patient data, medical literature, and guidelines to provide personalized recommendations [41]. Pharmacovigilance and Adverse Event Monitoring: AI, particularly natural language processing (NLP), is used to analyze unstructured data from various sources to identify and monitor adverse drug reactions. Automated systems help in early detection of potential safety issues. Personalized Medicine: AI analyzes genomic and clinical data to tailor drug therapies based on individual patient characteristics. Predictive modeling helps identify patient-specific responses to medications [42]. Medication Adherence Monitoring: AI applications monitor patient adherence to prescribed medications through data analysis of refill patterns, electronic health records, and patient-reported information. Interventions can be suggested to improve adherence and patient outcomes. Tele-pharmacy Services: AI-powered chat-bots and virtual assistants provide information on medications, answer patient queries, and support remote consultations [43]. Tele-pharmacy services improve accessibility and patient engagement. Inventory Management and Supply Chain Optimization: AI applications analyze historical data and predict demand patterns to optimize inventory levels. Supply chain optimization reduces the risk of stock-outs and minimizes excess inventory. Robotics and Automation: AI-driven robotics automated tasks in pharmacy operations, such as medication dispensing and inventory management [44]. Automation enhances efficiency, reduces errors, and allows pharmacists to focus on patient care. Block-chain for Drug Traceability: AI can be integrated with block-chain

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technology for secure and transparent drug traceability. This application ensures the authenticity of pharmaceutical products throughout the supply chain. Disease Diagnosis and Prediction: AI analyzes medical images, patient records, and diagnostic data to assist in disease diagnosis and prognosis. Predictive modeling helps in identifying disease risk factors and potential interventions. Educational Tools for Pharmacists: AI-powered educational tools provide pharmacists with updated information on medications, guidelines, and treatment protocols [45]. Continuous learning platforms support professional development. Continuous Monitoring of Patient Health: AI applications continuously monitor patient health data from wearable and other devices. Early detection of health issues enables timely interventions and improved patient outcomes. These applications collectively demonstrate the transformative potential of AI in pharmacy, enhancing both the scientific and operational aspects of the field. They contribute to more efficient drug discovery, improved patient care, and streamlined pharmacy operations.

Conclusion:

In conclusion, the integration of Artificial Intelligence (AI) in pharmacy holds tremendous promise and is reshaping the landscape of pharmaceutical research, patient care, and operational processes. The convergence of advanced technologies, big data, and sophisticated algorithms has ushered in a new era of efficiency, precision, and innovation. AI expedites the drug discovery process by analyzing vast datasets, predicting drug candidates, and optimizing molecular structures. This has the potential to bring new and effective medications to market more rapidly. Virtual screening, molecular docking, and QSAR modeling, powered by AI, enable more accurate predictions of drug-target interactions. This reduces the need for extensive experimental testing and accelerates the identification of potential therapeutic agents. AI analyzes genomic data and patient profiles to tailor drug therapies based on individual characteristics. This move toward personalized medicine improves treatment outcomes by considering genetic variations and other patient-specific factors. Clinical Decision Support Systems (CDSS) powered by AI assist healthcare professionals in making informed decisions about drug selection, dosing, and monitoring. This leads to more personalized and evidence-based patient care. AI applications, particularly natural language processing, facilitate the monitoring of adverse drug reactions and safety concerns. Early detection enhances patient safety and contributes to regulatory compliance. AI-driven Tele-pharmacy services, including virtual assistants, improve patient engagement and accessibility to healthcare services. Patients can receive information, consultations, and support remotely. Robotics and automation, guided by AI, streamline pharmacy operations such as medication dispensing and inventory management. This not only reduces errors but also allows pharmacists to focus more on patient care. AI optimizes inventory management and supply chains by predicting demand patterns. This leads to more efficient stock levels, reduced wastage, and improved overall logistics. AI provides pharmacists with educational tools that keep them updated on medications, guidelines, and best practices. Continuous learning platforms support ongoing professional development. AI applications monitor patient health continuously through wearable devices, improving adherence to prescribed medications. This contributes to better disease management and patient outcomes.

Integrating AI with block-chain enhances the traceability and authenticity of pharmaceutical products, addressing issues related to counterfeiting and ensuring the integrity of the supply chain. In essence, AI is driving a paradigm shift in pharmacy, empowering professionals with tools and insights that were once unimaginable. The synergy of computational power and healthcare expertise is opening up new frontiers, paving the way for more precise treatments, better patient outcomes, and a more efficient and secure pharmaceutical ecosystem. The ongoing collaboration between pharmacists, healthcare practitioners, data scientists, and technology experts will likely continue to yield groundbreaking advancements, making AI an indispensable force in the evolution of pharmacy.

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Conflict of Interest:

Authors declared for none conflict of interest.

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