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INTEGRATING ARTIFICIAL INTELLIGENCE IN FORMULATION RESEARCH: TOWARD INTELLIGENT AND PERSONALIZED DRUG DELIVERY SYSTEMS

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ABSTRACT

This article reviews the revolutionary function of artificial intelligence (AI) and machine learning (ML) in pharmaceutical formulation research, as they outdistance the traditional trial-and-error and empirical approaches. By combining the advanced computational methodologies, like artificial neural networks (ANNs), support vector machines (SVMs), neuro-fuzzy logic, random forest (RF), and genetic algorithms (GAs), we see that scientists are able to digest complex multidimensional data much more rapidly, successfully predict and optimize formulation parameters, like drug release, dissolution, and excipient choice. The review describes how AI models have successfully implemented across a wide variety of dosage forms (solid dispersions, controlled release tablets, immediate release tablets, capsule shells, emulsions, beads, nanoparticles) and have demonstrated improved formulation robustness, stability, and therapeutic effects. Among other caveats, the review acknowledges that implementation cost, such as a lack of a unique and comprehensive datasets, makes it increasingly difficult. Regardless, the review provides evidence of the versatility, predictiveness, and process efficiency that can be achieved with AI as applied to computational pharmaceutics. AI is reestablishing the pace of innovation in drug product design and personalized medicine, implying that the next step in developing a superior pharmaceutical formulation that benefits patients will require the use of both AI-based and AI-derived approaches.

KEYWORDS: Artificial Intelligence, Artificial Neural Networks, Pharmaceutical Formulation Development, Machine Learning, Drug Delivery Systems, Fuzzy Logic.

INTRODUCTION

A crucial element of pharmaceutical research is the development of formulations that ensure stability, safety, and efficacy. Traditionally, formulation scientists have relied on empirical methods and trial-and-error approaches to enhance combinations of drugs and excipients, as well as process parameters and dosage forms. These traditional techniques may not consistently produce the most reliable or effective results, and often require a substantial commitment of time and financial resources. Recently, the pharmaceutical sector has undergone a significant change due to the incorporation of artificial intelligence (AI) and machine learning (ML) technologies into drug formulation and development processes. These advanced technologies provide innovative strategies for improving predictive capabilities, streamlining the formulation process, and more precisely refining dosage form attributes and excipient selections.[3]

In recent years, a novel field known as 'computational pharmaceutics' employs computational methods, such as artificial intelligence (AI), big data, and multiscale modeling techniques, to create, refine, and evaluate medication formulations. AI systems can analyze the vast amounts of data generated by simulations or tests, providing valuable insights into the behavior of formulations. The incorporation of AI technology in pharmaceutics holds the promise of transforming pharmaceutical research by facilitating quicker, more efficient, and more precise drug formulation and assessment. Clearly, the design and evaluation of specific medication formulations have significantly benefited from the application of these AI prediction models. They are capable of predicting not just the fundamental physicochemical properties of active pharmaceutical ingredients (APIs), but also essential parameters of formulation systems by exploring the high-dimensional formulation space involving the drug/excipients/process combination. Additionally, the algorithms can evaluate the factors that influence the formulation to theoretically assist in designing it.[16] The key components of artificial intelligence were depicted in Fig. 1.

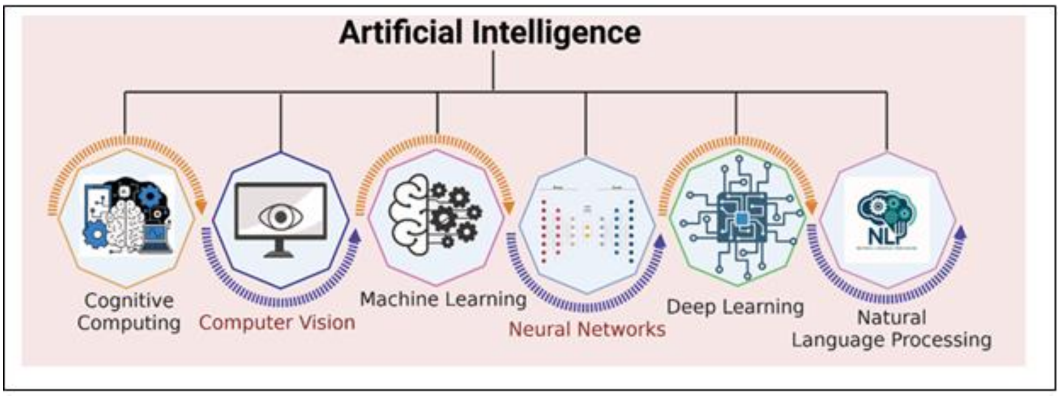

Fig. 1: Overview of how artificial intelligence works through key components such as cognitive computing, computer vision, machine learning, neural networks, deep learning, and natural language processing. [Created in https://BioRender.com]

The application of artificial intelligence (AI) in the areas of drug formulation, delivery, and targeting is increasingly becoming prominent. This encompasses the utilization of machine learning, design of experiments (DOE), molecular docking and simulations, along with various useful software and informatics tools. DOE aids in optimizing processes and formulations by uncovering the relationships between different key factors and responses throughout the manufacture, development, and discovery of drug products. Enhancing optimization boosts the efficiency and reliability of the pharmaceutical process while elevating the quality of drug products. Nonetheless, the DOE methodology can become intricate as the number of factors increases and when faced with nonlinear relationships. When examining datasets with complex multivariate interactions that are difficult to understand with traditional regression or rule-based models, machine learning (ML) is very helpful. Furthermore, machine learning is especially helpful in situations where runs or experiments are unplanned and deviate from predetermined patterns. ML techniques outperform the conventional DOE approach using statistical methods of optimization when analyzing complex interactions between several variables that do not follow a straightforward linear pattern. Furthermore, machine learning techniques can be used to analyze a wide range of information types, including text, pictures, and numerical data.[59]

MILESTONES IN AI

In 1956, the phrase "Artificial Intelligence" was introduced for the very first time. However, since 1950, the concept of artificial intelligence has been applied through both symbolic and problem-solving methods. The important milestones in the domain of artificial intelligence applications were listed in Table 1.[15]

Table 1: Important Milestones In The Area Of The Ai Uses.

Year	Events
1943	Neurons connected in a network can perform logical operations like "and," "or," and "not," as demonstrated by Walter Pitts and Warren McCulloch.
1956	The phrase "artificial intelligence" was initially used.
1958	Perceptrons, a type of neural network developed by Frank Rosenblatt, are capable of one-way information transmission.
1974	"First AI Winter" begins
1986	Back propagation method design, which is popular in deep learning, was promoted by Georey Hinton.
1987	Initiation of “AI winter”.
1997	IBM Deep Blue defeated Russian grandmaster Garry Kasparov.
2013	Google used British technology to conduct effective study on images.
2016	This year, Google DeepMind's AlphaGo AI defeated Go Champion Lee Sedol.

MILESTONES OF AI IN PHARMACY

The important milestones of artificial intelligence in the pharmacy were listed in Table 2.[25,52,31,45]

Table 2: Significant Turning Points For Ai In Pharmacy.

Year	Milestone	Description
1956	AI term coined	"Artificial Intelligence" coined at the Dartmouth Conference, laying foundation for all AI work in science.
1960-1970	Early Medical Expert Systems	DENDRAL (1965–70): First expert system used for chemical structure analysis; MYCIN (1970s): Assisted in antibiotics selection.
1971	INTERNIST-1	The first medical AI diagnostic consultant, used to assist clinicians in diagnosis based on patient symptoms.
1980	Introduction of ANN Models	Early use of Artificial Neural Networks in biomedical applications, making way for complex modeling.
	SUMEX-AIM Resource	National computing resource established for AI biomedical research at Stanford and Rutgers; enabled research networks.
1986	DXplain Medical Expert System	Expanded clinical diagnostic support and information databases for clinicians
1990	Computational Drug Design Begins	AI/ML algorithms start complementing molecular modeling and QSAR (quantitative structure-activity relationships) for drug design.
Late 1990	ML Algorithms for Formulation/Prediction	Machine learning used for predicting formulation properties, bioactivity, and early data mining in pharma.
2000	Pharmacy Management Systems	Early AI used in pharmacy operations for housing and processing patient utilization/drug data.
2010-2015	Early AI application in drug discovery	AI algorithms began accelerating identification of drug candidates and targets, reducing timelines.
2015-2018	Personalized medicine AI models	AI models predicting patient-specific drug responses, enhancing personalized treatment strategies.
2019-2021	AI-powered clinical trial optimization	Introduction of Al digital twins and predictive analytics for patient recruitment and trial design, leading to shorter and more efficient clinical trials.
2022-2023	AI and quantum computing integration	Combining AI with quantum computing enhanced prediction accuracy of protein–drug interactions.
2023	AI-driven formulation development	Launch of AI platforms predicting formulation properties, optimizing excipient combinations.
2023-2024	Collaborative Federated learning models for drug safety	AI models enable detection of rare adverse drug reactions across institutions without data sharing.
2024	AI in pharmaceutical manufacturing	Real-time AI analytics automate quality control and increase efficiency in drug manufacturing.
	Regulatory AI tools	AI assists in automating compliance checks, speeding regulatory approval processes.
2024-2025	Generative AI for molecule design	Use of generative AI to design and optimize novel drug molecules, accelerating innovation.
2025	Widespread adoption and market Growth	Growth in AI adoption across all pharma sectors, with expected multimillion-dollar economic impact by 2030.

TYPES OF ARTIFICIAL INTELLIGENCE

The concept of artificial intelligence is broad and can be categorized in several ways.

AI systems are categorized as follows according to their quality

1. **Weak intelligence or Artificial narrow intelligence (ANI)** – It is a system that has been trained to carry out a certain activity, including traffic signaling, chess, driving, or facial recognition. For instance, social media tagging and Apple SIRI virtual personal help.
2. **Artificial General Intelligence (AGI) or Human Level AI** - It is also called as Strong AI. It has the capacity to make human intelligence simpler. It is therefore capable of solving problems when presented with new tasks. AGI is capable of everything that humans can do.
3. **Artificial Super intelligence (ASI)** – It is a brain capacity that is more active than intelligent humans in every discipline, from science to art, including sketching, mathematics, and space. It varies from a computer that is only marginally more intelligent

than a human to one that is trillions of times more intelligent.

AI expert Arend Hintze categorized AI technologies according to their current and future states. They are as follows:

1. Type 1: This type of AI system is called Reactive machines. E.g. Deep Blue, an IBM chess program that hit chess champion Garry Kasparov in the 1990s. It has the capability to identify checkers on the chess board and can make prognostications; it doesn't have the memory to use once gests. It was created with a specific purpose in mind and is useless in other contexts. Another illustration is Google's Alpha Go.

2. Type 2: This type of AI systems is called Limited memory systems. This system has the capability to use the once gests for the present and unborn problems. In independent vehicles, some of the decision-making functions are designed by this system only. The recorded compliance are used to record the conduct passing in the future, similar to changing the lanes by auto. The compliance is not in the memory permanently.

3. Type 3: This type of AI system is called as “proposition of mind”. It means that all the humans have their own thinking, intentions and solicitations that impact the opinions they make. This is a non-existing AI.

4. Type 4: These are called as tone-mindfulness. The AI systems have the sense of tone and consciousness. However, it understands the condition and uses the ideas present in other's brain, If the machine has tone-mindfulness. This is a non-being AI.[42]

ADVANTAGES OF AI TECHNOLOGY

The potential advantages of AI technology are as follows

- **i) Difficult exploration:** AI exhibits its utility in the mining sector. It is also used in the energy disquisition sector. AI systems are able of probing the ocean by defeating the crimes caused by humans.
- **ii) Daily application:** AI is veritably useful for our diurnal acts and deeds. For exemplifications, GPS system is astronomically used in long drives. Installation of AI in androids helps to prognosticate what an existent is going to class. It also helps in correction of spelling miscalculations.
- **iii) Digital assistants:** Now-a-days, the advanced associations are using AI systems like ‘avatar’ (models of digital sidekicks) for the reduction of mortal requirements. The ‘avatar’ can follow the right logical opinions as these are completely impassive. mortal feelings and moods disturb the effectiveness of judgement, and this problem can be overcome by the uses of machine intelligence.
- **iv) Repetitive tasks:** Generally, mortal beings can perform one task at a time. In discrepancy to the mortal beings, machines are able of performing multi-tasking jobs and can dissect more fleetly in comparison to the mortal beings. Colorful machine parameters, i.e., speed and time can be acclimated according to their conditions.
- **v) Medical uses:** Generally, the croakers can assess the condition of cases and dissect the adverse goods and other health pitfalls associated with the drug with the help of the AI program. Trainee surgeons can gather knowledge by the operations of AI programs like colorful artificial surgery simulators (for exemplifications, gastrointestinal simulation, heart simulation, brain simulation, etc.).
- **vi) No breaks:** Unlike mortal beings who have the capacity of working for 8 h/ day with breaks, the machines are programed in such a way that they are able of performing the work in a nonstop manner for long hours devoid of any kinds of confusions and tedium.
- **vii) Increase technological growth rate:** AI technology is extensively used in utmost of the advanced technological inventions worldwide. It can produce different computational modeling programs and points for the invention of the newer molecules. AI technology is also being used in the development of medicine delivery phrasings.
- **viii) No risk:** In case of working at the parlous zone like fire stations, there are huge chances of causing detriment to the labor force engaged. For the machine literacy programs, if some mishap happens, also broken corridor can be fixable.
- **ix) Acts as aids:** AI technology has played a different function by serving children as well as elders on a 24x7 base. It can perform as tutoring and literacy sources for all.
- **x) Limitless functions:** Machines aren't confined to any boundaries. The impassive machines can do everything more efficiently and also produce more directly than the mortal beings.

DISADVANTAGES OF AI TECHNOLOGY

The important disadvantages of AI technology are as follows

- **i) Expensive:** The launch of AI causes huge plutocratic consumption. Complex designing of machine, conservation and repairing are largely cost-effective. For the designing of one AI machine, a long period is needed by the R&D division. AI machine needs streamlining the software programs, regularly. The reinstallation as well as recovery of the machine consume longer time and huge resources.
- **ii) No replicating humans:** Robots with the AI technology are associated with the power of allowing like mortal and being impassive as these add some advantages to perform the given task more directly without any judgement. However, robots cannot take the decision and give false reports if strange problems arise.
- **iii) No improvement with experience:** Mortal resource can be bettered with gests. In discrepancy, machines with AI technology cannot be enhanced with

experience. They are unfit to identify which one is hardworking and which one is nonworking.

iv) **No original creativity:** Machines with AI technology have neither perceptivity nor emotional intelligence. Humans have the capability to hear, see, feel, and suppose. They can use their creativity as well as studies. These features aren't attainable by the uses of machines.

v) **Unemployment:** The wide uses of AI technology in all the sectors may beget large scale severance. As because of the undesirable severance, mortal workers may lose their working habits and creativity[28,58]

TOOLS OF ARTIFICIAL INTELLIGENCE

1. Artificial neural networks (ANN)

Machine Learning (ML), an essential subdivision of Artificial Intelligence (AI), plays a significant role in data-driven problem-solving. A major part of ML is deep learning, which involves the use of artificial neural networks (ANNs). ANNs are biologically inspired systems made up of multilayer functional units that mimic how electrical impulses are transmitted in the human brain.

In biological neural systems, the fundamental component is the neuron—an electrochemical cell that receives signals from one neuron and transmits signals to others. Similarly, in an ANN, the primary component is the perceptron (or node). These nodes are arranged into layers, and each artificial neuron analyzes the input, processes the information primarily through summation, and produces an output that is transmitted to the next perceptron. ANNs can be categorized based on learning approaches into supervised learning (SL) and unsupervised learning.

In unsupervised learning, the network receives unlabeled input data and works to identify underlying patterns or structures, effectively condensing the data into a more compact and meaningful form.

In supervised learning, the network is given both input and output data, and it "learns" the connection between them with guidance. This approach is considered the most popular and valuable for formulation-related applications.

The arrangement of interconnected neurons in an ANN is referred to as its network architecture. Among the various architectures, the multilayer perceptron (MLP) is a prominent and widely used example. In this model, input variables (X1, X2, X3) are processed through hidden layers to generate an output (Y). The number of input, output, and hidden layers depends on the specific condition and the researcher’s design as depicted in Fig. 2.[46]

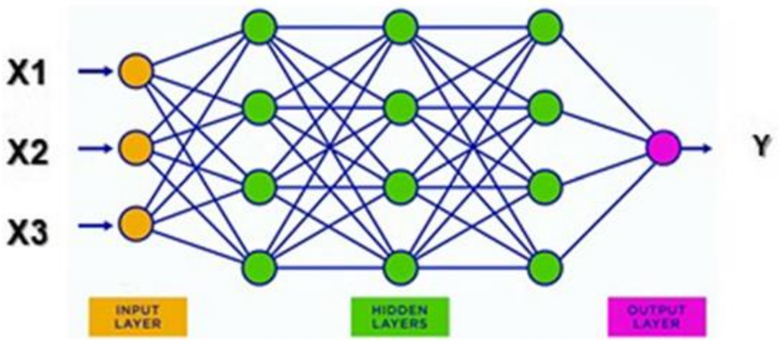

Fig. 2: Schematic diagram of artificial neural network.

2. Support vector machine (SVM)

The support vector machine (SVM) approach is primarily based on Statistical Learning Theory (SLT) and the concept of a hyperplane classifier for linearly separable data. The central aim of SVM is to identify an optimal linear hyperplane that maximizes the margin of separation between two classes.[11] The major advantages of the SVM approach are as follows:[24]

i) The solution is unique, optimal, and global, as the training process involves solving a linearly constrained quadratic optimization problem.
ii) Only two free parameters need to be selected, namely the kernel parameter and the upper bound parameter.
iii) SVM provides strong generalization performance and robust predictive quality.

In recent years, SVM has been widely applied across different domains due to these benefits. For instance, it has shown great promise in structure–activity relationship (SAR) analysis, highlighting its potential in drug discovery.[23,40] In a benchmark study by Burbidge et al. (2001), the performance of SVM was compared with several existing machine learning methods used in drug design. The results demonstrated that SVM significantly outperformed these conventional techniques, with the exception of a manually capacity-controlled neural network, which achieved comparable performance but required substantially longer training times.[10]

3. Fuzzy logic

Fuzzy logic is another AI technology. Fuzzy logic is widely used by people to solve problems. It collaborates to comprehend the formulation and optimization process when an ANN is present. Either "true" or "false" is what conventional sense depends on. This idea therefore lies somewhere between being true and being completely untrue. In the true set, the membership function is 1 since the premise is true; in the false set, it is 0.[18]

4. Neuro-fuzzy logic

Giving in basic forms is fuzzy logic's guiding principle. To form it, neural network modeling is required. Neural networks and fuzzy logic are the two main components of neuro-fuzzy logic, as the name suggests. It combines the generality of ANN's learning capabilities with fuzzy logic's power to investigate intricate ideas. Process data mining is ideally suited for neurofuzzy logic. It can articulate the IF_THEN principles in language and create accurate models from data.[34]

5. Random forest (RF)

Random forest constitutes an ensemble learning technique. Combining many base learners into ensemble learning techniques may improve models capacity for generalization compared to using only one basis learner. In many learning tasks, random forest typically performs better than other ensemble learning models. In random forest, the diversity of the base learners comes from both sample and attribute disturbances, increasing the difference between the base learners and enhancing their capacity for generalization.[64]

6. Genetic algorithms (GAs)

Genetic algorithms (GA) were first presented by John Holland in the 1970s. When creating a pharmaceutical product, an optimization strategy is required to determine the optimal mix of chemicals and methods. Scientists have demonstrated that ANN and GA together provide the necessary answers for creating dosage formulations. By simulating natural evolutionary processes, genetic algorithms are employed to address challenging optimization challenges in tablet formulation. To attain desired tablet properties like hardness and dissolve rate, GAs assist in determining the best mix of excipients and process variables. Researchers can reduce experimental workload and quickly converge on strong, high-quality formulations by combining GAs with artificial neural networks (ANNs).[8]

APPROACHES OF AI TOOLS IN PHARMACEUTICAL PRODUCT DEVELOPMENT

1. AI models for formulation optimization

Artificial neural networks (ANNs), support vector machines (SVMs), random forests (RF), and genetic algorithms (GAs) are some of the machine learning (ML) methods that have been extensively studied for optimizing drug formulations. These models are particularly useful for identifying complex, non-linear relationships between formulation inputs, such as the type and concentration of excipients and process factors, and outputs like stability, bioavailability, and dissolution rate, which are often hard to model with traditional approaches. Their ability to analyze large datasets makes them effective tools for uncovering these intricate connections.

Artificial neural networks have been applied in pharmaceutical formulation to predict key parameters such as encapsulation efficiency, drug release profiles, and disintegration time. For example, an ANN-based model was successfully used to optimize the formulation of sustained-release matrix tablets by accurately predicting in-vitro drug release.[47]

Support vector machines are another machine learning technique that can be used for both regression and classification tasks. They are especially effective at distinguishing between optimal and non-optimal formulation conditions due to their ability to create hyperplanes in high-dimensional spaces. In one study, SVMs outperformed regression-based models in predicting particle size and zeta potential during nanoparticle formulation optimization.[50]

Random forest, an ensemble learning technique, is known for its ability to handle missing data and resist overfitting. It has been used to predict optimal combinations of formulation components that achieve desired quality attributes and to determine the importance of various formulation variables. For instance, random forest was applied to model solid dispersion systems and accurately determined the excipient ratios that maximized solubility and dissolution rate.[49]

Genetic algorithms are commonly used for optimization tasks alongside predictive models. These bio-inspired algorithms mimic evolutionary processes to iteratively identify the best formulation conditions. They are frequently combined with ANNs or other ML models to develop hybrid systems that can both predict and optimize formulation outcomes.[54]

2. AI in drug formulation development

In addition to conventional dosage forms, pharmaceutical sciences have witnessed the emergence of other formulations, such as solid dispersions, extrudates, pellets, nanoparticles, and liposomes. These methods are referred to as "formulation techniques" because they facilitate the creation of formulations or add functionality to widely used dosage forms, such tablets. Because AI applications in formulation techniques can effectively address a range of API issues, including low solubility, stability, bioavailability, and production capability, they are even more valuable to research in order to develop next-generation drug products with desired efficacy and health outcome.[2]

i. AI in the formulation of solid dispersions

Solid carbamazepine dispersions have been created utilizing poloxamer 188 and Soluplus® in conjunction with ANN modeling and experimental design.[43] Enhancing the solubility and rate of dissolution of carbamazepine was the goal of creating solid dispersions. Solvent casting was used to create these carbamazepine-Soluplus®-poloxamer 188 solid dispersions. Research has already used ANN (feed-forward back propagation) modeling using the logistic sigmoid activation function to analyze the relationships between various variables and dissolution characteristics in order to optimize the drug's rate of dissolution. In this study, poly (vinyl pyrrolidone)/polyethylene glycol combinations were employed as carriers to create the solid drug dispersions. An adequate prediction for the solid dispersion preparations of medications with desirable dissolution qualities and long-lasting physical stability was achieved by the modeling helped by applied artificial neural networks.[7]

ii. AI in hard gelatin capsule formulation development

Hard gelatin capsules are made using special tools like artificial neural networks (ANN) and expert systems (ES). These computer programs are designed to mimic parts of how humans think, such as learning, generalizing, predicting outcomes, and abstracting information. During the research process, data and statistics are easily turned into useful knowledge with ANNs, which helps the formulator create guidelines for similar cases in the future or predict how a new formula might work.[21] In 2005, Wendy I. Wilson used an expert system to create a capsule shell for drugs classified as BCS class II. Although this system only provided a suggested formula, it was widely used worldwide for making powder-filled hard gelatin capsules. Several model drugs, including carbamazepine, ketoprofen, naproxen, diazepam, chlorpropamide, and ibuprofen, were developed, and their dissolving abilities were tested. The system initially had trouble making accurate predictions and had a large error rate. After retraining the ANN with a new dataset, the models achieved an R2 value of at least 70%. For these model drugs, the intelligent hybrid system predicted the amount of drug dissolved within a 5% margin. A cross-validation test used 10% of the new data, showing that the system could create a formulation that met its specific performance standards. The system considered factors like how well a drug mixes with water and its natural dissolving ability, and it was proven to work well for various BCS class II drugs.[63]

iii. AI in the formulation of emulsions and microemulsions

Additionally, ANNs have been used to formulate and create stable emulsions (oil/water). This study examined how to create emulsions (oil/water) by optimizing the fatty alcohol concentration. Time and lauryl alcohol concentrations were the unreliable variables (factors) examined in this study. The conductance, viscosity, zeta potential, and droplet size were the reliable variables (responses). ANN-predicted values were found to have an excellent correlation with the experiment's data based on validation tests.[33] ANNs have also been used in the formulation and design of microemulsions, where it was simple to examine the precision prediction based on the formula's microemulsion nature.[56] The microemulsion type and internal structural properties have also been highly accurately predicted using a combination of evolutionary artificial neural networks and genetic algorithms. In another study, the formulation of stable microemulsions containing antitubercular medications such as isoniazid and rifampicin for oral administration was predicted using artificial neural network (ANN) modeling. ANN modeling was tested and validated using data from the produced pseudo-ternary phase triangle-diagrams displaying the oil components and the surfactant combination.[1]

iv. AI in the formulation of tablets

Static and dynamic artificial neural networks (ANNs) have been used in matrix tablet design to model the dissolving profiles of various matrix tablets. For these ANN-based models, Monte Carlo simulations and the genetic algorithms optimizer tool were used in this study. The dissolution characteristics of hydrophilic and lipid-based matrix tablets with regulated drug release patterns were accurately predicted by the researcher using Elman dynamic neural networks and decision trees. Elman neural networks-based modeling showed effective modeling of drug releasing patterns by different formula of hydrophilic as well as lipid-based matrix tablets, in contrast to most widely used multilayer perceptron and static networks.[54] In one study, a multilayer perceptron using the feed forward back propagation approach was used to create matrix tablets for the prolonged release of the antidiabetic medication metformin HCl.[35] The optimized formulations were developed by optimizing the matrix tablets' in vitro metformin HCl release pattern. For network training, the dependable variables (responses) and independent variables (factors) were examined. Additionally, through a number of trials, the leave-one-out strategy was used to validate the model. In a different study, ANNs were used to optimize the formulation of nimodipine matrix tablets for use in controlled release.[6] The formulation design of glipizide-releasing osmotic pump tablets has used a combination of statistical optimization and ANN-based modeling.[67] Along with testing the glipizide-releasing osmotic pump tablets' dissolution, ANNs were used to optimize and assess the various formulation and process variables. For the formulation optimization of osmotic tablets containing isradipine, a combination of response surface methodology (RSM) and artificial neural network (ANN)-based modeling has been used. For the optimized isradipine osmotic tablets, the difference between the expected and observed dissolving outcomes was determined to be within the error limitations resulting from the experiment. Furthermore, there was no difference in the similarity or difference factors between the observed and predicted dissolution results, indicating that ANN-based modeling was suitable for achieving the desired dissolution pattern in the formulation development of the controlled isradipine releasing osmotic tablets.[51]

a) AI in the formulation of controlled-release tablets

Controlled release formulations are designed using pharmacokinetic simulations and artificial neural networks (ANN). The ANN model inputs have led to the usage of seven formulation factors and three alternative tablet variables, such as moisture, hardness, and particle size, for 22 tablet formulations of a model medicine. As outputs, the cumulative percentage of medication released in vitro at ten different sampling evaluation times has been used. With the aid of Chem software, the ANN model gains sophistication and proficiency from the input and output data units. Using two desired *in vitro* dissolution-time profiles and two desired *in vivo* release profiles, the expert ANN model is utilized to predict the most effective tablet formulations. The rate-limiting phase in the drug's *in vivo* absorption is the dissolution, and the amount of the drug absorbed *in vivo* is linearly related to the drug's *in vitro* dissolution. The main criteria used to observe *in vitro* release profiles are the distinguishing factor, f1, f2, and similarity factor.[48]

b) AI in the formulation of immediate-release tablets

Turkoglu created a direct compression tablet formulation using hydrochlorothiazide to increase tablet strength.[55] In a separate study, Kesavan and Peck created a model of a caffeine tablet formulation to explain the properties of the granules and tablets (disintegration time, hardness, and friability), processing variables (granulator type, binder addition technique), and the diluting agent and binder content in each formulation. Neural networks outperformed conventional statistical techniques, as these two investigations showed. Scholars have therefore reexamined Kesavan and Peck's findings using a range of neural networks and genetic algorithms.[30] This presentation illustrated how the limitations placed on the various component and processing variable tiers, along with the relative significance of the output attributes, determined the best formulation.[13]

v. AI in the formulation of multiparticulate beads

Multiparticulate verapamil beads were created using CAD/Chem software-assisted modeling. This study examined the effects of several formulation and process variables on the verapamil released by the beads in vitro. When compared to the expected outcomes derived from the ANN modeling, the optimized beads *in vitro* verapamil releasing data were shown to be in good agreement.[60] To increase stability and site-specific release, ANN modeling was used in a study to evaluate the impact of process variables on papain (enzyme) entrapment within alginate-based beads.[56]

vi. AI in the formulation of nanoparticles

ANN modeling was used in a study to construct albumin-loaded chitosan nanoparticles in order to analyze the effects of different unreliable variables (factors) on dependable variables (responses), such as the cytotoxicity profile and albumin loading efficiency.[5] Tri-block poly(lactide)–poly(ethylene glycol) poly(lactide) nanoparticle formation was investigated using ANN modeling based on a 3-layer feed forward back propagation.[4] The optimal analytical model for prediction was selected for training, testing, and data validation analysis in this work based on correlation coefficient (R2) and mean squared error (MSE) values. The polymer content in the copolymer-based nanoparticle formulation was shown to have the greatest influence among all the factors that were examined. The formulation development of polymer-lipid hybrid nanoparticles of verapamil HCl was conducted based on the central composite design (spherical), and the effects of several formulation parameters were examined. Using continuous genetic algorithms and validated ANNs, the multi-objective optimization of polymer-lipid hybrid nanoparticles of verapamil HCl was conducted. The analysis findings showed that the ANN model had superior analytical capabilities.[37]

It includes some current studies on the application of AI technology to the formulation and development of different types of medication delivery systems in Table 3.

Table 3: Some Recent Researches On The Uses Of Ai In The Development Of Drug Delivery Systems.

S.No.	Drug delivery systems	AI approaches used	References
1	Ibuprofen-sustained release from tablets based on different cellulose derivatives	Adaptive neural-fuzzy inference system	Rebouh et al. (2019)[55]
2	Novel granulated pellet-containing tablets and traditional pellet containing tablets	ANNs	Huang et al. (2015)[26]
3	Ultrasonic release of drug from liposomes	ANNs	Moussa et al. (2017)[55]
4	Doxycycline hydroxypropyl-β-cyclo dextrin inclusion complex	RSM, ANN and support vector machine (SVM) modeling	Wang et al. (2013)[62]
5	Oral disintegrating tablets	ANN and DNN	Han et al. (2018)[22]
6	Agar nanospheres of Bupropion	Genetic algorithm, ANN and RSM	Zaki et al. (2015)[66]
7	Ophthalmic flexible nano-liposomes of pilocarpine HCl	RSM and ANN	Zhao et al. (2018) [65]

8	Floating tablets of rosiglitazone maleate	ANNs	Güler et al. (2017)[57]
9	Nifedipine osmotic release tablets	Mechanistic gastro intestinal simulation and ANN	Ilić et al. (2014)[27]
10	Gelatin nanoparticles of diclofenac sodium	Central composite design and ANNs	Koletti et al. (2020)[32]
11	Timolol-loaded ultradeformable nanoliposome formulations	ANN and multiple linear regression (MLR) analysis	León Blanco et al. (2018)[36]
12	Transferosomal gel for transdermal insulin delivery	2^3 factorial design and RSM	Malakar et al. (2012) [39]
13	Besifloxacin HCl loaded liposomal gel	3^2 full factorial design and RSM	Bhattacharjee et al. (2020)[9]
14	Transferosomal gel for transdermal delivery of risperidone	Central composite design and RSM	Das et al. (2017)[14]
15	Multiple-unit pellet system of prednisone	Box–Behnken design, RSM and ANN	Manda et al. (2019)[41]
16	pH-dependent mesalamine matrix tablets	ANN, multi-layer perception (MLP) algorithm and RMSE	Khan et al. (2020)[29]
17	Voriconazole loaded nanostructured lipid carriers based topical delivery system	Box–Behnken design and QbD	Waghule et al. (2019)[41]
18	Modified starch (cationized)-alginate beads of aceclofenac	Central composite design and RSM	Malakar et al. (2013)[38]
19	Oil-entrapped sterculia gum-alginate beads of aceclofenac	3^2 factorial design and RSM	Guru et al. (2013)[20]
20	Sustained release matrix formulations of salbutamol sulfate	ANN	Chaibva et al. (2010)[12]

CONCLUSION

Pharmaceutical formulation research has been revolutionized into an advanced field through the use of artificial intelligence (AI) and machine learning (ML) that has enabled data-driven frameworks to predict and optimize important aspects of formulation. The field is currently interpreting meaningful complex relationships between drug, excipient, and process variables using various models that include sophisticated mathematics like artificial neural networks, support vector machines, fuzzy logic, and genetic algorithms. These advances allow for the more precise and effective design of an assortment of dosage forms including tablets, capsules, emulsions, beads, and nanoparticles, in addition to overcoming the limitations associated when using classical trial-and-error approaches. AI has enabled better predictive capability, process robustness, and innovation in optimization; for these reasons, AI models can provide objective key benefits in the development of the next generation of pharmaceutical products having improved efficacy, stability, and patient outcomes notwithstanding the variety of obstacles that may impede development such as resource implementation costs, and collaboration or access to datasets.

REFERENCES

1. Agatonovic-Kustrin S, Glass BD, Wisch MH, Alany RG. Prediction of a stable microemulsion formulation for the oral delivery of a combination of antitubercular drugs using ANN methodology. *Pharm Res.,2003;* 20, 1760–1765.
2. Al Kuwaiti A, Nazer K, Al-Reedy A, et al. A review of the role of artificial intelligence in healthcare. *J Pers Med*., 2023; 13, 951.
3. Anurag, Yadav AP, Singh G, Singh MK. Artificial Intelligence in Optimizing Formulations and Excipients: Revolutionizing Pharmaceutical Product Development. *J Adv Sci Res., 2025;* 16, 9–18.
4. Asadi H, Rostamizadeh K, Salari D, Hamidi M. Preparation of biodegradable nanoparticles of tri-block PLA–PEG–PLA copolymer and determination of factors controlling the particle size using artificial neural network. *J Microencapsul*, 2021128, 406–416.
5. Baharifar H, Amani A. Size, loading efficiency and cytotoxicity of albumin loaded chitosan nanoparticles: An artificial neural networks study. *J Pharm Sci., 2017;* 106, 411–417.
6. Barmpalexis P, Kanaze FI, Kachrimanis K, Georgarakis E. Artificial neural networks in the optimization of a nimodipine controlled release tablet formulation. *Eur J Pharm Biopharm*, 2010; 74, 316–323.
7. Barmpalexis P, Koutsidis I, Karavas E, Louk D. Development of PVP/PEG mixtures as carriers for solid dispersions and optimization of dissolution using neural networks. *Eur J Pharm Biopharm* 85, 1219–1231 (2013).
8. Bibhishan Mundhe K, Chitra V, Madasamy P. Tablet formulation using artificial neural networks and genetic algorithm. *Front Health Inform*, 202312, 331–342.
9. Bhattacharjee A, Das PJ, Dey S, et al. Besifloxacin HCl loaded liposomal gel optimized using factorial design. *Colloids Surf A*, 2020; 585: 124071.
10. Burbidge R, Trotter M, Buxton B, Holden S. Drug design by machine learning: SVMs for

pharmaceutical data analysis. *Comput Chem., 2001* 26, 5–14.

11. Burges CJC. A tutorial on support vector machines for pattern recognition. *Data Min Knowl Discov.*, 1998; 2, 121–167.
12. Chaibva F, Burton M, Walker RB. Optimization of salbutamol sulfate dissolution from sustained release matrices using ANN. *Pharmaceutics*, 2010;2, 182–198.
13. Colbourn EA, Rowe RC. Modelling and optimization of a tablet formulation using neural networks and genetic algorithms. *Pharm Technol Eur.*, 1996; 8, 46–55.
14. Das B, Sen SO, Maji AK, Nayak AK, Sen KK. Transferosomal gel for risperidone delivery: Optimization and ex vivo studies. *J Drug Deliv Sci Technol.*, 2017; 38, 59–71.
15. Das S, Dey R, Nayak AK. Artificial Intelligence in Pharmacy. *Indian J Pharm Educ Res.*, 2021; 55: 304–318.
16. Dong J, Wu Z, Xu H, Ouyang D. Formulation AI: A web-based platform for drug formulation design. *Brief Bioinform* bbad419 (2023).
17. Gao M, Liu S, Chen J, et al. Raman spectroscopy in facilitating formulation development—an AI perspective. *Int J Pharm.,2021;* 597: 120334.
18. Guru PR, Nayak AK, Sahu RK. Oil-entrapped sterculia gum–alginate buoyant systems of aceclofenac. *Colloids Surf B*., 2013; 104: 268–275.
19. Guo M, Kalra G, Wilson W, Peng Y, Augsburger L. Intelligent hybrid system for capsule formulation development. *Pharm Technol* 44–52 (2002).
20. Han R, Yang Y, Li X, Ouyang D. Predicting ODT formulations using ANN. *Asian J Pharm Sci*., 2018; 13: 336–342.
21. Heikamp K, Bajorath J. Support vector machines for drug discovery. *Expert Opin Drug Discov* 9, 93–104 (2014).
22. Heba FE, Darwish A, Hassanien AE, Abraham A. PCA–SVM intrusion detection system. *Int Conf Intell Sy Design Appl., 2010;* 363–367.
23. Hirani R, Noruzi K, Khuram H, et al. Artificial Intelligence and Healthcare: Past–Present–Future. *Life, 2024;* 14, 557.
24. Huang Y, Yao Q, Zhu C, et al. ANN comparing novel pellets vs traditional pellets. *Pharm Dev Technol*., 2015; 20: 670–675.
25. Ilić M, Đuriš J, Kovačević I, Ibrić S, Parojčić J. In vitro–in silico–in vivo absorption modeling via ANN. *Eur J Pharm Sci., 2014;* 62: 212–218.
26. Jiang F, Jiang Y, Zhi H, et al. Artificial intelligence in healthcare: Past, present, future. *Stroke Vasc Neurol., 2017;* 2: 230–243.
27. Khan AM, Hanif M, Bukhari NI, et al. ANN to optimize pH-dependent mesalamine matrix tablet. *Drug Des Devel Ther., 2020;* 14: 2435–2448.
28. Kesavan J, Peck G. Neural networks for granulation and tableting. *Pharm Dev Technol., 1996;* 1: 391–404.
29. Kiran TN, Kumar NS, Lakshmi GVN, Naseema S, Bhargav SB, Mohiddien SM. Artificial intelligence in pharmacy. *Der Pharm Lett* 13, 6–14 (2021).
30. Koletti AE, Tsarouchi E, Kapourani A, et al. Gelatin nanoparticles for NSAIDs: QbD + ANN. *Int J Pharm., 2020;* 578, 1–14.
31. Kumar KJ, Panpalia GM, Priyadarshini S. ANN optimization of fatty alcohol in O/W emulsions. *Acta Pharm., 2011;* 61: 249–256.
32. Landin M, Rowe RC. ANN to model and optimize formulations. In: *Formulation Tools for Pharmaceutical Development*, 2013; 7–37.
33. Mandal U, Gowda V, Ghosh A, Bose A, Bhaumik U, Chatterjee B. Optimization of metformin HCl 500 mg sustained release matrix tablets using ANN based on MLP model. *Chem Pharm Bull., 2008;* 56: 150–155.
34. León BJM, González RPL, Arroyo GCM, et al. ANN as tool for minimizing error in ultradeformable nanoliposomes. *Drug Dev Ind Pharm., 2018;* 44: 135–143.
35. Li Y, Abbaspour MR, Grootendorst PV, Rauth AM, Wu XY. ANN–GA–RSM for verapamil nanoparticles. *Eur J Pharm Biopharm.,2015;* 94, 170–179.
36. Malakar J, Nayak AK, Das A. Modified starch–alginate beads: Optimization via CCD. *Starch., 2013;* 65: 603–612.
37. Malakar J, Sen SO, Nayak AK, Sen KK. Transferosomal gel for insulin delivery. *Saudi Pharm J*., 2012; 20: 355–363.
38. Maltarollo VG, Kronenberger T, Espinoza GZ, et al. Advances in SVM for novel drug discovery. *Expert Opin Drug Discov*., 2020; 14: 23–33.
39. Manda A, Walker RB, Khamanga SMM. ANN predicting prednisone release. *Pharmaceutics, 2019;* 11: 109.
40. Manikiran SS, Prasanthi NL. AI in pharma: milestones and role. *Pharma Times, 2019;* 51.
41. Medarevic DP, Kleinebudde P, Djuris J, Djuric Z, Ibric S. ANN + mixture design for solid dispersions. *Drug Dev Ind Pharm, 2016;* 42: 389–402.
42. Moussa HG, Husseini GA, Abel-Jabbar N, Ahmad SE. ANN + MPC to optimize ultrasonic drug release. *IEEE Trans Nanobiosci., 2017;* 16, 149–156.
43. Mrunal K, Kandhare P. AI in pharmaceutical sciences: Review. *Med Nov Technol Devices, 2025;* 27: 100375.
44. Mohin SK, Mondal P, Goswami S, Ghosh S, Choudhuri S. AI in modern pharmaceutical formulation. *Future J Pharm Sci*., (2024).
45. Muneer R, Hashmet MR, Pourafshary P, Shakeel M. AI for accurate zeta potential prediction. *Nanomaterials, 2023;* 13: 1209.
46. Nagalakshmi S. AI: A new paradigm for formulation development. *Indian J Pharm Educ Res* 54, 843–846 (2020).

47. Noorain, Srivastava V, Parveen B, Parveen R. AI in drug formulation: applications & prospects. *Curr Drug Metab, 2023;* 24: 622–634.
48. Öztürk K, Kaplan M, Çalış S. Effects of nanoparticle characteristics on drug delivery. *Int J Pharm., 2024;* 666: 124799.
49. Patel A, Mehta T, Patel M, Patel K, Patel N. Design of porosity osmotic tablets using ANN. *Curr Drug Deliv., 2012;* 9: 459–467.
50. Patel VL, Shortliffe EH, Stefanelli M, et al. Coming of age of AI in medicine. *Artif Intell Med*., 2009; 46, 5–17.
51. Petrovic J, Ibric S, Betz G, Duric Z. Optimization of matrix tablets via Elman neural networks. *Int J Pharm* 428, 57–67 (2012).
52. Prital S, Khanvilkar VV. Pharmaceutical applications of AI. *Int J Pharm Res Health Sci., 2018;* 6: 2342–2345.
53. Podlogar F, Sibanc R, Gasperlin M. Evolutionary artificial neural networks as tools for predicting the internal structure of microemulsions. *J Pharm Pharmaceut Sci., 2018;* 11(1): 67–76.
54. Rao RV, Savsani VJ. Mechanical Design Optimization Using Advanced Optimization Techniques. Springer London (2012).
55. Rebouh S et al. Neuro-fuzzy modeling of ibuprofen sustained release tablets. *Drug Deliv Transl Res., 2019;* 9: 162–77.
56. Sankalia MG, Mashru RC, Sankalia JM, Sutariya VB. Papain entrapment in alginate beads for stability improvement and site-specific delivery: physicochemical characterization and factorial optimization using neural network modeling. *AAPS Pharm Sci Tech., 2005;* 6(2): E209–E222.
57. Güler GK, Eroğlu H. Development and formulation of floating tablet formulation containing rosiglitazone maleate using artificial neural network. *J Drug Deliv Sci Technol., 2017;* 29: 385–3973.
58. Silver D, Schrittwieser J, Simonyan K, et al. Mastering Go without human knowledge. *Nature, 2017;* 550: 354–359.
59. Singh A, Saharan VA, Hathout RM. AI in drug formulation & delivery: Future perspectives. *Arch Pharm Sci ASU., 2017;* 9: 209–222.
60. Vaithiyalingam S, Khan MA. Controlled-release beads with CAB dispersion. *Int J Pharm.,* 2002; 234: 179–193.
61. Waghule T, Rapalli VK, Singhvi G, et al. Voriconazole-loaded NLC topical system: QbD. *J Drug Deliv Sci Technol., 2019;* 52: 303–315.
62. Wang Z, He Z, Zhang L, et al. Optimization of doxycycline–HP-β-CD inclusion complex. *Acta Pharm Sin B., 2013;* 3, 130–139.
63. Wilson W, Peng Y, Augsburger L. Prototype hybrid system for capsule development. *Pharm Technol., 2002;* 44–52.
64. Yang Y, Ye Z, Su Y, et al. Deep learning for formulation prediction. *Acta Pharm Sin B., 2019;* 9: 177–185.
65. Zhao F, Lu J, Jin X, Wang Z, Sun Y, Gao D, et al. Comparison of response surface methodology and artificial neural network to optimize novel ophthalmic flexible nano-liposomes: Characterization, evaluation, in vivo pharmacokinetics and molecular dynamics simulation. *Colloids Surf B Biointerf* ., 2018; 172: 288–297.
66. Zaki MR, Varshosaz J, Fathi M. Agar nanospheres: ANN vs RSM with GA. *Carbohydr Polym., 2015;* 122: 314–320.
67. Zhang ZH et al. Development of glipizide push-pull osmotic pump controlled release tablets. *Yao Xue Xue Bao., 2012;* 47: 1687–95.