IJCRT.ORG ISSN : 2320-2882

INTERNATIONAL JOURNAL OF CREATIVE RESEARCH THOUGHTS (IJCRT)

An International Open Access, Peer-reviewed, Refereed Journal

REVIEW ON REVOLUTIONIZING PHARMACEUTICALS: THE ROLE OF ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY AND DEVELOPMENT

[1]Meghana Kasana, [2]Ameena Ayesha Shaik, [3]Kavya Gangireddy

Designation:[1,2,3] Pharm.D Intern, Chalapathi Institute of Pharmaceutical Sciences (Autonomous), Chalapathi Nagar, Lam, Guntur, Andhra Pradesh, India 522034

Department: Pharmacy practice

Organization: Chalapathi Institute of Pharmaceutical Sciences (Autonomous), Guntur, Andhra Pradesh, India

Abstract: Research on drug development is crucial for scientists and pharmaceutical companies. However, there are obstacles and difficulties that affect medication design and development, such as low efficacy, off-target delivery, time consumption, and excessive cost. Big and complex data from clinical trials, proteomics, microarray, and genomes all represent a challenge to the drug discovery process. Drug development and discovery heavily rely on artificial intelligence and machine learning technologies. Stated differently, the field has been modernized by artificial neural networks and deep learning algorithms. Peptide synthesis, structure-based virtual screening, ligand-based virtual screening, toxicity prediction, drug monitoring and release, pharmacophore modelling, quantitative structure–activity relationship, drug repositioning, poly-pharmacology, and physiochemical activity and other drug discovery processes have all made use of machine learning and deep learning algorithms. Additionally, by accelerating research and development procedures, Artificial intelligence (AI) can help lower development costs. Pharmacokinetics and toxicity of potential drugs can be predicted using machine learning algorithms, which also help with experimental design. This capacity lessens the need for extensive and expensive animal research by enabling the prioritization and optimization of lead compounds. AI algorithms that evaluate real-world patient data can support personalized medicine strategies, improving patient adherence and treatment outcomes. This thorough analysis examines the many uses of AI in medication development, dosage form designs for drug delivery, process optimization, testing. In conclusion, AI in the pharmaceutical sector provides previously unattainable improvements in drug development, clinical trial design, manufacturing, and regulatory affairs. AI has the potential to revolutionize pharmaceutical research and development by speeding up procedures, improving decision-making, and increasing overall efficiency.

Index Terms: Artificial intelligence, Clinical Research, Pharmaceutical Industry, Clinical trial design.

I. INTRODUCTION:

AI's role in the entire process of creating a pharmaceutical product, from initial development to practical application, is conceivable. It can contribute by facilitating rational drug design, aiding in decision-making processes, identifying personalized therapies for patients, and effectively managing and utilizing clinical data for future drug development.

1.1 AI in Drug Discovery

The large chemical space, with more than more than 10^{60} molecules, makes it easier to investigate a wide range of potential drugs. However, the lack of technological advances makes the medication development process more difficult and expensive[1]. AI offers a way to overcome this obstacle . It can be used to find exciting substances for more research, validate drug targets more quickly, and optimize drug structure design more quickly, all of which contribute to a quicker and more effective drug development process[2].

AI has many benefits, but it also has considerable data challenges. These challenges include the volume, diversity, growth, and ambiguity of the data. Millions of compounds may be included in the drug development data sets available to pharmaceutical corporations; conventional machine learning algorithms may not be able to handle these kinds of data sets of information[3]. A computational model based on the quantitative structure-activity relationship (QSAR) can predict a large number of compounds or basic physicochemical characteristics like log P or log D very quickly[9]. These models, however, fall well short of accurately predicting intricate biological characteristics like a compound's effectiveness and side effects. Small training sets, experimental data inaccuracy in training sets, and a dearth of experimental validations are further issues that QSAR-based models deal with[4]. To overcome these challenges, recently developed AI techniques for large data modelling and analysis, including as deep learning (DL) and pertinent modelling studies, can be applied to safety and efficacy assessments of chemical substances[5]. In addition to structure- and ligand-based techniques, a variety of in computational techniques for virtual screening compounds from virtual chemical spaces offer improved profile analysis and quicker elimination of non-lead chemicals and therapeutic molecule selection, at a lower cost[8]. To choose a lead ingredient, drug design algorithms consider the physical, chemical, and toxicological profiles, such as coulomb matrices and molecular fingerprint recognition[6-7].

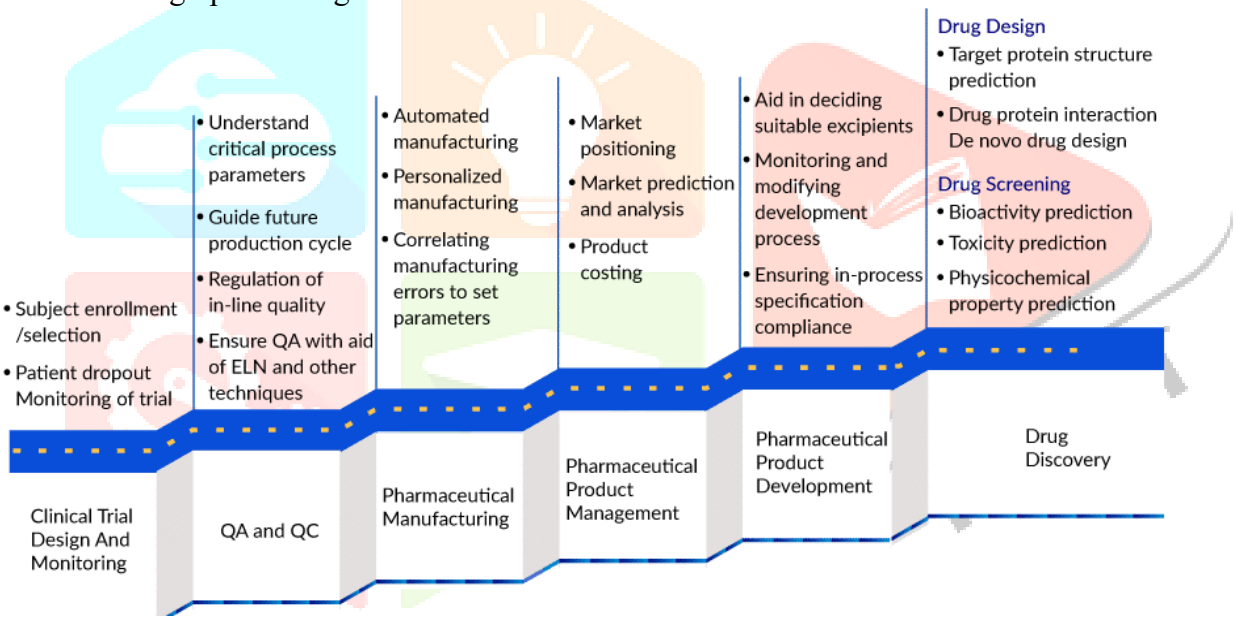

fig 1 applications of artificial intelligence in different subfields of the pharmaceutical industry

1.2 AI in Drug Screening

The average cost of finding and developing a medicine is US$2.8 billion, and the process can take more than ten years. Even Nevertheless, nine out of ten medicinal compounds are not approved by regulators or pass Phase II clinical studies. Based on synthesis feasibility, algorithms including Random Forest, Supporrt vector machine (SVMs), deep neural networks(DNN), and Nearest-Neighbour classifiers have been applied for VS. These algorithms can also predict in vivo activity and toxicity[10-12].

1.3 Physicochemical Properties

Drug physicochemical characteristics, including solubility, partition coefficient (log P), degree of ionization, and intrinsic permeability, influence the drug's pharmacokinetics and target receptor family in an indirect way, so they must be considered when Developing a Novel Drug. Physicochemical qualities can be predicted using a variety of AI-based methods[13]. For instance, machine learning (ML) trains its algorithms using massive data sets generated via earlier compound optimization[15]. Molecular descriptors, such as Simplified Molecular Input Line Entry System (SMILES) strings, potential energy measurements, electron density surrounding the molecule, and coordinates of atoms in three dimensions, are used by drug design algorithms to create viable molecules via DNN and subsequently anticipate the characteristics of those molecules[14-15].

To estimate the acid dissociation constant of substances, ANN-based models, graph kernels, and kernel ridge-based models were constructed in multiple cases. Similar to this, cell lines including human colon adenocarcinoma (Caco-2) cells and canine kidney cells from Madin-Darby have been used to produce data on the cellular permeability of a variety of classes of compounds. These data are then fed into AI-assisted predictors[16-17].

1.4 Bioactivity

The affinity of drug molecules for the target protein or receptor determines how effective they are. The therapeutic effect cannot be produced by drug molecules that have no contact with or affinity for the targeted protein. It is also possible that produced medication molecules occasionally connect with undesirable proteins or receptors, which can be harmful. Therefore, in order to predict drug-target interactions, drug target binding affinity (DTBA) is essential[18]. AI-based techniques can calculate a drug's binding affinity by considering the characteristics or similarities between the drug and its target. Feature-based interactions identify the target and medication's chemical moieties to produce feature vectors. In contrast, in an interaction based on similarity, the medication and target's resemblance factors are considered, and it is anticipated that comparable medications will interact with the same targets[19].To anticipate drug-target interactions, web programs like ChemMapper and the similarity ensemble technique (SEA) are available.

1.5 Toxicity

Considering in vitro and in vivo investigations are labour-intensive and time-consuming, they highlight the limitations of traditional methodologies and the need of forecasting drug toxicity in the drug development process. It draws attention to the moral dilemmas and hefty expenses related to animal testing, which has prompted the creation of substitute strategies, especially in silico toxicology techniques. The use of artificial intelligence (AI), more especially machine learning (ML) and deep learning (DL) algorithms, in forecasting medication toxicity is then the main topic of discussion[20]. Artificial intelligence (AI)-based models that make use of neural networks and other methods are seen to be promising instruments for early detection of possible hazardous effects. By bypassing expensive and time-consuming animal testing, this could result in a more effective drug development process.

1.6 AI in Pharmaceutical Drug Development

Once a novel therapeutic molecule has been discovered, it must be incorporated into an appropriate dosage form with the necessary delivery properties. AI can take the role of the more traditional trial-and-error method in this field[21]. With the use of QSPR, a variety of computational techniques can address challenges in the formulation design field, including dissolution, porosity, stability concerns, and so forth. Decision-support tools work through a feedback loop to monitor the entire process and make sporadic modifications[22]. They pick the type, nature, and quantity of excipients based on the physicochemical properties of the medicine using rule-based systems[23].

1.7 AI in Pharmaceutical Product Management

Market positioning, which is the process of giving a product a distinct identity in the marketplace to entice customers to purchase it, is a crucial component of almost all business strategies for organizations looking to forge their own distinctive identity. Technology and e-commerce as a platform have made it simpler for businesses to establish their brand's organic recognition in the public domain[24]. As the Internet Advertising Bureau has also revealed, businesses use search engines as one of the technology platforms to take center stage in online marketing and aid in the positioning of the product in the market. Businesses constantly want to rank their websites higher than those of their competitors in order to quickly establish their brand. Additional tools that gave a better understanding of markets included statistical analysis techniques and particle swarm optimization algorithms (introduced by Eberhart and Kennedy in 1995) combined with NNs. They can assist in selecting the product's marketing plan based on precise predictions of consumer demand. The problems with the pharmaceutical industry's research and development (R&D) , which attributes the drop to a failure to implement new marketing technology. It emphasizes how crucial ongoing improvement and expansion are to a business' success. One of the most important factors in overcoming these obstacles is the rise of the "Fourth Industrial Revolution," which is characterized by advancements in digital technologies. It is stressed that creative digitalized marketing should be adopted using a multicriteria decision-making process[25]. This method entails gathering, evaluating, and combining mathematical and statistical data with individual judgments to produce AI-based decision-making models. These models investigate novel marketing strategies, offering a more successful and efficient way to connect with target markets.

Artificial Intelligence (AI) is recognized for its ability to perform thorough customer-centric studies of product requirements and comprehend market demands. Artificial intelligence (AI)-powered prediction tools support decision-making by helping businesses project sales and examine market trends. The text also emphasizes how tailored marketing using AI-based software engage consumers and increase physician awareness. The paragraph also discusses how natural language processing methods are used to analyze keywords entered by customers in order to estimate the possibility that they would make a purchase. It is explained how self-service technology can be integrated into business-to-business (B2B) businesses to facilitate free health product browsing, simple specification-based searches, order placement, and shipment tracking. It is observed that pharma businesses are increasingly releasing web apps like Medline, Ask Apollo, 1 mg, Net meds and pharm easy.

1.8 AI in Pharmaceutical Manufacturing

Modern manufacturing systems are attempting to transfer human expertise to machines in order to meet the growing demands for efficiency and higher-quality products, as well as the growing complexity of production processes . The pharmaceutical business may benefit from the application of AI in manufacturing. Utilizing the automation of many pharmaceutical processes, tools like computational fluid dynamics study the effects of agitation and stress levels in various equipment (such stirred tanks) by using Reynolds-Averaged Navier-Stokes solvers technology. Similar systems, such large-eddy, and direct numerical simulations, use sophisticated techniques to resolve challenging flow issues in production[26].

Within the pharmaceutical industry, A digital elevation model has been widely applied. Examples of its use include studying the segregation of powders in a binary mixture, analyzing the time spent by tablets under the spray zone, predicting the possible path of the tablets during the coating process, and examining the effects of varying blade speed and shape. Artificial neural networks (ANNs) and fuzzy models investigated the relationship between machine parameters and the capping issue in order to minimize tablet capping on the production line. Artificial intelligence (AI) tools called meta-classifier and tablet-classifier assist in regulating the final product's quality standard by detecting potential production errors in tablets.

1.9 AI in Quality Control and Quality Assurance

A number of factors must be balanced in order to manufacture the desired product from the raw ingredients. Manual intervention is needed to maintain batch-to-batch consistency and conduct quality control tests on the products. This may not be the optimal course of action in every situation, highlighting the necessity of using AI at this time. In order to comprehend the crucial function and particular standards that determine the ultimate quality of the pharmaceutical product, the FDA modified the Current Good Manufacturing Practices (cGMP) by implementing a "Quality by Design" approach[26].

Artificial Intelligence (AI) has the potential to regulate in-line manufacturing processes in order to get the intended level of product quality. Utilizing a combination of local search, backpropagation, and self-adaptive evolution, ANN-based monitoring of the freeze-drying process is used. This can be used to forecast the temperature and thickness of the desiccated cake at a later time point (t + Dt) given a specific set of operating parameters, hence assisting in the quality control of the finished product. The quality assurance of the product can be guaranteed by using advanced, intelligent approaches in conjunction with an automated data entry platform, like as Electronic Lab Notebook. Additionally, the Total Quality Management expert system's data mining and other knowledge discovery techniques can be useful tools for making difficult judgments and developing new technologies for intelligent quality control.

1.10 AI in Regulatory Affairs

Drug regulatory issues is a complicated topic that calls for expertise across numerous academic fields. By automating repetitive and error-prone processes, artificial intelligence (AI) can assist streamline this process and free up human specialist’s time to concentrate on more difficult work. AI can also assist in identifying opportunities and hazards related to regulations, enabling a business to adjust its development plan. Artificial Intelligence is gradually transforming the drug regulatory affairs sector, and the FDA is incorporating AI technologies to expedite and improve the accuracy of new medication reviews[27].

1.11 AI in Regulatory Publishing

In a few years, artificial intelligence will introduce a huge upheaval to the regulatory publishing sector. Regulatory publishing is the process of submitting data to regulatory bodies, including the FDA, and other health agencies, as well as posting regulatory information about a drug in XML format. The procedure takes a long time and a lot of labour from people. Machine learning ideas will automate and improve the efficiency

of collecting and connecting. AI in Regulatory Submissions By minimizing the need for capital expenditures for compliance and regulation, artificial intelligence (AI) will help pharmaceutical businesses save time and money by automating the regulatory submission process. Artificial intelligence (AI) can assist in this process by automating some tedious and time-consuming human processes. AI can be used, for instance, to automatically extract data from clinical trials or create regulatory paperwork based on templates. Massive amounts of information can be analyzed by AI to find patterns and relationships that are impossible for people to find on their own. AI will aid in expediting the regulatory affairs review process for creating and releasing new medications more quickly.

1.12 AI in clinical trial design

Clinical trials take six to seven years and a significant financial commitment to establish the safety and efficacy of a medicinal product in people for a specific medical condition. Although only a single in ten of the compounds that are put through these trials end up getting cleared, which is a huge loss for the industry .These errors may be the consequence of bad infrastructure, insufficient technical requirements, or improper patient selection. But with the abundance of digital medical data at our disposal, these mistakes can be minimized by using AI.

Thirty percent of the clinical trial timeline is devoted to patient enrolment. Recruiting appropriate participants is crucial to the success of a clinical study, since it prevents around 86% of failure cases. Using patient-specific genome-exposome profile analysis, AI can help select only a particular diseased population for recruitment in Phase II and III clinical trials. This can help in early prediction of the possible therapeutic targets in the selected patients. Preclinical drug discovery and early lead compound prediction using other AI features, like predictive machine learning and other reasoning techniques, aid in the early identification of lead compounds that would pass clinical trials while taking the chosen patient population into account[28]. Thirty percent of clinical trials fail due to patient dropout, which causes additional recruiting requirements to be met for the experiment to be completed and wastes time and money. By closely monitoring the patients and assisting them in adhering to the intended protocol of the clinical research, this can be prevented. Ai Cure created mobile software to track schizophrenia patients' consistent medication intake throughout a Phase II trial[29]. This resulted in a 25% increase in patient adherence and the successful completion of the clinical trial.

India was one of the many countries in the world where pharmaceutical companies was using AI techniques and technologies. Nevertheless, consider that AI is a quickly developing area, and new tools might have appeared since then. The pharmaceutical sector in India made use of the following typical AI technologies and applications:

Drugs Discovery and Design:

- Machine Learning Algorithms: These are employed in the analysis of chemical and biological data to find possible candidates for drugs.
- Deep Learning: Neural networks have the potential to improve chemical architectures and anticipate drug-target interactions.
- Virtual Screening: Artificial intelligence assists in sifting through enormous chemical databases to find chemicals that may have medicinal benefits.

Clinical trial performance:

- Predictive analytics: AI systems assist with patient recruiting, tracking, and result prediction.
- Natural Language Processing (NLP): This technique is used in scholarly publications and electronic health records to extract insightful information from unstructured clinical data

Regulatory Compliance:

- AI-driven Compliance Management Systems: assist make sure that techniques used in the pharmaceutical industry adhere to legal requirements.

Customer Support and Engagement:

- Chatbots and Virtual Assistants: For answering consumer questions, providing pharmacological information, and facilitating communication with medical experts.

II. DISCUSSION:

Drug Discovery and Development Artificial intelligence (AI) is essential for rational drug design, optimal drug structure, and accelerated drug development. Although there are over 10^{60} compounds in the huge chemical universe, AI technologies like virtual screening and deep learning make it easier to find possible medications, validate targets, and enhance lead selection. However, issues with volume, variation, and complexity of data present challenges for AI. Large datasets may present obstacles for traditional machine learning algorithms, but newer AI methods like deep learning- solve these issues and improve safety and efficacy evaluations. In order to track the benefits of deep learning (DL) in the pharmaceutical industry's drug discovery process, Merck sponsored a Quantitative Structure Activity ML competition in 2012. In comparison to conventional ML techniques, DL models demonstrated a notable degree of predictivity for absorption, distribution, metabolism, excretion, and toxicity (ADMET)[6-7].

Drug Screening AI-driven algorithms are invaluable in the medication development process because of the significant cost and duration involved. Toxicological assessments, in vivo activity prediction, virtual screening, and nearest-neighbour classifiers are conducted using random forests, support vector machines, deep neural networks, and nearest-neighbour classifiers. Important factors to consider include physicochemical qualities, bioactivity, and toxicity. Artificial intelligence models help forecast and optimize these attributes. The Estimation Program Interface (EPI) Suite, which is a collection of six physicochemical properties of environmental chemicals received from the Environmental Protection Agency (EPA), was developed by Zang et al. using a quantitative structure - property relationship (QSPR) methodology. The ADMET predictor and ALGOPS program-based neural networks have been utilized to forecast the lipophilicity and solubility of different substances[15]. Molecule solubility has been predicted using DL techniques including graph-based convolutional neural networks (CVNN) and undirected graph recursive neural networks[30-31].

In Pharmaceutical Drug Development AI assists formulation design by handling stability, porosity, and dissolving issues. The concepts of Quality by Design are implemented, and excipient selection based on physicochemical attributes is guided by decision-support tools built on rule-based systems. In order to design a hybrid system for the production of piroxicam hard gelatin capsules that fill out directly, Guo et al. merged Expert Systems (ES) and ANN according to the requirements of its dissolving profile. Based on the input parameters, the MODEL EXPERT SYSTEM (MES) renders judgments and suggestions for formulation development[21]. In contrast, to enable hassle-free formulation creation, ANN uses backpropagation learning to link formulation parameters to the intended response, jointly regulated by the control module.

In Pharmaceutical Product Management the efficiency of a company depends on its market placement, and AI techniques such as particle swarm optimization algorithms and statistical analysis aid in understanding the changing circumstances of the market. The Fourth Industrial Revolution highlights the value of digital technologies in marketing, and artificial intelligence (AI) facilitates the formulation of winning market strategies. In Pharmaceutical Manufacturing Digital elevation models and computational fluid dynamics are two ways artificial intelligence is used in manufacturing operations to maximize output. Probabilistic models and artificial neural networks are used to identify possible mistakes in tablet manufacturing, which helps control product quality.

In Quality Control and Assurance AI plays a critical role in upholding product quality, automating production processes in-line, and guaranteeing adherence to Current Good Manufacturing Practices (cGMP). Intelligent methods and ANN-based models for process monitoring during freeze-drying improve quality assurance. Gams et al. created decision trees and assessed preliminary data from production batches using a combination of human and artificial intelligence[26]. To further direct the production cycle going forward, these were further translated into rules and examined by the operators . Using artificial neural networks (ANNs), Goh et al. investigated the dissolution profile of theophylline pellets as a measure of batch-to-batch consistency. The artificial neural networks accurately predicted the tested formulation's dissolution with an error of less than 8%[32].

In Regulatory Affairs AI plays a critical role in upholding product quality, automating production processes in-line, and guaranteeing adherence to Current Good Manufacturing Practices (cGMP). Intelligent methods and ANN-based models for process monitoring during freeze-drying improve quality assurance. Gams et al. created decision trees and assessed preliminary data from production batches using a combination of human and artificial intelligence. To further direct the production cycle going forward, these were further

translated into rules and examined by the operators . Using artificial neural networks (ANNs), Goh et al. investigated the dissolution profile of theophylline pellets as a measure of batch-to-batch consistency. The artificial neural networks accurately predicted the tested formulation's dissolution with an error of less than 8%.

In Clinical Trial Design by increasing patient recruitment, anticipating results, and reducing patient dropout rates, AI decreases the duration of clinical trials. Clinical trial efficiency is increased by patient-specific genome-exposome profile analysis, natural language processing, and predictive analytics.

III. CONCLUSION:

The pharmaceutical business is experiencing a surge in startups because to the revolutionary changes it is bringing about in the areas of medication research and production through the integration of AI. This development tackles issues like growing prescription expense and the requirement for substantial reforms in the healthcare system. Artificial Intelligence (AI) in pharmaceutical manufacturing enables customized drugs based on each patient's requirements, including doses, release parameters, and other important factors. The integration of artificial intelligence (AI) technologies results in expedited product development timeframes, improved product quality, safety, and resource efficiency, and an automated and cost-effective solution. Artificial Intelligence plays a significant role in hit compound identification, synthesis method suggestions, chemical structure prediction, drug-target interaction understanding, and structure-activity relationship (SAR) comprehension. Furthermore, AI is essential for improving medication dose formulations, guaranteeing batch-to-batch consistency, accelerating the process of making decisions and enabling the production of high-quality goods more quickly.

AI is useful for determining a product's safety and effectiveness in clinical trials, analyzing the market, and forecasting prices and positioning. Although there aren't any AI-developed medications on the market now, it's expected that AI will grow to be a vital tool in the pharmaceutical sector, helping to solve particular implementation-related issues. All things considered, artificial intelligence is going to be a big part of how drug research and discovery are done in the future, and it will be very beneficial to the industry.

IV. ACKNOWLEDGMENT:

I would like to express my gratitude to the Chalapathi Institute of Pharmaceutical Sciences for their constant support and guidance.

REFERENCES:

1. Duch, W. et al. (2007) Artificial intelligence approaches for rational drug design and discovery. Curr. Pharm. Des. 13, 1497–1508
2. Blasiak, A. et al. (2020) CURATE. AI: optimizing personalized medicine with artificial intelligence. SLAS Technol. 25, 95–105
3. Vyas, M. et al. (2018) Artificial intelligence:the beginning of a new era in pharmacy profession. Asian J. Pharm. 12, 72–76
4. Mak, K.-K. and Pichika, M.R. (2019) Artificial intelligence in drug development: present status and future prospects. Drug Discovery Today 24, 773–780 20
5. Sellwood, M.A. et al. (2018) Artificial intelligence in drug discovery. Fut. Sci. 10, 2025–2028
6. Zhu, H. (2020) Big data and artificial intelligence modeling for drug discovery. Annu. Rev. Pharmacol. Toxicol. 60, 573–589 22
7. Ciallella, H.L. and Zhu, H. (2019) Advancing computational toxicology in the big data era by artificial intelligence: data-driven and mechanism-driven modeling for chemical toxicity. Chem. Res. Toxicol. 32, 536–547
8. Chan, H.S. et al. (2019) Advancing drug discovery via artificial intelligence. Trends Pharmacol. Sci. 40 (8), 592–604
9. Mak, K.-K. and Pichika, M.R. (2019) Artificial intelligence in drug development: present status and future prospects. Drug Discovery Today 24, 773–780
10. A´lvarez-Machancoses, O´ and Ferna´ndez-Martı´nez, J.L. (2019) Using artificial intelligence methods to speed up drug discovery. Expert Opin. Drug Discovery 14, 769–777
11. Fleming, N. (2018) How artificial intelligence is changing drug discovery. Nature 557 S55–S55

12. Dana, D. et al. (2018) Deep learning in drug discovery and medicine; scratching the surface. Molecules 23, 2384
13. Zang, Q. et al. (2017) In silico prediction of physicochemical properties of environmental chemicals using molecular fingerprints and machine learning. J. Chem. Inf. Model. 57, 36–49
14. Hessler, G. and Baringhaus, K.-H. (2018) Artificial intelligence in drug design. Molecules 23, 2520
15. Zang, Q. et al. (2017) In silico prediction of physicochemical properties of environmental chemicals using molecular fingerprints and machine learning. J. Chem. Inf. Model. 57, 36–49
16. Rupp, M. et al. (2010) Estimation of acid dissociation constants using graph kernels. Mol. Inf. 29, 731–740
17. Rupp, M. et al. (2010) Estimation of acid dissociation constants using graph kernels. Mol. Inf. 29, 731–740
18. Lounkine, E. et al. (2012) Large-scale prediction and testing of drug activity on side-effect targets. Nature 486, 361–367
19. O¨ ztu¨rk, H. et al. (2018) DeepDTA: deep drug–target binding affinity prediction. Bioinformatics 34, i821–i829
20. Basile, A.O. et al. (2019) Artificial intelligence for drug toxicity and safety. Trends Pharmacol. Sci. 40, 624–635
21. Guo, M. et al. (2002) A prototype intelligent hybrid system for hard gelatin capsule formulation development. Pharm. Technol. 6, 44–52
22. Mehta, C.H. et al. (2019) Computational modeling for formulation design. Drug Discovery Today 24, 781–788
23. Zhao, C. et al. (2006) Toward intelligent decision support for pharmaceutical product development. J. Pharm. Innovation 1, 23–35
24. Ding, M. et al. (2016) Innovation and Marketing in the Pharmaceutical Industry. Springe
25. Toker, D. et al. (2013) A decision model for pharmaceutical marketing and a case study in Turkey. Ekonomska Istraivanja 26, 101–114
26. Gams, M. et al. (2014) Integrating artificial and human intelligence into tablet production process. AAPS PharmSciTech 15, 1447–1453
27. Patil RS, Kulkarni SB, Gaikwad VL. Artificial intelligence in pharmaceutical regulatory affairs. Drug Discov Today. 2023 Sep;28(9):103700. doi: 10.1016/j.drudis.2023.103700. Epub 2023 Jul 12. PMID: 37442291.
28. Hay, M. et al. (2014) Clinical development success rates for investigational drugs. Nat. Biotechnol. 32, 40–51
29. Harrer, S. et al. (2019) Artificial intelligence for clinical trial design. Trends Pharmacol. Sci. 40, 577–591
30. Lusci, A. et al. (2013) Deep architectures and deep learning in chemoinformatics: the prediction of aqueous solubility for drug-like molecules. J. Chem. Inf. Model. 53, 1563–1575
31. Kumar, R. et al. (2017) Prediction of human intestinal absorption of compounds using artificial intelligence techniques. Curr. Drug Discovery Technol. 14, 244–254
32. Goh, W.Y. et al. (2002) Application of a recurrent neural network to prediction of drug dissolution profiles. Neural Comput. Appl. 10, 311–317