ejpmr, 2025, 12(7), 295-305

EUROPEAN JOURNAL OF PHARMACEUTICAL AND MEDICAL RESEARCH

www.ejpmr.com

SJIF Impact Factor 7.065

Review Article

ISSN (O): 2394-3211

ISSN (P): 3051-2573

GENERATIVE AI IN DRUG DISCOVERY: FROM MOLECULAR GENERATION TO POST MARKETING SURVEILLANCE

Kavitha R.[a]*, Arundathi P.[a], Hemalatha K. K.[a] and Allen D.[b]

[a,b]KMCH College of Pharmacy, Coimbatore 641048, India.

***Corresponding Author: Kavitha R.**

KMCH College of Pharmacy, Coimbatore 641048, India.

Article Received on 20/05/2025 **Article Revised on 10/06/2025** **Article Accepted on 30/06/2025**

ABSTARCT

Pharmaceutical industries experience revolutionary changes through artificial intelligence integration which transforms all pharmaceutical activities from discovery processes through post-market surveillance. Artificial intelligence algorithms use large amounts of data to discover new therapeutic targets and predict molecular interactions with highly accurate precision which leads to faster drug discovery processes. Through formulation optimization AI finds ideal excipients that prove effective for enhancing drug absorption as it determines compound stability better than manual testing methods. Intelligent automation in pharmaceutical manufacturing supports real-time process optimization and predictive maintaining while reducing waste which leads to high-quality cost-effective drug production. AI quality control systems built with predictive analytics and computer vision capabilities discover manufacturing deviations while checking that regulatory needs remain in compliance. AI-based pharmacovigilance operates as a transformative tool for post-market surveillance to discover drug side effects quickly and track treatment performance using big data analysis methods. The full potential of AI depends on resolving key hurdles that include clear algorithm processes as well as secure data and adaptable regulatory environments. The study shows how AI technologies transform pharmaceutical sciences by creating a smarter and more efficient patient-centered path for future pharmaceutical work.

KEYWORDS: AI in Pharma, Intelligent Drug Discovery, Smart Formulation, AI-Driven Manufacturing, Predictive Quality Control.

INTRODUCTION

Different industries maintain their continuous growth through various methods which satisfy customer needs. The pharmaceutical domain serves as an essential industry because it protects human life directly. Through enduring innovation and new technologies the pharmaceutical industry manages global healthcare crises as well as medical emergency situations including the current pandemic.[1] Deep research and development operations drive pharmaceutical innovation through technology development and packaging operations and market-oriented strategy development. New pharmaceutical products consist of drug molecules and biologic representatives that show better stability and efficacy for unmet medical needs. Extensive investigation combined with future study is necessary to evaluate substantial drug toxicity because of its major concerns. The primary objective focuses on creating drug substances that yield optimal healthcare advantages as well as industrial implementation compatibility. Managed healthcare delivery requires technological improvements because pharmaceutical companies deal with various operational problems within their worldwide medical operations.

Artificial intelligence brought profound changes to the pharmaceutical industry since it affected all stages of drug innovation and formulation development and manufacturing and inspection processes and regulatory requirements. Various effects of AI-powered solutions on pharmaceutical drug development through complete product creation receive extensive examination. The paper demonstrates how machine learning algorithms and data analytics tools, prediction modeling frameworks boost discovery methods and formulation designs and manufacturing operations and quality control programs and post-market surveillance techniques. AI enables essential pharmaceutical evaluation through a review of its current advancements and future opportunities that exist alongside existing implementation barriers for pharmaceutical drug development.[2]

The pharmaceutical industry quickly adopts artificial intelligence (AI) combined with machine learning (ML) techniques to obtain advanced data analysis capabilities and better decision-making tools. Artificial intelligence contains methods that include natural language processing and computer vision as well as robotics and focuses on machine learning to produce algorithms

which analyze data for prediction without human programming.

Deep learning functions within machine learning to turn artificial neural networks into systems that recognize complex data relationships in extensive datasets similarly to human brain processing. The leading-edge technologies processing images and understanding language along with identifying speech rely on advanced deep-learning functions. Researches can use the table in Figure 1 to understand the main differences between AI, ML, and DL as well as their role in advancing drug discoveries and enhancing delivery techniques.[3]

HISTORY AND TIMELINE OF AI

Herbert A Simon and Allen Newell created the Logic Theorist application during the well-known 1956 Dartmouth college conference. The Artificial Intelligence market is expected to grow tenfold during the period from 2017 through 2022. Research shows the natural language processing industry will increase its earnings by 28.5% throughout 2017. The worldwide market value of business analysis and big data generated US$ 122 billion in 2015 yet analysts project this market to exceed US$ 200 billion by 2020. Artificial intelligence experienced its initial turbulent period in the 1950s. Deep Blue from IBM proved the power of artificial intelligence as it defeated chess champion Garry Kasparov during matches in 1997 thus transitioning from dreamer to reality. The new Watson supercomputer developed by IBM managed to win the US$1m game-show prize through its Jeopardy victory back in 2011. An essential drug discovery milestone for Watson happened when Pfizer partnered with it in 2016 to fast-track their immuno-oncology work. In December 2016 researchers received access to medical documents via partnership between Pfizer and IBM through which they could create precise representations of data relations in different files.[4]

GOALS OF AI, ML, DL

Artificial Intelligence (AI) together with Machine Learning (ML) and Deep Learning (DL) have established themselves as disruptive technologies which transform operations in pharmaceuticals and healthcare and biotechnology sectors. The main objective of AI involves developing systems which execute intellectual operations previously handled by humans throughout problem-solving tasks alongside pattern recognition and decision-making functions. Machine Learning operates as an AI subset which develops data learning algorithms that allow systems to adjust their operational methods according to new inputs while making determinations without human code intervention. Multiple technologies collaborate to improve solution performance by increasing efficiency while attaining better accuracy thresholds and expanded scale for pharmaceutical drug discovery programs alongside personalized medicine applications along with clinical trial enhancement systems as well as patient care administration programs. The application of sophisticated computational models combined with large data volumes helps AI and ML with DL achieve new findings that lead to automated processes which produce improved healthcare and pharmaceutical results. The continuous advancement work aims to produce systems which learn and adapt automatically and deliver immediate actionable solutions within various fields.[5]

IMPORTANCE OF AI IN PHARMACEUTICAL INDUSTRY

The pharmaceutical sector experienced a tremendous rise in data digitalization during the last few years. The process of digitalization presents a difficulty to obtain and evaluate information for solving intricate clinical situations. The ability of AI to automatically process extensive data quantities makes it an ideal solution for this task. The technology-based system that involves many advanced tools and networks functions as a system able to mimic human intelligence. The system exists without endangering human contact although it operates without full human presence. The technology of AI operates through software and systems which process data inputs to autonomously generate independent decisions toward specific functional targets. The pharmaceutical field demonstrates expanding applications of this technology according to the information presented in this review. McKinsey Global Institute publishes research indicating that fast-moving AI automation will reshape work culture at all levels of society.

Neural networks became the initial use of AI in drug product development activities during the 1990s to forecast disintegration time and dissolution rate of immediate-release oral tablets. Research expanded toward modern delivery systems which targeted clinical API barriers and managed gastrointestinal discharge rates. AI helps develop micro- and nanoparticle drug delivery systems by efficiently processing formulation optimization parameters which are complicated to handle.

The discussion investigates how AI transforms pharmaceutical operations beginning from drug compound creation until product delivery (Fig. 2). Drugs benefit from AI by getting faster more precise drug development while pharmaceutical scientists utilize AI to enhance both formulation stability and drug absorption rates. The manufacturing performance through its capability to forecast dimensional quality changes and establish solid product consistency standards. The detection of defects and the evaluation of safety and efficacy are both enhanced through AI for final product quality assurance. CEO Strategic Decisions aims to maximize supply chain management operations along with logistics and distribution functions for pharmaceutical delivery timing. Through post-market surveillance evaluation AI performs real-time drug reaction analysis which sustains pharmaceutical safety

from product launch until its end of life. The evaluation shows how Artificial Intelligence develops pharmaceutical industry sectors while enabling more effective individualized healthcare systems accessible for all patients.

AI IN THE LIFECYCLE OF PHARMACEUTICAL PRODUCT

Given its capability to contribute to drug development from the laboratory to patient treatment AI involvement becomes plausible through its support for designing medications logically and making decisions for defining healthcare solutions alongside managing medical data for future medication development. The analytical and decision-making E-VAI platform from Eularis applies competitive market evaluation using ML methodology for predicting pharmaceutical sales drivers through interface-based analytical road mapping that incorporates company competitors along with stakeholders and present market share information.[6] This platform assists marketing executives to direct resources for reaching their maximum market share potential while understanding which investments will be most beneficial.

AI IN DRUG DISCOVERY

More than 1060 possible molecules exist within the chemical space to create numerous drug molecules. The drug development process faces slow and costly procedures because of lacking advanced technologies but AI implements solutions to manage these issues. AI systems have the ability to detect both hit and lead compounds while speeding up the drug target validation process along with drug structure optimization.[7]

The extensive data liabilities that AI handles include unparalleled dataset volume together with its rapid expansion and diverse nature and unpredictable quality. Pharmaceutical companies struggle to process their drug development data sets which consist of millions of compounds through traditional ML tools. The QSAR-based computational model functions to produce quick predictions of extensive chemical compounds along with basic parameters like log P or log D. The existing computational models remain distant from establishing predictions regarding compound efficacy along with their adverse side effects. ště of QSAR-based models remain a challenge because they work with small training sets and have errors in experimental training data along with a lack of experimental verification. The safety and efficacy testing of drug molecules requires the implementation of DL and relevant modelling approaches based on big data modelling and analysis to handle current challenges. The pharmaceutical company Merck created a QSAR ML challenge during 2012 to showcase how DL benefits drug discovery operations within the pharmaceutical sector. The DL predictive models exhibited stronger performance than conventional ML methods when predicting 15 ADMET data sets of drug candidates.[8]

The combination of in silico methods which screen digital compounds virtually through structure and ligand-based approaches results in better profiling analysis and faster nonlead compound elimination and more economical drug molecule selection. The drug design algorithms choose lead compounds based on physical chemical and toxicological properties through algorithms which incorporate both coulomb matrices and molecular fingerprint recognition functions. The prediction of suitable compound chemical forms requires multiple elements that include predictive models with molecular similarity analysis and computer simulations along with the generation methods. The Mult objective automated replacement algorithm utilized by researchers optimizes the potency profile of cyclin-dependent kinase-2 inhibitors by examining their shape similarity in combination with biochemical activity and physicochemical properties.

PREDICTION OF PHYSIOCHEMICAL PROPERTIES

Artificial Intelligence tools exist to perform predictions of various drug properties. During compound optimization previous operations produced vast datasets that ML uses to develop its program. A drug design algorithm requires molecular descriptors such as SMILES strings and potential energy measurements and electron density measurements and atomic coordinate data to create feasible molecules via DNN for predicting drug properties.[9]

Drugs created digitally through virtual screening enable fast profile evaluations while swiftly eliminating potential unsafe compounds and afford cheaper drug selections. Both molecular fingerprint recognition functions alongside coulomb matrices present in the drug design algorithms enable selection of lead compounds based on their physical chemical and toxicological attributes. The prediction of suitable compound chemical forms requires multiple elements that include predictive models with molecular similarity analysis and computer simulations along with the generation methods. The Mult objective automated replacement algorithm utilized by researchers optimizes the potency profile of cyclin-dependent kinase-2 inhibitors by examining their shape similarity in combination with biochemical activity and physicochemical properties.[10]

PREDICTION OF BIOACTIVITY

A drug molecule must demonstrate strong receptor affinity to demonstrate its therapeutic effectiveness. A drug molecule which fails to establish any attachment to the target protein will lose its capacity to trigger therapeutic outcomes. The improper interaction of developed drug molecules with alternative proteins or receptors at times leads to toxicity. The prediction of drug–target inter actions depends critically on drug target binding affinity (DTBA). AI-based approaches use two different methods for measuring drug–target binding affinity through identifying either drug characteristics or

target similarities. The identification of chemical components within drug molecules and target moieties occurs during feature-based interaction to establish feature vectors. Similarity-based interaction analyzes the drug-target similarities but maintains the belief that identical drugs will bind to equivalent targets.[11]

The approaches of DeepAffinity and Protein and Drug Molecule interaction prediction (PADME) serve similar purposes with previously mentioned models. The interpretable DeepAffinity model takes unlabelled and labelled data through a deep learning architecture made of RNN functions and CNN structures. A protein sequence analysis together with the compound expressed in the SMILES format forms the basis for this approach. PADME operates as a DL-based system which uses feed-forward neural networks for predicting drug target interactions (DTIs). The model accepts drug and protein features as inputs to predict their interaction strength as output. The drug is represented by SMILES while PSC provides the sequence data for the target entities. The unsupervised ML approaches MANTRA and PREDICT enable predictions of therapeutic outcomes for drugs with known and unknown pharmaceutical ingredients for drug repurposing and understanding therapeutic mechanisms. Through the CMap data set MANTRA conducts group clustering to identify compounds sharing similar mechanism of action and biological pathways. ADME information constitutes an important element of drug bioactivity data. XenoSite and FAME alongside SMARTCyp assist researchers in determining the metabolic sites of pharmaceutical compounds. The software collection of CypRules along with MetaSite and MetaPred and SMARTCyp and WhichCyp enables researchers to determine specific CYP450 isoforms which participate in drug metabolic processes. SVM-based predictors achieved high accuracy scores in clearing the pathway processes for 141 approved drugs.[12]

PREDICTION OF PHARMACOKINETICS OF DRUG CANDIDATES

AI algorithms run predictive models and perform simulations to boost the outcome success of clinical trials. These assessment tools enable early-stage safe and effective drug candidate evaluation before launching full-scale clinical trials. By utilizing AI-powered models scientists can determine how drug candidates behave inside the body and anticipate the pharmacokinetic and pharmacodynamic effects which leads to identification of possible adverse reactions. The clinical data aids developers optimize their drug development paths.[13]

Drug–target binding affinity (DTBA) functions as an approach to predict bioactivities in new drug candidates through analysing strength levels which drugs bind with their targets. AI-based platform tools measure drug binding affinity by using structure-based and feature-based methods. The exploration of possible binding sites through three-dimensional molecule and protein structures takes place in structure-based method. Two well-known methods fall under these examples: docking techniques together with molecular dynamics simulations. The techniques demand large amounts of time alongside essential known protein structures for successful implementation. Feature-based methods create feature vectors from both ligands and proteins before using them to train ML/DL models. Neural networks succeed at handling significant datasets after proper training and at resolving numerous obstacles therefore they deliver higher effectiveness than conventional systems. DL techniques employed for DTBA assessment consist of DeepDTA, WideDTA, PADME and DeepAffinity and GraphDTA.

Artificial intelligence serves multiple capabilities in the prediction of generic drug pharmacokinetic properties. AI models processes extensive databases with physicochemical characteristics together with drug-related historical information and clinical trials results to make accurate predictions about absorption distribution metabolism and excretion (ADME) profiles of drugs.AI achieves several impacts through its ability to identify biosimilars, research drug compound crystal structures and execute salt and polymorph screening. Predictive analytics-driven generic drug development benefits from ML-based applications that boost accuracy and efficiency of the development process.AI shows potential as a tool for searching new therapeutic applications of generic pharmaceuticals. Through its AI tool Reboot Rx led by Laura Kleiman develops software to seek generic drugs that might show anticancer capabilities whereas the main focus is prostate cancer. Kleiman creates a platform to reuse generic non-cancer drugs for cancer treatment through ML analytic assessment of existing medical literature to discover promising candidates while motivated by her mother's multiple myeloma diagnosis. Only a minority of the 1000 off-patent drugs receive cancer care applications because researchers have not focused on their potential. Patient advocate Brian McCloskey works with Reboot Rx to instruct its AI platform to analyze research quality and study pertinence using only evidence-based reports that measure well in clinical environments. The initiative aims to lower the cost of cancer medication while promoting government-sponsored trials for drug rediscovery. This campaign seeks both financial accessibility and clinical resourcing for drug innovation.[14]

PREDICTION OF DRUG TOXICITY

Determining the toxicity of drug molecules remains essential for the purpose of preventing toxic side effects. Chemical evaluations happen first through cellular models then animals receive further work to discover toxic effects which drives up drug development expenses. The cost of drug development can be reduced through several web-based tools including LimTox and pkCSM and admetSAR together with Toxtree. The latest AI-based methods allocate compounds into toxicity categories through automated feature detection.

AI IN DESIGNING DRUG MOLECULES

PREDICTION OF TARGET PROTEIN STRUCTURE

Before achieving successful treatment, doctors must establish the correct target when creating new drug molecules. The disease development requires multiple proteins and some of these proteins show overexpression patterns. The successful targeting of diseases demands that scientists predict target protein structures which enables them to create drug molecules. The design corresponds to target protein environmental chemistry thereby allowing AI to forecast compound action while evaluating safety aspects before synthesis or production. AlphaFold uses DNNs to analyze both amino acid distances and bond angles for target protein structure predictions leading to 25 correct out of 43 successful predictions.[15]

Protein structure prediction happened through RNN technologies according to AlQurashi. The author designed three operational phases naming them recurrent geometric network (RGN) which included computation followed by geometry and assessment. The backbone output provided new structural information to the current target residue after receiving as input both encoded protein sequence data and torsional angles obtained from the preceding geometric unit. The production of 3D structures finished the procedure as the most decisive outcome. Sensorial evaluation of predicted and experimental structures utilized distance-based root mean square deviation (dRMSD) as the assessment metric. The RGN operating parameters underwent optimization to minimize the dRMSD between actual and predicted molecular structures. AlQurashi estimated that the estimated protein structure calculation speed of his AI method would surpass AlphaFold. The accuracy rate of AlphaFold remains higher for structures whose reference sequences match the input structures.

The 2D structure prediction of proteins involved MATLAB as well as a feed-forward supervised learning algorithm and backpropagation error algorithm delivered through a nonlinear three-layered NN toolbox. The NN system learned from databases that MATLAB accepted through its training procedure and operated as dual performance assessment and learning mechanism. The 2D structure prediction accuracy reached 62.72% as reported.[16]

PREDICTING DRUG – PROTEIN INTERACTIONS

Success in therapy strongly depends on drug–protein interactions. Predicting drug-protein interactions serves to evaluate drug potency, enables drug product diversification while also minimizing pharmaceutical polypharmacology. The accurate prediction of ligand–protein interactions relies on different AI methods which deliver better therapeutic results. The research from Wang et al. presented an SVM-based model that used 15,000 protein–ligand interactions for training to discover nine new compounds and their binding to four vital targets.

Placing drug molecules together with proteins allows scientists to estimate polypharmacology risk factors that produce undesirable effects between multiple receptors. A new molecule can be designed with polypharmacology principles using AI assistance which produces safer drug molecules. Through the combination of SOM AI platforms and available extensive databases multiple compounds can be related to different targets and off-target elements. Pharmacological drug profiles linked to their potential targets are analyzed by Bayesian classifiers and SEA algorithms.[17]

THE ROLE OF AI IN PHARMACEUTICAL FORMULATION OPTIMIZATION AND DEVELOPMENT

Drug discovery and development needs pharmaceutical formulation development to be a fundamental step. By designing drug formulations pharmaceutical experts can enhance the key features of novel medications including improved bioavailability together with targeted delivery. The current standard for formulating drugs implements a time-consuming research methodology that needs numerous laboratory screenings together with experiments on living beings. AI technology integration into pharmaceutical formulation development has generated a new efficient process that delivers accurate results at reduced costs. Pharmaceutical products' quality characteristics together with their formulation variables and operating parameters linkages can be detected by AI algorithms through experimental data. The models established through AI determine multiple predictions about these systems by measuring excipient-induced API solubility effects whereas API release rates from dosing vehicles and pharmaceutical product physical stability assessments become possible. The three distinct groups where artificial intelligence supports pharmaceutical formulation include conventional dosage forms alongside advanced oral drug delivery and micro/nanoparticles for drug delivery.

CONVENTIONAL DOSAGE FORM

The first application of AI through ML and ANN techniques happened during the initial stages of conventional pharmaceutical dosage form development to estimate drug formulation effectiveness. AI technology allowed the prediction of multiple drug behavioral aspects including mechanical properties and dissolution rates as well as stability and bioavailability to optimize conventional formulations of tablets and capsules. These computational models learned excipient and operating parameter effects during product development to speed up pharmaceutical processes thus researchers achieved faster new product formulation cycles and better optimized formulations for market-safe drug delivery.

CONTROLLED RELEASE TABLET FORMULATION

The development of controlled-release formulations relies on pharmacokinetic simulations combined with ANN functionality. Therefore, with Chem software the ANN model develops complex abilities from processing input along with output data units. The sophisticated ANN model enables researchers to determine the optimal tablet formulations while considering two desired in vitro dissolution time profiles together with two in vivo release profiles. Medical drug absorption in the human body depends on dissolution rates because in vivo drug amount directly correlates with this process. Various in vitro release patterns get identified through the analysis of difference factors (f1) and similarity factor (f2).[18]

IMMEDIATE RELEASE TABLETS FORMULATION

Both analysis methods showed neural network systems delivered superior results than standard statistical assessment methods. The research work of Kesavan and Peck received additional academic analysis through genetic algorithms and neural networks testing. The relative importance between output attributes together with process factor limitations helped determine optimal formulations according to this presentation. Research methods involving neuro-fuzzy computing analyzed the same data while generating beneficial rules to show significant aspects of each product.[19]

HARD GELATIN CAPSULE SHELL FORMULATION

Production of hard gelatin capsule formulations needs executive tools including ANN and expert systems (ES). ANN activates human mental processes that include generalization and learning alongside prediction and abstraction of domain knowledge. The manufacturer can quickly develop specialised strategies for future events and predict theoretical preparation characteristics by swiftly applying data and statistics gathered during investigations using ANNs. Wendy I. Wilson developed a capsule shell production method for Biopharmaceutical Classification System II drugs through the Expert Network and analysis in 2005. She focused on creating the manufacturing procedure for carbamazepine, ketoprofen, naproxen and ibuprofen. The worldwide use of Capsugel's expert system for developing hard gelatin capsule powders showed only limited success since it provided just proposed compositions. The system performed poorly at its initial release because it generated inaccurate predictions alongside extensive errors. The new dataset training of the ANN achieved prediction models with an R2 value of less than 70%. In its predictions for model drugs the smart hybrid system determined drug solubility to be near 5%. Research findings demonstrated the system's capability to develop formulations that met performance requirements based on validating its results with only 10% of newly generated data. The system demonstrated its analysis capabilities for diverse BCS class II drugs by evaluating their wettability and intrinsic dissolving properties according to research.[20]

SOLID DISPERSIONS (SD)

A solid matrix containing dispersed APIs makes up solid dispersions. The technique represents an accessible method to improve drug solubility and bioavailability at present. The pharmaceutical sector and academic institutions have widely adopted them as a solution to address solubility issues with APIs. Various SD formulation studies have utilized ANNs as the main artificial intelligence method for optimization purposes. A group of scientists employed ANNs to increase floating ability and drug release behaviour in Nimodipine SD prepared using PEG and effervescent mixtures. The authors applied ANNs to study the influence between API concentration and PEG molar mass and temperature input factors for PVP-based SD systems. Scientific researchers established a forecasting model which uses ML techniques to determine SD stability. Researchers examined eight ML methods while using twenty molecular descriptors for evaluation. The RF model achieved maximum precision when producing estimates while delivering complete comprehension of all provided inputs. The researchers studied twenty descriptors to identify drug loading ratios together with relative ambient humidity and storage temperature and preparation temperature and molecular weight of polymers as the five main contributors.

THE ROLE OF AI IN QUALITY CONTROL OF PHARMACEUTICAL PRODUCTS

Product or quality control receives transformation through AI technologies since it functions as a vital operation for pharmaceutical manufacturing in the pharmaceutical industry. The evaluation of product security alongside operation efficiency necessitates exact attention. The present quality control methods function effectively yet require extensive work and expose humans to mistakes. AI technologies led to an essential quality control transformation when ML and computer vision features were incorporated. AI systems use their fast and precise abilities to identify manufacturing shortcomings along with unstandardized elements and packaging irregularities in pharmaceutical operations. Through AI implementation organizations have achieved both faster inspections and reduced mistakes. Through its implementation AI has elevated product safety in the market launch process and maintained patient health protection. Inserting AI technology into pharmaceutical product regulation leads to problems regarding how much trust can be placed in AI-driven quality management methods to confirm that products meet specified requirements. An AI system works most effectively when it receives good quality information which covers a wide range of sources for its training or operational use. To validate the reliability and precision of AI-based quality control data in pharmaceutical product processes testing and research must be performed for AI system implementation.

THE ROLE OF AI IN PHARMACEUTICAL MANUFACTURING

Production management through continual manufacturing practices generates worthwhile reductions of product quality differences between various batches. The FDA endorses production without interruptions to prevent variations in both end products and patient results. Several process analytical technologies (PAT) allow efficient cost-effective control of uninterrupted production. The combination of AI technology with PAT through automated ML generates operational enhancements which maintain proper control of manufacturing production processes. Biopharmaceutical product manufacturers achieve business advantages through data science by incorporating logistics system integration into their manufacturing operations. Extended maintenance of these factors should be recognized as a vital regulatory aspect since engineered living cells underlie biopharmaceutical manufacturing operations. A successful manufacturing process requires continuous observance and management of various elements to produce pure steady products. The world's top chemical organizations use big data to boost vaccine output numbers and monitor product quality standards on a regular basis.

THE ROLE OF AI IN POST-MARKET SURVEILLANCE

Continuous post-approval monitoring of drug and medical device safety and effectiveness receives essential support from artificial intelligence advances in post-market surveillance. After market launch PMS acts as a necessary procedure to protect patient health and safety of medical devices that include in vitro diagnostic medical devices. The implementation of AI tools within PMS leads to dramatic improvements across all surveillance domains including data acquisition and analysis and detection of signals and risk assessments as well as patient relationship initiatives. The collection and analysis of huge real-world data through electronic health records social media and patient registries becomes possible with AI thereby providing additional insights beyond standard clinical trials. The recognition of complex patterns by algorithms makes data analysis more thorough than what is possible with limited information. AI improves both signal detection and risk assessment processes through datasets analysis which allows identification of safety issues and drug side effects in patient reports alongside social media interactions thus enabling early detection and regulatory steps. Through predictive analytics powered by AI doctors can evaluate patients who face risks for adverse events as they use this data for decision-making and prevention strategies. Virtual assistants equipped with AI-powered technology deliver medication safety information to patients while enhancing their pharmacovigilance participation. The generation of real-world evidence by AI becomes vital to perform benefit–risk assessments through real-world evidence analysis for ascertaining drug safety and efficacy over long durations. The combination of AI capabilities helps organizations meet regulatory requirements through automated data handling and allows for transparent knowledge sharing of both data insights and risk analyses with regulatory bodies and health service providers. AI fundamentally transforms and optimizes PMS systems to establish a new generation of drug safety monitoring which focuses on patient needs.

DISCUSSION

The pharmaceutical industry will experience significant transformation from AI because the technology shows great potential for drug discovery and product development as well as industry administration and regulatory requirements and PMS. Through AI simulations laboratories can foresee drug interactions with biological systems to run clinical trials at better efficiency and reduced cost. The implementation of AI tools helps optimize supply chain operations and achieves maximum regulatory compliance along with automated formulation procedures and production processes. The identification of optimal practical AI-driven applications with commercial potential will occur in the future. The pharmaceutical industry faces assured transformation through the integration of AI technology because advancements in technology will shape both innovation and medical results in healthcare. .Through continuous advancements in AI technology, it will become increasingly important for researchers to identify new drug targets and predictive patient outcomes because the technology will offer better support for drug research and development. Greater development in AI systems leads to better simulation capabilities that enable researchers to build individualized and performance-driven therapeutic treatments. The development of better targeted medications and personalized healthcare approaches becomes achievable through this advancement leading to increased efficiency in drug development processes. Research using AI capabilities enables advanced exploration of complex diseases therefore leading to better treatments that will achieve improved patient health worldwide. The convergence of AI with technologies like blockchain, quantum computing, and the Internet of Things (IoT) will further unlock new possibilities, ultimately shaping the future of pharmaceutical innovation and global healthcare.

CONCLUSION

Compared to conventional research methodologies, where drug discovery takes years with high attrition rates, AI-driven approaches have significantly reduced timelines and improved success rates, as evidenced by recent breakthroughs in AI-assisted drug design, such as AlphaFold's impact on protein structure prediction. The pharmaceutical sector has accumulated more than 1000 research publications and review papers regarding the application of AI systems during the past five years. Such research counts emphasize the importance of improving and speed maturing present operational methods in pharmaceutical research. Modern

pharmaceutical formulation and development industries rely on expanding AI applications for numerous advantages across their operations. Testing has already shown that artificial intelligence processes both extensive information databases while optimizing medications through improved formulae and speeding up medical research trials.AI applications in pharmaceutical formulation and development are proven to be transformative for the industry while promising continued industrial revolution during the next years.

Table 1: A compilation of AI tools used in drug discovery.

AI MODEL TOOLS	SUMMARY
DeepChem	A free library supplies extensive resources for drug discovery containing deep learning algorithms to forecast molecular properties and execute screening procedures and chemical prospecting operations.
RDKit	An open-source cheminformatics library known for its wide usage provides functionalities to handle molecules and search for substructures along with descriptor computation capabilities. Drug discovery applications benefit from machine learning frameworks through integration of the open-source cheminformatics library.
ChemBERTa	This model specializes in drug discovery applications through its specialized drug development design structure. The Transformer-based framework operates on extensive biomedical and chemical text databases during pretraining which enables it to create new molecules while performing molecular property assessments as well as contribute to lead development processes.
GraphConv	The model uses a machine learning structure built for molecular graphs. The predictive characteristics of properties such as bioactivity and toxicity have been reliably predicted by using structural data within the graph representation of molecules.
AutoDock Vina	The machine learning-based prediction software Autodock Vina serves as a popular choice for estimating small molecule-proteins binding affinity through its advanced techniques. Virtual screening and lead optimization during drug discovery gain support from this software.
SMILES Transformer	Autodock Vina operates as a widely adopted machine learning tool for predicting protein-small molecule binding strength through its powerful methodology. The screening phase and lead optimization phase of drug discovery find support through this software.
Schrödinger Suite	The program serves as a complete software system for drug research featuring different AI functions. The software package contains modules for molecular modeling together with virtual screening modules and both ligand-based and structure-based drug design functions and predictive modeling capabilities.
IBMRXNfor Chemistry	An AImodeldesigned to predict chemical reactions. The framework leverages deep learning methods together with extensive reaction information to predict feasible reaction products thereby supporting new synthetic pathway creation and compound development.
scape-DB	The information retrieval system called Escape-DB (Extraction of Chemical and Physical Properties from the Literature-DrugBank) has been created to extract chemical and biological data from scientific publications using natural language processing with automated learning techniques. Research efforts for drug discovery gain significant value from this database.
GENTRL (Generative Tensorial Reinforcement Learning)	The Adeeplearning system connects reinforcement learning to generative chemistry for creating new molecules possessing specific properties. Rephrase The System Functions To Create Novel Molecules As Well As Optimize Existing Ones And Design New Medical Compounds From Scratch.

Table 2: List of commonly explored AI models in pharmaceutical product development.

AI/Machine Learning Models	Description/usage
Genetic Algorithms	The optimization technique known as genetic algorithms draws its concepts from natural selection together with genetics principles. The optimization techniques based on genetic algorithms enable formulators to develop desired dosage forms by applying them to various formulation compositions along with drug release profiles and process parameters.

Artificial Neural Networks (ANNs)	Researchers use ANN to model drug release kinetics from multiple dosage forms. The predictive modeling through ANN assists pharmaceutical scientists to determine optimal formulation compositions together with API release behavior predictions under different conditions.
Support Vector Machines (SVMs)	The application of SVMs in dosage form optimization helps predict relationships between formulation variables that include excipient composition and processing parameters and drug release profiles. Such tools help refine the area where formulation developers should concentrate their efforts.
Particle Swarm Optimization (PSO)	PSO represents a population-based optimization method dedicated for dosage form optimization tasks. Designers have implemented PSO to optimize various formulation parameters as well as dissolution profiles and particle size distributions.
Artificial Intelligence-based Expert Systems	Expert systems implement artificial intelligence through rule-based systems alongside fuzzy logic to model expert decision procedures. Their utilization involves addressing several formulation together with processing variables for dosage form optimization.
Monte Carlo Simulation	Drugs show improved product performance through Monte Carlo simulation techniques used to handle unpredictability and random variation in product formulation parameters. Such methods enable resilient formulation and process planning.
Computational Fluid Dynamics (CFD)	CFD simulations help improve fluid flow and mixing performance inside dosage form manufacturing operations such as granulation and coating and drying operations. The simulation helps generate efficient processes that operate in uniform ways.
Response Surface Methodology (RSM)	The statistical method of RSM enables objective optimization of dosage form formulations by creating mathematical models which analyze formulation response behavior. Formulation parameters become clearer with the help of this statistical technique which also enables optimization.
Multivariate Analysis Techniques	The optimization of dosage forms benefits from two multivariate analysis methods called principal component analysis (PCA) and partial least squares (PLS). These methods help identify essential formulation variables as well as decrease complexity while improving formulation functionality.

FIGURES

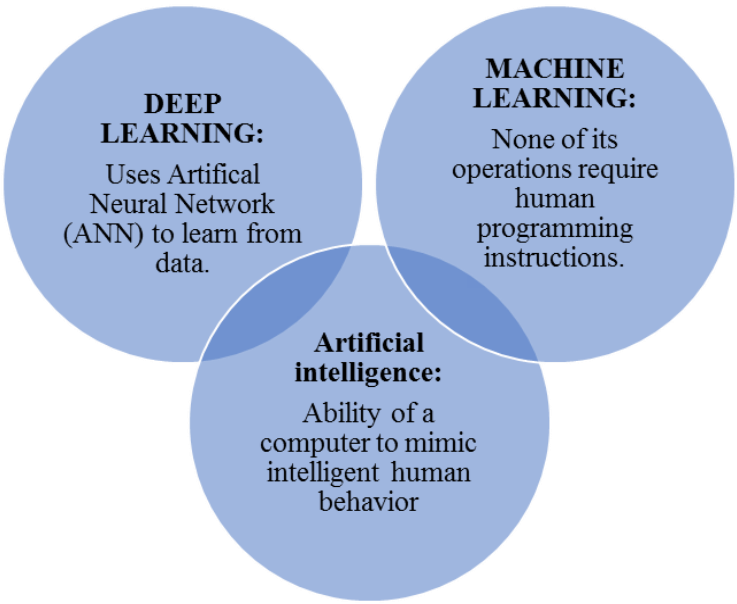

Figure 1: Definitions of AI, ML, and DP.

Figure 2: Artificial intelligence applications improve various stages of drug development and distribution.

ACKNOWLEDGEMENTS

I want to sincerely thank everyone who helped me finish this review essay. I would like to start by expressing my gratitude to my mentors and coworkers for their insightful conversations and invaluable advice, which have greatly influenced the course of this work.

I am also appreciative of the authors of the studies that I have cited, whose work served as the basis for my evaluation. We would especially like to thank [name of any financial organization or institution, if relevant] for their assistance. Finally, I would want to thank my friends and family for their support during this journey.

REFERENCE

1. Krikorian, G.; Torreele, E. We Cannot Win the Access to Medicines Struggle Using the Same Thinking That Causes the Chronic Access Crisis. Health Hum. Rights, 2021; 23: 119–127.
2. Scannell, J.W.; Blanckley, A.; Boldon, H.; Warrington, B. Diagnosing the Decline in Pharmaceutical R&D Efficiency. Nat. Rev. Drug Discov, 2012; 11: 191–200. [CrossRef] [PubMed]
3. Mak, K.-K.; Pichika, M.R. Artificial Intelligence in Drug Development: Present Status and Future Prospects. Drug Discov. Today, 2019; 24: 773–780. [CrossRef]
4. Markoff J. On 'Jeopardy' Watson win is all but trivial. The New York Times, 2017.
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. doi: 10.1038/s41573-019-00098-4.
6. Baronzio, G. et al. Overview of methods for overcoming hindrance to drug delivery to tumors, with special attention to tumor interstitial fluid. Front. Oncol, 2015; 5: 165.
7. Sellwood, M.A. et al. Artificial intelligence in drug discovery. Fut. Sci., 2018; 10: 2025–2028.
8. Ciallella, H.L. and Zhu, H. Advancing computational toxicology in the big data era by artificial intelligence: data-driven and mechanism-driven modeling for chemical toxicity. Chem. Res. Toxicol, 2019; 32: 536–547 23.
9. Mak, K.-K. and Pichika, M.R. Artificial intelligence in drug development: present status and future prospects. Drug Discovery Today, 2019; 24: 773–780 20.
10. Thafar, M. et al. Comparison study of computational prediction tools for drug–target binding affinities. Frontiers Chem., 2019; 7: 1–19.
11. O ¨ztu ¨rk, H. et al. DeepDTA: deep drug–target binding affinity prediction. Bioinformatics, 2018; 34: i821–i829.
12. Pu, L. et al. eToxPred: a machine learning-based approach to estimate the toxicity of drug candidates. BMC Pharmacol. Toxicol, 2019; 20: 2.
13. Chou, W.-C., Lin, Z., Machine learning and artificial intelligence in physiologically based pharmacokinetic modeling. Toxicol. Sci., 2023; 191: 1–14.
14. Drug Discovery News, 2024. AI's Role in Shaping Future Therapeutics. https://www.drugdiscoverynews.com/ai-s-role-in-shaping-future-therapeutics-15877#:~:text=By%20using%20machine%20learning%20and,to%20address%20unmet%20clinical%20needs. accessed 15 January 2024.
15. Mayr, A. et al. DeepTox: toxicity prediction using deep learning. Frontiers Environ. Sci., 2016; 3: 80.

16. Wang, F. et al. Computational screening for active compounds targeting protein sequences: methodology and experimental validation. J. Chem. Inf. Model., 2011; 51: 2821–2828.
17. Hamet P, Tremblay J. Artificial intelligence in medicine. Metabo lism, 2017; 69: S36–S40. https://doi.org/10.1016/j.metabol.2017.01.011
18. Artificial intelligence for drug toxicity and safety. Trends Pharmacol. Sci., September, 40((9)): 624–635. http://dx.doi.org/10.1016/j.tips.2019.07.005 Epub 2019 Aug 2. PMID: 31383376; PMCID: PMC6710127
19. Emig D, Ivliev A, Pustovalova O et al. Drug target prediction and repositioning using an integrated network-based approach. PLoS One, 2013; 8: e60618. https://doi.org/10.1371/journal.pone.0060618
20. Serajuddin ATM Solid dispersion of poorly water-soluble drugs: early promises, subsequent problems, and recent breakthroughs. J Pharm Sci., 1999; 88: 1058–1066. https://doi.org/10.1021/js980403l