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Artificial Intelligence in Pharmacy

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Abstract: *Artificial intelligence use in pharmaceutical technology has increased over the years, and the use of technology can save time and money while providing a better understanding of the relationships between different formulations and processes parameters. Artificial intelligence is a branch of the computer science that deals with the problem-solving by the aid of symbolized programming. It has greatly evolved in to a science of problems - solving with the hug applications in business, health care, and engineering. The article is describes the drugs discovery, tools of AI, manufacturing execution systems automated control processes systems ,AI to predict new treatment ,development of novel peptides from natural foods, treatment and management of rare diseases, drug adherence and dosage ,challenges to adoption of AI in pharma.*

Keywords: Drug Discovery, tools of AI, MES, ACPS, treatment and management of rare diseases, drug adherence and dosage, challenges to adoption of AI in pharma.

I. INTRODUCTION

Artificial Intelligence (AI) is a stream of science related to intelligent machine learning, mainly intelligent computer programs, which provides results in the similar way to human attention process.[1] This process generally comprises obtaining data, developing efficient systems for the uses of obtained data, illustrating definite or approximate conclusions and self-corrections/adjustments.[2] In general, AI is used for analyzing the machine learning to imitate the cognitive tasks of individuals.[2,3] AI technology is exercised to perform more accurate analyses as well as to attain which enormously contributes its efficacy tothe industry.

Recently, AI technology becomes a very fundamental part of industry for the useful applications in many technical and research fields.[3,4] The emergent initiative of accepting the applications of AI technology in pharmacy including drug discovery, drug delivery formulation development and other healthcare applications have already been shifted from hype to hope.[5,6] The uses of AI models also make possible to predict the *in vivo* responses, pharmacokinetic parameters of the therapeutics, suitable dosing, *etc*.

In this perspective, various useful statistical models as well as computational intelligence are combined in the AI technology.[4] The progress and innovation of AI applications are often associated to the fear of unemployment threat. However, almost all advancements inthe applications of AI technology are being celebrated on account of the confidence, of pharmacokinetic prediction of drugs, the uses of *in silico* models facilitate their effectiveness and inexpensiveness in the drug research.[8] There are two key classes of AI technology developments.[9] The firstone comprises the conventional computing methodologies including expert systems, which are capable of simulating the human experiences and illustrating the conclusions from the principles, like expert systems.[10] The second one comprises the systems, which can model the modeof brain functioning employing the artificial neural networks (ANNs).[9] In specific, various ANNs like deepneural networks (DNNs) or recurrent neural networks(RNNs) control the evolutions of AI technology. In Merck Kaggle[11] and NIH Tox21 challenge,[12] DNN issues show the greater predictivity than the baseline machine learning methodologies.[3,14] The machine learning employs suitable statistical methodologies with the capability to learn with or devoid of being unequivocally programmed.[13] In addition, *de novo* design promotes the invention of newer drug molecules withregard to optimal or desired qualities.[14] In the current review article, the uses of AI in pharmacy, especially in drug discovery, drug delivery formulation development, polypharmacology and hospital pharmacy are discussed.

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II. MILESTONES IN AI

The first use of the phrase "Artificial Intelligence" was appeared in 1956. However, the concept of AI was employed since 1950 with the uses of problem-solving as well as symbolic methodologies.[5] important milestonesin the area of the AI uses are presented in Table 1.

Important milestones in the area of the AIuses.

Year	Events
1943	Walter Pitts and Warren McCulloch proved that logicaloperations like "and", "or" or "not" can be done by neurons connected in a network
1956	The term „artificial intelligence" was first appeared.
1958	Frank Rosenblatt created neuronal networks calledPerceptrons which can transmit information in one direction.
1974	Initiation of "First AI Winter".
1986	Georey Hinton promoted Back propagation algorithmdesign which is widely used in deep learning.
1987	Initiation of "AI winter".
1997	Garry Kasparov (Russian grandmaster) was defeatedby IBM Deep blue.
2013	Google carried out efficient research on pictures by utilizing the British technology.
2016	In this year, the Go Champion Lee Sedol was defeatedby Google DeepMind, software AlphaGo.

2.1 Classification of AI

AI can be classified into two different ways: according tocalibre and their presence (Figure 1).[15,16] According to their ability, AI can be categorized as:

1. Artificial Narrow Intelligence (ANI) or Weak AI: It performs a narrow range task, i.e., facial identification, steering a car, practicing chess, traffic signalling, etc.
2. Artificial General Intelligence (AGI) or Strong AI: It performs all the things as humans and also knownas human level AI. It can simplify human intellectualabilities and able to do unfamiliar task.
3. Artificial Super Intelligence (ASI): It is smarter than humans and has much more activity than humans drawing, mathematics, space, etc.

According to their presence and not yet present, AI can be classified as follows:

1. Type 1: It is used for narrow purpose applications, which cannot use past experiences as it has no memory system. It is known as reactive machine. There are some examples of this memory, such as a IBM chess program, which can recognize the checkers on the chess playing board and capable of making predictions.
2. Type 2: It has limited memory system, which can apply the previous experiences for solving different problems. In automatic vehicles, this systemis capable of making decisions there are some recorded observations, which are used to record further actions, but these records are not stored permanently.
3. Type 3: It is based upon "Theory of Mind". It means that the decisions that human beings makeare impinged by their individual thinking, intentionsand desires. This system is non-existing AI.
4. iv). Type 4: It has self-awareness, i.e., the sense of self andconsciousness. This system is also non-existing AI.

2.2 Neural networks and ANNs

The learning algorithm of neural networks (from input data) takes two different forms mainly. The classes of neural networks are as follows (Figure 2):[9,17]

1. Unsupervised learning: Here the neural network is submitted with input data having recognised pattern. It is used for organizational purpose.

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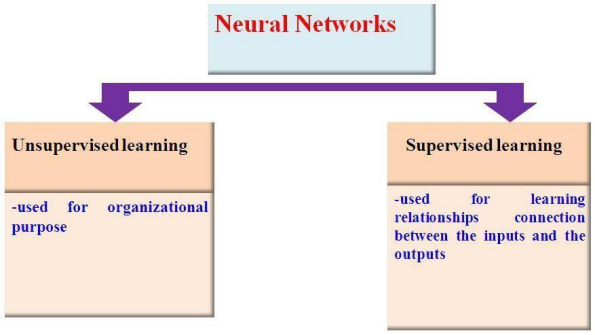

Figure 1: Classification of neural networks.

The unsupervised learning algorithm uses „Self Organizing Map" or Kohonen".[9] This is known as very useful modeling for the searching of relationships amongst the complex data sets.

2. *Supervised learning:* This kind of neural network is illustrated with the sequences of harmonizing inputs and outputs. It is used for learning relationship- connection between the inputs and the outputs. It shows its usefulness in formulation to measure the cause and effects linking between input-output. It is the most frequently employed ANNs and is entirely linked with the back propagation learning rule. This learning algorithm is known as the outstanding methodology for the prediction as well as classification jobs.[9]

A simple mathematical processing unit called neuron is the main part of the neural network.[17] Every input possesses an associated weight having relative importance and calculates the weighted sum of all the inputs as output. This output is then forwarded to another neuron after being modified by a transformation function. The whole processing is called a perceptron(a feed-forward system). A neural network having manyneurons is organized into network architectures.[9] The most famous and prosperous network is multilayer perceptron network. In this network system, the identicalneurons are arranged in such a way that in one layer, the outputs are presented and in the subsequent layer, the inputs are presented. There are one or more secretlayers, which can be introduced between the input andoutput layers. In theory, amount of secret layers can be attached according to solitary need. In practice, multiple layers are needed in case of applications with extensive nonlinear behaviour.

ANN is one of the computational modelling figured from hundreds of single units of artificial neurones associated with the constituents comprising the neuralstructure, which are known as processing elements asthey participate in information processing.[2,9,18] ANN methodology presents a potential modeling procedure,in particular for the data sets of non-linear links commonly encountered in the pharmaceutical research.[19-21] For the model specification analyses, ANNs don"t necessitate acquaintance of the data source. However, they frequentlyhave many weightages that should be analyzed. They also necessitate larger training sets. Additionally, ANNscan mix as well as add in both the literature and the investigational data to resolve the problems.

Recently, ANN models are being hybridized with other kinds of simpler models.[22] For example, a recently proposed combination of neural networks and logistic regression allow the generation of hybrid linear/ nonlinear classification surfaces and the identification of possible strong interactions that may exist between the attributes (also known as covariates in the Logistic Regression literature) which define the classification problem. All these hybrid models perform reasonablewell for a given set of databases.[22]

The prospective uses of ANNs in pharmacy are wide-ranged from the data analyses *via* the modeling of pharmaceutical quality control.[21,23] ANNs are also provedfunctional for the uses in the drug designing, especially in molecular modeling and QSAR.[1,24] It is also used in formulation optimization processes for dosage form designing and in biopharmaceutical analyses, such as pharmacokinetic modeling, pharmacodynamic modeling,*in vitro-in vivo* correlation analysis, *etc.*[7,21-23,25]

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2.3 Fuzzy LOGIC and neurOFUZZY logic

According to the conventional logic, proposal may betrue or false. The hypothesis behind the logic lies either in or totally outside the "true" set. When the hypothesislies within the "true" set, the membership function is denoted as "1" and when the hypothesis lies outside the "true" set, the membership function is denoted as "0". The basic concept of fuzzy logic is promoted by Lotfi Zadeh in the 1960s.[26] In contrast to the conventional logic, the fuzzy logic is not limited to be 0 or 1. However, anycontinuous value in-between these limits can be taken here. When 20°C temperature is taken as "comfortable", according to the conventional logic temperature of 19 or21°C, which remain outside this set, are "uncomfortable".But, according to fuzzy logic, 17°C may obtain amembership of 0.4 in the "hot" set as well as 0.6 in the"cold" set. This logic is very useful in process control.[26] For the automated circulations by the arteries andvenous, the automated system based on fuzzy logic for drug releasing has been framed and analyzed.[27] Fuzzy hemodynamic management modules have already been employed for the assessment of the condition of patients to report the regulation of the arterial as well as pulmonary pressures. This can be used to monitorthe cardiac output of patients. The fuzzy logic-basedautomated system offers a comparative faster reaction and more effectual haemodynamic control.[27] In addition, the uses of supervisory-fuzzy rule-dependent adaptive control system is considered as a potential way for controlling the multiple drug hemodynamic process.[28] When the fuzzy logic system is strongly combined witha neural network, it is called as neurofuzzy logic system. Here, the capability of neural networks of learning from data and the ability of fuzzy logic of expressing complex concepts intuitively are combined properly. It has datamining capability. The neurofuzzy logic also presentsneural network having 2 extra layers for the fuzzification of inputs as well as defuzzification of outputs. In a research, the simulation of probucol absorption *via*the lipid formulations has been studied by means ofneurofuzzy networkings.[29] According to the outcomeof the research, the probucol releasing rate from thelipid formulations was found to be significantly lesser in comparison with that of the self-emulsifying formulations.The adaptive neurofuzzy network model together with*in vitro-in vivo* correlation tool demonstrated the competent predictive presentation and the prospective for the development of complex relationships as well asinterpolates the pharmacokinetic constraints.[29]

2.4 Principal Component Analysis (PCA)

PCA is another AI based model for decreasing the dataset-dimensionality by preserving as much „variability" (*i.e.,* statistical information) as possible and at the same time, PCA modelling minimizes the loss of information. PCA modelling translates into searching newer variables,which are linear functions of those in the original datasetby generating newer uncorrelated variables so that maximize the variance, successively.[30] Searching of such newer variables, the principal components reduce the resolving of an eigenvector or eigenvalue problem.[30,31] PCA can be based on either the covariance matrix or the correlation matrix and the main applications of PCA are descriptive in nature, rather than the inferential uses. Recent years, PCA is well- known for using as a „hypothesis generating" AI tool generating a useful statistical mechanics frame for modelling of biological systems without therequirement for strong a priori theoretical assumptions, which makes PCA of paramount significance for drugdiscovery research by a systemic perspective overcomingtoo narrow reductionist approaches.[32]

2.5 Support Vector Machine (SVM)

SVM approach is based on the idea of a hyper plane classifier or linearly separability. It is mostly dependent on Statistical Learning Theory (SLT). The aim of SVM is to discover a linear optimal hyper plane in order to that the margin of separation in-between the two classifications is maximized.[33] SVM approach has recently been employed in many applications asit encompasses some potential benefits over various conventional machine learning methods. The important benefits of SVM approach are identified as:[34]

1. The solution of SVM approach is exclusive, optimaland global since the training of a SVM is done bysolving a linearly confined quadratic problem.
2. Only two free parameters are required to be chosen. These are known as: the kernel parameter and the upper bound parameter.

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3. SVM approach is capable of facilitating excellent generalization performance and good qualityrobustness.

Recent years, SVM approach has been employed for structure–activity relationship analysis and it proves its potential in drug discovery field.[35,36] Burbidge *et al.* (2001) tested a benchmark test, where SVM approach was compared to several currently used machine learningtechniques in the drug design field.[37] The results of this research demonstrated that the SVM approach is significantly better as compared to these tested machinelearning techniques currently used in drug designing, bara manually capacity-controlled neural network, which takes considerably longer to train.

2.6 Hammeistern Weiner (HW)

HW modeling approach is one of the unrelated tophysiological AI models.[38] This is more flexible andbetter able to adapt to data, which results in a superiorfitting when compared to different methods.[38,39] HW model is implemented if a cascade of two staticnonlinear blocks and one linear block are employed.Only the linear block contains the dynamic elements.[39] In a research, Shokrollahi *et al*. (2018) evaluated the useof a nonlinear Hammerstein-Wiener modeling in the development and control of a magneto-rheological fluidhaptic device, which can be potentially used for roboticbone biopsy.[40] The validation testing performed in thisresearch found that the HW modeling is able to predict theperformance of the magneto-rheological fluid devicewith an accuracy of 95% and the HW modeling is capableof eliminating the hysteresis in a closed-loop controlsystem.

A. Advantages of AI technology

The potential advantages of AI technology are asfollows:[6,15,41]

1. Error minimization: AI assists to decrease the errorsand increase the accuracy with more precision. Intelligent robots are made of resistant metal bodies and capable of tolerating the aggressive atmosphericspace, therefore, they are sent to explore space.
2. Difficult exploration: AI exhibits its usefulness in the mining sector. It is also used in the fuel exploration sector. AI systems are capable of investigating theocean by defeating the errors caused by humans.
3. Daily application: AI is very useful for our daily acts and deeds. For examples, GPS system is broadly used in long drives. Installation of AI in Androidshelps to predict what an individual is going to type. It also helps in correction of spelling mistakes.
4. Digital assistants: Now-a-days, the advanced organizations are using AI systems like „avatar" (models of digital assistants) for the reduction of human needs. The „avatar" can follow the right logical decisions as these are totally emotionless. Human emotions and moods disturb the efficiencyof judgement and this problem can be overcome by the uses of machine intelligence.
5. Repetitive tasks: In general, human beings can perform single task at a time. In contrast to the human beings, machines are capable of performing multi-tasking jobs and can analyze more rapidly in comparison to the human beings. Various machine parameters, i.e.,speed and time can be adjusted according to their requirements.
6. Medical uses:In general, the physicians can assess the condition of patients and analyze the adverse effectsand other health risks associated with the medicationwith the help of AI program. Trainee surgeons can gather knowledge by the applications of AI programs like various artificial surgery simulators (for examples, gastrointestinal simulation, heart simulation, brain simulation, etc.
7. No breaks: Unlike human beings who have the capacity of working for 8 h/day with breaks, the machines are programmed in such a way that theseare capable of performing the work in a continuous manner for long hours devoid of any kinds of confusions and boredom.
8. Increase technological growth rate: AI technology is widely used in most of the advanced technological innovations worldwide. It is capable of producingdifferent computational modelling programs and aims for the invention of the newer molecules. AItechnology is also being used in the development of drug delivery formulations.
9. No risk: In case of working at the risky zone like firestations, there are huge chances of causing harm to the personnel engaged. For the machine learningprograms, if some mishap happens then broken parts can be repairable.

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10. Acts as aids: AI technology has played a different function by serving children as well as elders on a24x7 basis. It can perform as teaching and learning sources for all.
11. Limitless functions: Machines are not restricted to any boundaries. The emotionless machines can doeverything more efficiently and, also produce more accurately than the human beings.

B. Disadvantages of AI technology

The important disadvantages of AI technology are as follows:[6,15,41]

1. Expensive: The launch of AI causes huge money consumption. Complex designing of machine, maintenance and repairing are highly cost effective. For the designing of one AI machine, a long period of time is required by the R&D division. AI machine needs updating the software programmes,regularly. The reinstallations as well as recovery of the machine consume longer time and huge money.
2. No replicating humans: Robots with the AI technology are associated with the power of thinking like human and being emotionless as these add some advantagesto perform the given task more accurately withoutany judgement. If unfamiliar problems arise, robots cannot take the decision and provide false report.
3. No improvement with experience: Human resource can be improved with experiences. In contrast, machines with AI technology cannot be enhanced with experience. They are unable to identify which individual is hard working and which one isnonworking.
4. No original creativity: Machines with AI technology have neither sensitivity nor the emotional intelligence. Humans have
5. the ability to hear, see,feel and think. They can use their creativity as wellas thoughts. These features are not achievable by theuses of machines.
6. Unemployment: The widespread uses of AI technology in all the sectors may cause large scale unemployment.As because of the undesirable unemployment, human workers may lose their working habits andcreativity.

III. Artificial Intelligence in Drug Discovery

Drug discovery often takes a long time to test compounds against samples of diseased cells. Finding compounds that are biologically active and are worth investigating further requires even more analysis. To speed up this screening process, Novartis research teams use images from machine learning algorithms to predict which untested compounds might be worth exploring in more details. As computers are far quicker compared to traditional human analysis and laboratory experiments in uncovering new data sets, new and effective drugs can be made available sooner, while also reducing the operational costs associated with the manual investigation of each compound [3]. The current AI initiative by the top biopharmaceutical companies include:

1. mobile platform to improve health outcomes –the ability to recommend patients by means of real time data collection and thus improve patient outcomes.
2. drug discovery- pharma companies in conjunction with software companies are trying to implement the most cutting –edge technologies in the costly and extensive process of drugdiscovery [42].

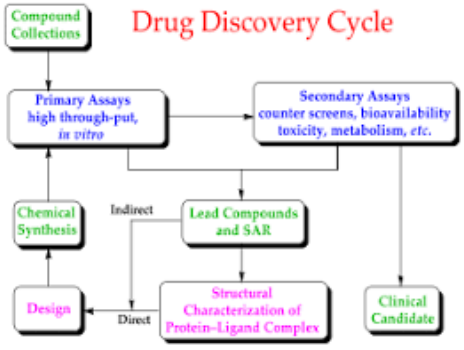

Figure 2: Drug discovery cycle

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3.1 Tools of AI

A. Robot Pharmacy

The objective of improving the safety of patients, UCSF Medical Center uses robotic technologyfor the preparation and tracking of medications. According to them, the technology has prepared 3, 50, 000 medication doses without any error.The robot has proved to be far better than humans both in size as well as its ability to deliver accurate medications. The abilities of the robotic technology include preparation of oral as well as injectable medicines which include chemotherapy drugs that are toxic. This has given freedom to the pharmacists and nurses of UCSF so that they can utilize their expertise by focusing on direct patient care and working with the physicians [43].

Figure 3: Robot pharmacy

B. MEDi Robot

MEDi is a short form for medicine and engineering designing intelligence. Tools of AIThe pain management robot was developed as part of a project led by Tanya Beran, professor of Community Health Sciences at the University of Calgary in Alberta. She got the idea after working in hospitals where children scream during medical procedures. The robot first builds a rapport with the children and then tells them what to expect during a medical procedure [44], although the robot cannot think, plan, or reason, it can be programmed such that it shows to have AI [45].

C. Erica Robot

Erica is a new care robot that has been developed in Japan by Hiroshi Ishiguro, a professor at Osaka University.) It was developed in collaboration with the Japan Science and Technology Agency, Kyoto University, and the Advanced Telecommunications Research Institute International (ATR). It can speak Japanese and has a blend of European and Asian facial feature [46]. Like any normal human being, it likes animated films, desire to visit south-east Asia, and wants a life partner who would chat with it. The robot cannot walk independently; however, it has been developed with the ability to understand and answer questions with human-like facial expressions. Erica is the “most beautiful and intelligent” android as Ishiguro fixed up the features of 30 beautiful women and used the average for designing the robot‟s nose, eyes, and so on [47].

D. TUG Robots

Aethon TUG robots are designed to autonomously travel through the hospital and deliver medications, meals, specimens, materials, and haul carry heavy loads such as linen and trash. It has two configurations, i.e., fixed and secured carts as well as exchange base platform that can be used to carry racks, bins, and carts. The fixed carts are used for delivering medications, sensitive materials, and laboratory specimens, whereas, the exchange platform is employed to Vyas, et al.: Artificial Intelligence: New era in pharmacy profession transport materials that can be loaded on different racks. The TUG can deliver several types of carts or racks thus making it a very flexible and utilizable resource [48].

E. Automated Control Process System [ACPS]:

The elements of [ACPS] include:

- Sensing process variables‟ value.
- Transmission of signal to measuring element.
- Measure process variable.

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- Presenting the value of the measured variable.
- Set the value of the desired variable.
- Comparison of desired and measured values.
- control signal transmission to final control element. and
- Control of manipulated value.

F. Berg

Berg is Boston-based biotech and is one of the key players employing AI in its various processes. It has an AI-based platform for drug discovery, which has a huge database of patients and this is used to find as well as validate the various biomarkers responsible for causing diseases and then decides therapies according to the obtained data. The motto of the company is to speed up the process of drug discovery and to bring about a reduction in the cost with the aid of AI as it obliterates guesswork that is involved in the process of drug development [49].

IV. MANUFACTURING EXECUTION SYSTEM (MES)

The benefits of using MES include compliance with guaranteed legal regulations, minimized risks, increased transparency, shortened production cycles, optimized resource utilization, controlled, and monitored production steps, and optimized up to batch release [50].

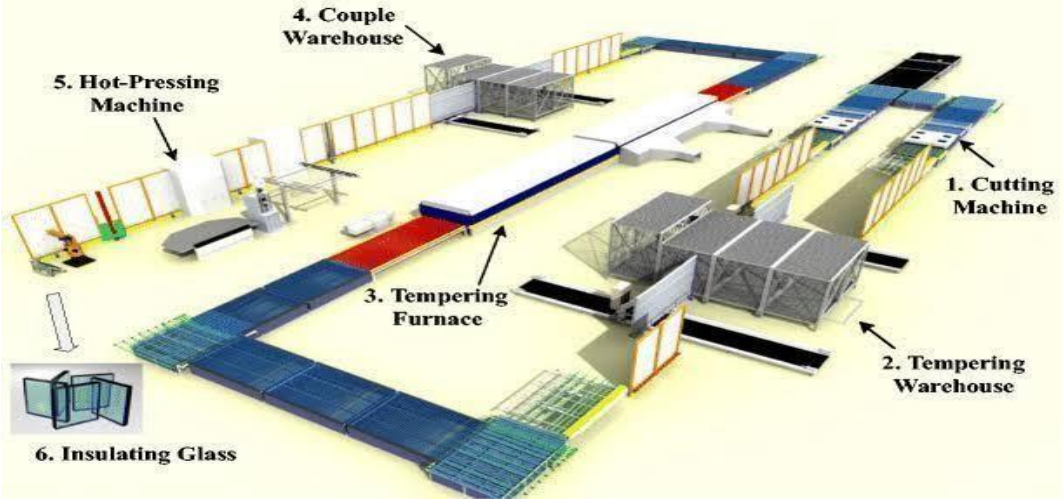

Figure 4: Manufacturing execution systems

4.1 AI to Predict New Treatments

Verge is using automated data gathering and analysis to tackle main problems in drug discovery. In other words, they are taking an algorithmic approach to map out hundreds of genes that play complex roles in brain diseases like Alzheimer‟s, Parkinson‟s or ALS. Verge‟s hypothesis is that gathering & analyzing gene data will positively impact the drug discovery phase starting with the preclinical trials. The idea is that Verge can use AI to monitor the impact that specific drug treatments have on the human brain starting with the preclinical phase. As a result, drug manufacturers can get a better picture early on about the effectiveness of a drug on human cells. More specifically, Verge uses artificial intelligence to keep track of the impact certain therapies on the human brain with a particular focus on the preclinical phase [51].

4.2 Development of Novel Peptides from Natural food

The Irish start up Nerites leverages AI and other novel technologies facilitate the discovery of new and more robust food and healthy ingredients. BASF (Baden Aniline and Soda Factory”) willtake advantage of this partnership to develop novel functional peptides derived from natural foods. In practice, BASF uses Nuritas AI and DNA analysis capabilities to predict, analyze, and validate peptides from natural sources. The main goal of BASF is to discover and deliver to the market peptide-based therapies that‟ll help treat conditions like diabetes.

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4.3 Treatment and Management of Rare Diseases

Advances in AI, renewed interest in rare disease treatments. Currently, there are over 350 million people with over 7,000 rare diseases around the world. However, it‟s not all gloom and doom for patients with rare diseases as Heal, a UK-based biotech firm, has secured $10 million in Series A funding to use AI to develop innovative drugs for rare conditions. Thera chon, another Swiss biotech company that leverage AI to develop drugs for the treatment of rare genetic diseases, has received $60 million in funding.

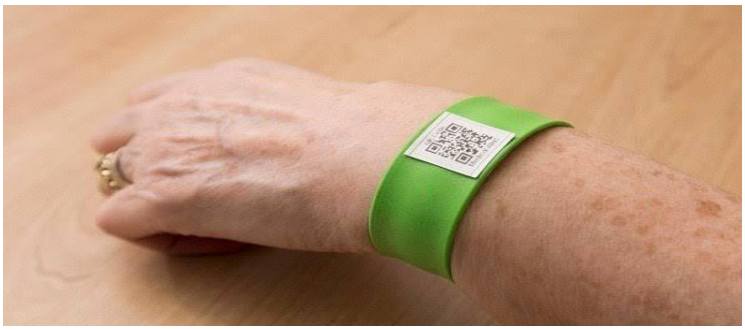

Figure 5: Treatment and management of rare disease

Having to go through physical enrollment. It‟s a clinical research ecosystem designed around its two flagship products, the iPhone and the Apple Watch. Duke University, for instance, uses patient data collected by these Apple devices and AI-driven facial recognition algorithm to identify children with autism. Research kit has made it easy to make better sense of collected health data.

4.4 Finding More Reliable Patients Faster for Clinical Trials

Although there‟s a lot of patient data out there, recruiting the right patients for clinical trials is a difficult process for big pharma. For instance, finding and enrolling ideal candidates can make clinical trials last an average of 7.5 years, costing between $161 million and $2 billion per drug. Unfortunately, 80 percent of clinical trials fail to make deadlines. With over 18,000 clinical studies currently recruiting candidates in the US, the $65 billion clinical trial market needs an overhaul. Extracting useful data from patients‟ records is perhaps the biggest challenge for pharmaceutical companies. Thankfully, that‟s where AI and machine learning comes into the picture

4.5 Challenges to Adoption of AI In Pharma

While AI has an extensive potential to help redefine the pharmaceutical industry, the adoption itself is not an easy walk in the park.

A. Challenges that Pharma Companies Face while Trying to Adopt AI

- The unfamiliarity of the technology – for many pharma companies, AI still seems like a “black box” owing to its newness and esoteric nature.
- Lack of proper IT infrastructure – that‟s because most IT applications and infrastructure currently in use weren‟t developed or designed with artificial intelligence in mind. Even worse, pharma firms have to spend lots of money to upgrade their IT system.
- Much of the data is in a free text format – that means pharma companies have to go above and beyond to collate and put this data into a form that‟s able to be analyzed. Despite all these limitations, one thing is for certain: AI is already redefining biotech and pharma.And ten years from now, Pharma will simply look at artificial intelligence as a basic, everyday, technology.

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Figure 6: Challenges to adoption of AI in pharma

B. Artificial Intelligence in Pharma is a Good Idea

Pharmaceutical Industry can accelerate innovation by using technological advancements. The recent technological advancement that comes to mind would be artificial intelligence, development of computer systems able to perform tasks normally requiring human intelligence, such as visual perception, speech recognition, decision-making, and translation between languages. An estimate by IBM shows that entire Healthcare domain has approx. 161 billion GB of data as of 2011. With humongous data available in this domain, artificial intelligence can be of real help in analyzing the data and presenting results that would help out in decision making, saving Human effort, time, money and thus help save Lives. Epidermic outbreak prediction; usingmechine learning /artificial intelligence one can study the history of epidermic outbreak, analyse the social media activity and predict where and when epidermic can effect with cocidarable accuracy.Apart from the a fore mentioned use-cases there are numerous others like: Personalizing the treatment Help build new tools for the patient , physicians etc. Clinical trials research : applying predictive analytics to identify candidates for the trial throughsocial media and doctor vists.

V. Application

5.1 In Formulation

Controlled release tablets: The first work in the use of neural networks for modeling pharmaceutical formulations was performed by Hussain and coworkers at the University of Cincinnati (OH, USA). In various studies they modelled the in vitro release characteristics ofa range of drugs dispersed in matrices prepared from various hydrophilic polymers. In all cases, neural networks [17] with a single hidden layer were found to offer reasonable performance in the prediction of drug release.

In a more recent study involving the formulation of diclofenac sodium from a matrix tablet prepared from cetyl alcohol, personnel from the pharmaceutical company KRKA dd (Smerjeska, Slovenia) and the University of Ljubljana (Slovenia) have used neural networks to predict the rate of drug release and to undertake optimization using two- and three-dimensional response surface analysis [52].

Immediate release tablets: Work in this area began only some three years ago with two studies. One by Turkoglu and coworkers from the University of Marmara (Turkey) and the University of Cincinnati11 used both neural networks and statistics to model tablet formulations of hydrochlorothiazide.

The networks produced were used to prepare three-dimensional plots of massing time, compression pressure and crushing strength, or drug release, massing time and compression pressure in an attempt to maximize tablet strength or to select the best lubricant [53]. Although trends were observed no optimal formulations were given. The trends were comparable to those generated by statistical procedures. Comparable neural network models were generated and then optimized using

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genetic algorithms. It was found that the optimum formulation depended on the constraints applied to ingredient levels used in the formulation and the relative importance placed on the output parameters. A high tablet strength and low friability could only be obtained at the expense of disintegration time. In all cases lactose was the preferred diluents and fluidized bed the preferred granulating technique [54].

5.2 In Product Development

The pharmaceutical product development process is a multivariate optimization problem. It involves the optimization of formulation and process variables. One of the most useful properties of artificial neural networks is their ability to generalize. These features make them suitable for solving problems in the area of optimization of formulations in pharmaceutical product development [21]. ANN models showed better fitting and predicting abilities in the development of solid dosage forms in investigations of the effects of several factors (such as formulation, compression parameters) on tablet properties (such as dissolution). ANNs provided a useful tool for the development of micro emulsion-based drug-delivery systems in which experimental effort was minimized.

5.3 AI in Hospital Pharmacy

There are several applications of AI in hospital pharmacy- based health care system in organizing dosage forms for individualized patients, selection of the suitable oravailable administration routes or treatment policies.[55]

1. Maintaining of medical records:
2. Treatment plan designing:
3. Health support and medication assistance:
4. AI helps to people in health care system

5.4 AI approaches for Drug Discovery

The drug discovery procedure begins from the available results attained from different resources like high- throughput screening modelling, fragment screening modelling, computational modelling and existing data reported.[55] A schematic outline of the drug discovery procedure is shown in Figure 3. In drug discovery procedure, the structural characterization of drug molecules can directly or indirectly be analyzed by computer-assisted design approaches and after this, organic synthesis of drug molecules is done. The synthesized drug molecules or collected drug compounds are subjected to high throughput screening in primaryassay and then, these are counter screened and evaluatedfor their bioavailability in secondary assays along with successful structure activity relationship (SAR) analysis. The drug discovery interchanges amongst induction and deduction processes. Thus, the interchangeable cycle of inductive–deductive process ultimately guides to attain the optimized lead molecules.[1] The automation of specificportions of the inductive–deductive cycle decreases the unpredictability and inaccuracy; thus, improves the effectiveness of drug discovery procedure. Chemical and pharmaceutical manufacturers examine and derive numerous patents as well as genomic data-based scientific science information by applying the deep learning software, *e.g.,* "NVIDIA DGX-1". Human beings cannotoperate total available information for the advancement of scientific research. AI supercomputers are able to receive and examine the information for identification the association in-between the compounds to offer newer drug molecules.[56,57]

The applications of AI in drug discovery process concerns the use of chemical space. In fact, the chemicalspace offers the phase for the identification of new molecules since it is achievable to computationally itemise the desired molecules.In addition, the machinelearning and related predictive tools also help for the identifications of target-specific effective molecules.The process of selecting a successful new drug moleculefrom large quantity of pharmacological active chemical entities is the toughest part of the whole phenomenon. Benevolent AI is utilized for the purpose of processingfewer molecules with much more surety about their activity. In this regard, *de novo* design necessitate the understanding of organic chemistry for the synthesis of *in silico* molecules and the virtual screening modellingthat perform as the replacements for many biochemical as well as biological testing to measure the efficiency as well as toxicity profiles.[58,59] The aim of *de novo* design in the drug discovery is the invention of newer active molecules without the uses of reference molecules.[60,61]Finally, the active learning algorithms permit the discoveryof new molecules with the potential actions against thetarget-setting of diseases or disorders. Several *in silico* methods for the selection of profiles like ligand-based

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design approaches or molecular structure-based design approaches may be employed along with the accessible information on the small molecule modulator probes or the features of structural biology.[62]*In silico* molecules is obtaining the next generation AI. There are various proposals and software solutions accessible for it. This design is not useful in drug discovery; but, it is connected to the generation of components possessing difficulty in synthesis.

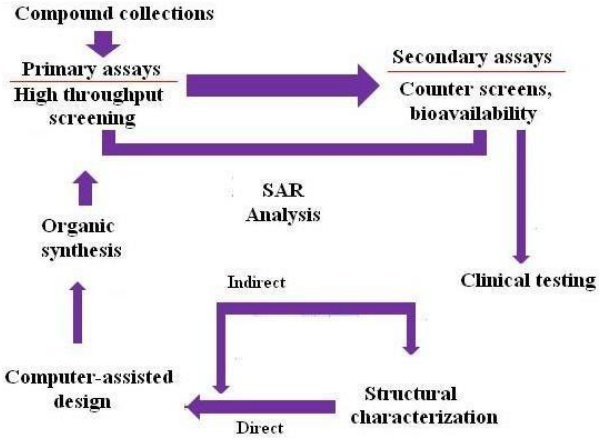

Figure 7: A schematic outline of the drug discovery procedure.

Although recursive neural networks are applied for *de novo* design, it is mainly introduced in the field of natural language processing.[63]The sequential information is taken as input by recursive neural networks. As the molecular structures are encoded as a series of letters bySMILES strings, recursive neural networks are employedfor generating the chemical structures of molecules. Theneural networks are taught the grammar of SMILES strings by mean of training recursive neural networks with a wider setting of chemical compounds from the existing/available chemical compounds from existing compound collections (*e.g.,* ChEMBL). The recursive neural networks have the capability for the processing of a high fraction of authentic SMILES strings.[64]Thisapproach is also applied for the creation of newer peptidestructures.[65]The reinforcement learning is also usedin favour of the generated chemical molecule towards the desired characteristics.[66]Another useful strategy istransfer learning used for generation of newer chemical structures processing a proper biological characteristics. This strategy possesses two steps. The step1 consists oftraining of the network for learning SMILES grammar.The step 2 consists of continued training with compoundspossessing proper desired property. Such few extra epochs of training are enough in favour of the generationof newer compounds as into a chemical space possessed bythe active molecules. Depending upon these approaches, in a work, synthesis of five molecules is done with theconformation of the design activity for four moleculesagainst the nuclear hormone receptors.[67]

There is a fascinating method in the sphere of AI named„Variational Autoencoder‟ having 2 neural networks:

(i) encoder networks and (ii) decoder networks. The translation of chemical structures is illustrated by SMILES. This represents into a real-value continuousvector as the latent space and translation of vectors from which the latent space into the chemical structures are performed by encoder networks as well as decoder networks, respectively. The latent extent description isrequired by the authors for the training of a model whichis dependent on synthetic accessibility score (SAS) and QED drug-likeness score.[68] It is then possible to acquire a passage of molecules with upgraded target properties. In a published report, the comparison of „Variational Autoencoder‟ with an „Adversarial Autoencoder‟ was shown according to their performance.The „Adversarial Autoencoder‟ has greater capability for producing appreciably more authentic molecularstructures in comparison with that by the „VariationalAutoencoder‟ during their generation mode.

Generative adversarial networks (GANs) are capable for the designing of drug molecules. The technology can prepare photo-realistic pictures from the text representation. In a work, Kadurin *et al.* (2017) employed GAN for suggesting compounds having anticancer characteristics.[69]Imagination or creations of new data can also be done by this technology based on the real data. Next generation AI is not dependent on the learning from large data sets. The new AI chnology is capableto handle all the problems that are difficult to solve previously .[70] The scientists and researchers are assisted by this new technology in the identification and selectionof promising chemical agents on the basis of their efficacy, safety and

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selection of patients to the clinicaltrials.[71,72]Therefore, AI is helpful in drug delivery becauseof its capability of prioritising the molecules according to the simplicity of syntheses or development of usefultools, which have been proved effectual for the most favourable synthetic technique.[73]A list of important synthesized *via* the solvent casting technique. Ina research, a modeling of ANN (a feed-forward back propagation) with the logistic sigmoid activation functionhas already been employed for the analyses of linkingamongst different variables as well as dissolution properties for the optimization of dissolution rate of drug. In this work, to prepare the solid dispersions of drug, poly (vinyl pyrrolidone)/polyethylene glycol mixtures were used as carriers. The applied ANNs- assisted modeling established an appropriate prediction for the solid dispersion preparations of drugs with desired dissolution properties with along-standing physical stability.[77]

Table 2: List of important AI-based computer-assisted tools used in drug discovery.

AI-based computer- assisted tools used indrug discovery	Websites	Descriptions
Chemputer	https://zenodo.org/record/1481731	More standardized set-up for reporting chemical synthesis
ODDT	https://github.com/oddt/oddt	For use in chemo informatics and Molecular modelling
ORGANIC	https://github.com/aspuru-guzik-group/ORGANIC	Molecular generation tool to create molecules withdesired characteristics
DeepChem	https://github.com/deepchem/deepchem	A python-based AI tool for drug discovery predictions
DeepNeuralNet- QSAR	https://github.com/Merck/DeepNeuralNet-QSAR	Predictions of molecular activity
Neural Graph Finger prints	https://github.com/HIPS/neural-fingerprint	Property prediction of novel molecules
Hit Dexter	http://hitdexter2.zbh.uni-hamburg.de	Machine learning models for the prediction of molecules, which might respond to biochemicalassays
NNScore	http://rocce-vm0.ucsd.edu/data/sw/hosted/nnscore/	Analysis of neural network-based scoring function for protein–ligand interactions
DeepTox	www.bioinf.jku.at/research/DeepTox	Prediction of toxicity and biocompatibility
PotentialNet	https://pubs.acs.org/doi/full/10.1021/acscentsci.8b00507	Ligand-binding affinity prediction based on a graph convolutional neural network
REINVENT	https://github.com/MarcusOlivecrona/REINVENT	Molecular de novo design using RNN and reinforcement learning
DeltaVina	https://github.com/chengwang88/deltavina	A scoring function for rescoring protein–ligand binding affinity
AlphaFold	https://deepmind.com/blog/alphafold	Prediction of protein 3D structure prediction

***Emulsions and microemulsions*:** ANNs have also been utilized for the formulation development of stable emulsions (oil/water).[78] The optimization of the fatty alcohol concentration to formulate emulsions (oil/water) was analyzed in this work. The independable variables (factors) analyzed in this work were concentrationsof lauryl alcohol and time. The dependable variables (responses) were droplet size, zeta potential, viscosity and conductance. On the basis of validation testing, ANN-predicted values were found in excellent correlationwith the data obtained from the experiment.[79]ANNs have also been applied in the formulation designing of microemulsions, where the prediction of precision based on the microemulsion nature from the formula was easily analyzed.[80]By means of the mixture of genetic algorithms and

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evolutionary ANNs, interior structural features and the microemulsion nature havealso been forecasted with the high level of precision. In another work, an ANN modeling has been employed to forecast the formulation of stable microemulsions loaded with antitubercular drugs like rifampicin and isoniazid for oral administrations.[81]Data obtained from the constructed pseudo-ternary phase triangle-diagrams presenting the oil components and the surfactant mixturewere used for the testing as well as validation of the ANN modeling.

Tablets: In the designing of matrix tablets, static anddynamic ANNs have been applied for the dissolutionprofile modeling of different matrix tablets.[82]In this work,Monte Carlo simulations and the genetic algorithms optimizer tool were applied for these modelings based on ANN algorithm. The researcher used the Elman dynamic neural networks and decision trees, which appropriately predicted the dissolution properties of hydrophilic as well as lipid-based matrix tablets exhibitingcontrolled drug releasing pattern. As compared to the majority of commonly employed multilayer perceptron and static networks, the Elman neural networks-basedmodeling demonstrated the efficient modeling of drugreleasing patterns by various formula of hydrophilic as well as lipid-based matrix tablets.[83]In a research, matrixtablets for sustained release of an antidiabetic drug, metformin HCl, was developed by means of multilayer perceptron with feed forward back propagationtechnique.[84] The *in vitro* metformin HCl releasing pattern by the matrix tablets was optimized to develop the optimized formulations. The independent variables(factors) and dependable variables (responses) were analyzed for network training. In addition, the leave- one-out technique was employed for the model validationprocess by means of several trials. In another work, ANNs was applied for the formulation optimization of nimodipine matrix tablets for controlled releasing application.[85]A combination of ANN-based modelingand statistical optimization process has been employedfor the formulation designing of glipizide releasing osmotic pump tablets.[86]In addition to the dissolution testing of these glipizide releasing osmotic pump tablets, the different formulation variables and process variables were optimized and analyzed by means of ANNs. A mixture of response surface methodology (RSM) and ANN-based modeling has been applied for the formulation optimization of osmotic tablets containing isradipine.[87]The disparity amongst the predicted dissolution results and observed dissolutionresults for the optimized is radipine osmotic tablets was found to be within the experimentally caused errorlimits. In addition, the difference as well as similarityfactors did not have any difference among the predicted dissolution results and observed dissolution results, demonstrating the appropriateness of ANN-based modeling to achieve the desired dissolution pattern forthe formulation development of the controlled is radipinereleasing osmotic tablets.

Multiparticulates (beads, microparticles and nanoparticles): By employing CAD/Chem software- assisted modeling, multiparticulate beads of verapamil was developed.[88]In this work, the influences of various formulation variables as well as process variables on the *in vitro* verapamil releasing by the beads were analyzed. The *in vitro* verapamil releasing data for the optimized beads were found to be in the line of good agreement in comparison with that of the predicted results obtainedby the ANN modeling.[89]In a work, ANN modeling was applied to assess the influence of process variables on the papain (enzyme) entrapment within alginate-based beads for the improvement of stability as well as site-specific release.[90]

The combination of ANN and RSM was applied to optimize alginate-based floating microspheres of aspirin, where the quantities of excipient materials, drug releasing and buoyant rate of microspheres were analyzed. ANN model was more precisely predicted *in vitro* aspirin releasing pattern in comparison with that of RSM.[91]Ina work, both the ANN model and factorial model as multivariate methods were used to develop the polymeric microspheres of verapamil HCl.[92]The mutual impacts of external phase pH, initial loading of verapamil HCl and concentration of polymer used on various propertiesof microspheres was analyzed. The results of the study clearly demonstrated that ANN model showed the better fitting abilities with comparatively less biased and more accurate predictability in comparison to thefactorial model.

RSM by full 3^2 factorial design was employed for the formulation development of tamarind seed polysaccharide- alginate composite beads loaded with diclofenac sodium, where the impact of sodium alginate totamarind seed polysaccharide ratio and cross-linker (calciumchloride) concentration as independent formulation variables on the drug encapsulation efficiency and drug release were statistically analyzed.[71] Suitable polynomial equation involving independent formulation variables

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(factors) and their interactions was analyzed based onthe estimation of several statistical parameters, such as correlation coefficient (R^2), predicted correlation coefficient (predicted R^2), adjusted correlation coefficient(adjusted R^2) and predicted residual sum of squares (PRESS), provided by the Design-Expert® Software. In this research, two quadratic models were selected as suitable statistical modeling for optimization for drug encapsulation efficiency and drug release as responses, as because both the responses analyzed hadthe negligible PRESS values. PRESS is well-known statistical parameter for the measure of model fit to the data points and the smaller PRESS statistic indicates the better model fit to the data points. The predicted values obtained from the full 3^2 factorial designs werecoincided well with the observed responses.[93]

In a research, central composite design and RSM wereemployed for the formulation optimization of alginate–methylcellulose mucoadhesive microcapsules loaded with gliclazide, where the impact of sodium alginate to methylcellulose ratio and cross-linker (calcium chloride)concentration as independent formulation variables on the drug encapsulation efficiency and drug release were statistically analyzed.[94] The statistical modeling was evaluated by one-way ANOVA (p<0.05) and the model analysis was evaluated lack of fit and R^2 analysis and PRESS value for measured responses. In this work, for the formulation optimization, the quadratic modelwas selected based on the statistically insignificant lack of fit and smallest values of PRESS for encapsulationefficiency and drug release.

Malakar and Nayak (2012) developed a multiple-unit floating system, which was mainly low density oil (liquid paraffin)-entrapped calcium alginate-magnesium stearatebeads loaded with ibuprofen by employing 2^3 factorial design, where the effects of three independent processvariables like amount of sodium alginate, magnesium stearate and liquid paraffin on density, ibuprofen entrapment and ibuprofen release were statistically analyzed by one-way ANOVA (p <0.05).[73] The results of ANOVA indicated that all models were significant (p < 0.05) for all the responses (namely density, ibuprofen entrapment and ibuprofen release).The *in vitro* drug release data were evaluated kinetically using variousmathematical models.

The R^2 and root mean squared error (RMSE) values of these mathematical models were computed using KinetDS 3.0 Rev. 2010 software for accuracy as well asprediction capability of these mathematical models. When the respective R^2 were compared, the Korsmeyer–Peppasmodel was found as best-fit kinetic model. However, it was also observed to be closest to zero order model, Weibull model and Baker–Lonsdale model. Finally, the best fitting of the Korsmeyer–Peppas model was verified by comparing RMSE values for each tested models, where the minimum RMSE values (0.12–0.68) was found.

In a work of development of albumin-loaded chitosannano particles, ANN modeling was employed for the analyses of the impacts of various independable variables (factors) on the dependable variables (responses) like albumin loading efficiency and cytotoxicity profile.[95]A 3 layer feed forward back propagation-based ANN modeling was studied for the development of nano- particles of tri-block poly(lactide)–poly(ethylene glycol)–poly(lactide) copolymer.[96]In this work, on the basis of correlation coefficient (R^2) and mean squared error (MSE) values, the best analytical model for prediction was chosen for training, test as well as data validationanalysis. Amongst all the investigated variables, the concentration of polymer in the copolymer-based nano- particle formulation was revealed as the most impacted factor. On the basis of central composite design (spherical),the formulation development of polymer-lipid hybridnanoparticles of verapamil HCl was carried out, where the impacts of various formulation factors were analyzed.[97]The multi-objective optimization of polymer-lipid hybrid nanoparticles of verapamil HCl was carried outemploying the validated ANNs and continuous genetic algorithms and the analyses results indicated the betteranalytical capability of ANN model.

Some recent researches on the uses of AI technology in the formulation development of various kinds of drug delivery systems are also presented in Table 3.

AI Approaches in Polypharmacology

Now a day, „one-disease-multiple-targets" concept governs over the „one-disease-one -targets" concept for the advanced realization of pathological process in various disorders at their molecular basis. The phenomenon of „one-disease- multiple-targets" is known as polypharmacology.[98,99] There are numerous and useful databases, for examples, PubChem, KEGG, ChEMBL, ZINC, STITCH, Ligand Expo, PDB, Drugbank, Supertarget, Binding DB, *etc*, which are accessiblefor the

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accomplishment of a variety of important and useful information related to the structure of crystals, chemical features, biological properties, molecular pathways, binding affinities, disease concern, drug targets, *etc*. AI also helps to discover the databases tosketch polypharmacological molecules/agents.

Table 3: Some recent researches on the uses of AI in the development of drug delivery systems.[100-131]

Drug delivery systems	**AI approaches used**
Ibuprofen-sustained release from tablets based on different cellulose derivatives	Adaptive neural-fuzzy inferencesystem
Novel granulated pellet-containing tablets and traditional pellet-containing tablets	ANNs
Ultrasonic release of drug from liposomes	ANNs
Doxycycline hydroxypropyl-β-cyclodextrin inclusion complex	RSM, ANN and support vectormachine (SVM) modeling
Oral disintegrating tablets	ANN and DNN
Agar nanospheres of Bupropion	Genetic algorithm, ANN and RSM
Ophthalmic flexible nano-liposomes of pilocarpine HCl	RSM and ANN
Floating tablets of rosiglitazone maleate	ANNs
Nifedipine osmotic release tablets	Mechanistic gastrointestinalsimulation and ANN
Gelatin nanoparticles of diclofenac sodium	Central composite design and ANNs
Hydroxyapatite (HAp)-ciprofloxacin bone-implants	Quality by Design (QbD) and 2^3 factorial design
Alginate-PVP K 30 microbeads of diclofenac sodium	Central composite design and RSM
Timolol-loaded ultradeformable nanoliposome formulations	ANN and multiple linear regression(MLR) analysis
Transferosomal gel for transdermal insulin delivery	2^3 factorial design and RSM
Besifloxacin HCl loaded liposomal gel	3^2 full factorial design and RSM
Transferosomal gel for transdermal delivery of risperidone	Central composite design and RSM
Multiple-unit pellet system of prednisone	Box–Behnken design, RSM andANN
pH-dependent mesalamine matrix tablets	ANN, multi-layer perception (MLP)algorithm and RMSE
Voriconazole loaded nanostructured lipid carriers based topicaldelivery system	Box–Behnken design and QbD
Calcium alginate-gum Arabic beads of glibenclamide	Central composite design and RSM
Modified starch (cationized)-alginate beads of aceclofenac	Central composite design and RSM
Oil-entrapped sterculia gum-alginate beads ofaceclofenac	32 factorial design and RSM
HAp-ofloxacin bone implants	32 factorial design and RSM
Pioglitazone-loaded jackfruit seed starch-alginate beads	32 factorial design and RSM
Ionotropically-gelled mucoadhesive beads for oral metformin HCldelivery	32 factorial design and RSM
Oral disintegrating tablet formulations	ANN and DNN
Sustained release matrix formulations of salbutamol sulfate	ANN
Jackfruit seed starch-alginate mucoadhesive beads of metformin HCl	32 factorial design and RSM
Jackfruit seed starch-pectin mucoadhesive beads of metformin HCl	32 factorial design and RSM
Emulsion-gelled floating beads of diclofenac sodium	23 factorial design and RSM
Aceclofenac-loaded pectinate-poly (vinyl pyrrolidone) beads	32 factorial design and RSM
Floating capsules containing alginate-based beads of salbutamolsulfate	32 factorial design and RSM
Granulated pellet-containing tablets and traditional pellet-containingtablets	ANN

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VI. CONCLUSION

During past few years, a considerable amount of increasing interest towards the uses of AI technology has been identified for analyzing as well as interpreting some important fields of pharmacy like drug discovery, dosage form designing, polypharmacology, hospital pharmacy, etc., as the AI technological approaches believe like human beings imagining knowledge, cracking problems and decision making. The uses of automated workflows and databases for the effective analyses employing AI approaches have been proved useful. As a result of the uses of AI approaches, the designing of the new hypotheses, strategies, prediction and analyses of various associated factors can easily be done with the facility of less time consumption and inexpensiveness.

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