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Review Article

Artificial Intelligence (AI) in Pharmacy: An Overview of Innovations: Review Article

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ABSTRACT

Artificial Intelligence (AI) is a tool for data analysis and data related problems. This advancement has led to several technological achievements in virtually all fields from engineering to architecture, education, accounting, business, health, and many more. Intelligent modeling is the main goal of Artificial Intelligence (AI), which aids with knowledge envisioning, problem solving, and decision making. AI has recently become significant in a number of pharmacy-related domains, including hospital pharmacy, polypharmacology, drug delivery formulation development, and drug discovery. Different Artificial Neural Networks (ANNs), such as Deep Neural Networks (DNNs) or Recurrent Neural Networks (RNNs), are used in drug discovery and drug delivery formulation development. The power of the technology in Quantitative Structure-Activity Relationship (QSAR) or Quantitative Structure-Property Relationship (QSPR) has been examined in a number of drug discovery applications. The applications of AI in pharmacy, particularly in drug discovery, drug delivery formulation development, polypharmacology, and hospital pharmacy, are covered in the current review paper.

Keywords: Artificial Intelligence, Artificial Neural Network, Drug Discovery, Drug Delivery Research, Hospital Pharmacy.

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INTRODUCTION

Artificial Intelligence (AI) is a branch of study that deals with intelligent machine learning, mostly intelligent computer programs that produce outcomes that resemble human attention processes (Mak and Pichika, 2019). In general, this process entails gathering data, creating effective methods for using the data, and demonstrating precise or approximative findings and self-corrections/adjustments (Hassanzadeh *et al*., 2019). AI is typically used to analyze machine learning to mimic human cognitive activities (Hassanzadeh *et al*., 2019; Russel *et al*., 2015). AI technology is used to achieve both helpful interpretation and more accurate analyses (Russel *et al*., 2015). According to this viewpoint, AI technology combines computer intelligence with a number of practical statistical models (Duch *et al*., 2004). However, the confidence that greatly adds to AI technology's effectiveness in the industry is the reason why nearly all advances in its applications are being welcomed. AI technology has recently become a highly important component of industry for the beneficial uses in numerous technical and research fields (Russel *et al*., 2015; Duch *et al*., 2004). The rising effort of accepting the uses of AI technology in pharmacy including drug discovery, drug delivery formulation development and other healthcare applications have already been converted from hype to hope (Table 1) (Dasta, 1992; Jiang *et al*., 2017). The applications of AI models also enable the prediction of *in vivo* reactions, pharmacokinetic therapeutic parameters, appropriate dosage, etc., (Hassanzadeh *et al*., 2019; Gobburu and Chen, 1996). Given the significance of pharmacokinetic drug prediction, the use of *in silico* models facilitates their efficacy and affordability in drug research (Sakiyama, 2009). AI technology advancements fall into two main categories (Agatonovic-Kustrin and Beresford, 2000). The first one consists of traditional computing techniques, such as expert systems, which can mimic human experiences and show the conclusions drawn from the principles (Zhang *et al*., 2012). The second one consists of systems that use Artificial Neural Networks (ANNs) to simulate how the brain functions (Agatonovic-Kustrin and Beresford, 2000). In specific, several ANNs like Deep Neural Networks (DNNs) or Recurrent Neural Networks (RNNs) manage the evolutions of AI technology. DNN problems demonstrate higher predictivity than the baseline machine learning approaches in the Merck Kaggle11 and NIH Tox21 challenges (Russel *et al*., 2015; Merk *et al*., 2018). Machine learning uses appropriate statistical techniques that can learn with or without explicit programming (Bishop, 2013). De novo design also encourages the creation of novel pharmacological compounds with optimal or desired properties (Merk *et al*., 2018). The applications of AI in pharmacy, particularly in drug

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discovery and drug delivery formulation development, are discussed in the current review paper. Hospital pharmacy and polypharmacology are discussed.

METHODOLOGY

To gather pertinent published research on the use of Artificial Intelligence (AI) in pharmacy, a thorough literature search was carried out. A thorough search was conducted for publications published between 2010 and 2025 using electronic databases such as PubMed, Scopus, Google Scholar, ScienceDirect, and Web of Science.

The following terms and combinations were used in the search:

"AI in Pharmacy," "AI in Drug Discovery," "Artificial Neural Networks in Drug Delivery," "Machine Learning in Pharmaceutical Sciences," "AI in Hospital Pharmacy," "Polypharmacology and Artificial Intelligence," "Deep Learning in Drug Design," and "QSAR and AI in Drug Discovery"

The search approach was refined using Boolean operators like AND, OR, and NOT. Title, abstract, and full-text availability were used to filter pertinent review articles, original research papers, and computational studies.

Criteria for Inclusion

1. Peer-reviewed journal articles.
2. Research on the use of AI in pharmacy.
3. Drug delivery, Polypharmacology, Drug development, and Hospital pharmacy research.
4. English-language articles.
5. Research with computational, Experimental, or Review-based evidence.

Exclusion Standards

1. Repeated research.
2. Abstracts of conferences without full texts.
3. Articles written in languages other than English.
4. Research unrelated to AI's use in medicine.
5. Articles containing inadequate scientific information.

DISCUSSION/REVIEW OF LITERATURE

Classification of AI

AI can be divided into two categories based on its presence and quality (Figure 1) (Manikiran and Prasanthi, 2019; Cherkasov *et al.*, 2009). Based on their capabilities, AI can be classified as:

i) Artificial Narrow Intelligence (ANI) or Weak AI: It carries out tasks that are limited in scope, such as traffic signaling, chess practice, car steering, and facial recognition.

ii) Artificial General Intelligence (AGI) or Strong AI: Also referred to as human-level AI, it is capable of all human functions. It can perform new tasks and simplify human cognitive capacities.

iii) Artificial Super Intelligence (ASI): It is far more intelligent and active than humans in areas such as mathematics, sketching, and space exploration.

AI can be categorized as follows based on whether it is present or not:

i) Type 1: Because it lacks a memory system, it is utilized for specialized applications that are unable to leverage prior knowledge. It's referred to as a reactive machine. Examples of this memory include an IBM chess program that can identify the checkers on the chess board and make predictions.

ii) Type 2: It features a constrained memory system that can use prior knowledge to solve various issues. The system in autonomous cars has the ability to make judgments based on some recorded observations that are used to document subsequent actions. However, these recordings are not kept indefinitely.

iii) Type 3: It is predicated on "Theory of Mind," which implies that people's decisions are influenced by their unique thoughts, intentions and aspirations. AI does not exist in this system.

iv). Type 4: It possesses self-awareness, or consciousness and a sense of self. Additionally, this system is nonexistent AI.

AI in hospital pharmacy

AI is used in hospital pharmacy-based healthcare systems in a number of ways, including organizing dose forms for specific patients, choosing the appropriate or accessible methods of administration or treatment guidelines (Jiang *et al.*, 2017; Manikiran and Prasanthi, 2019).

i) Maintaining medical records: Keeping up with patients' medical records is a challenging endeavor. The collection, storing normalization, tracing of data are made easy by applying the AI system. Google's Deep Mind health initiative helps quickly uncover medical records. Hence, this initiative is a valuable one for better and faster health treatment. The Moor Fields Eye hospital NHS is assisted by this project for development of eye treatment.

ii) Creating treatment plans: AI technology makes it feasible to create efficient treatment plans (Manikiran and Prasanthi, 2019). When a patient's situation is critical emerges and choosing an appropriate course of therapy becomes challenging, the AI system is required to manage the issue. The treatment plan that this technology suggests takes into account all of the prior data and

reports, clinical expertise, etc. IBM Watson launches a program to assist oncologists.

iii) Helping with repetitive jobs: AI technology also helps with certain repetitive duties, such analyzing radiography, X-ray imaging, ECHO, ECG, etc., for the detection and diagnosis of the illnesses or conditions (Manikiran and Prasanthi, 2019).

The IBM algorithm Medical Sieve is a "cognitive assistant" with strong analytical and reasoning skills. A medical start-up is important for the improvement of patient condition by combining deep learning with medical data. Every bodily part has a unique computer software that is employed for certain medical disorders. Nearly all imaging analyses, including X-rays, CT scans, ECHOs, ECGs, etc., may be performed using deep learning.

iv) Health support and medication assistance: Recent years, the uses of AI technology are acknowledged efficient in health support services and also, for the medication assistances (Jiang *et al.*, 2017). Molly (a start-up built virtual nurse) receives a lovely voice together with a kind visage. Its goal is to support patients with chronic conditions in between doctor appointments and to assist them in guiding their treatment. A smartphone webcam app called Ai Cure keeps an eye on patients and helps them manage their diseases.

v) AI benefits patients in the healthcare system by gathering and analyzing data via social awareness algorithms (Jiang *et al.*, 2017). The huge information recorded in healthcare system covers the medical history of the patients together with the treatment history profile from the birth, habits as well as life-styles of the patients.

AI techniques for finding new drugs

The accessible findings from many resources, such as high-throughput screening modeling, fragment screening modeling, computational modeling, and published data, are where the drug discovery process starts (Mak and Pichika, 2019; Fleming, 2018). Figures 2 and 3 depicts a schematic representation of the drug discovery process. Computer-assisted design techniques may be used to directly or indirectly examine the structural characterization of drug molecules throughout the drug discovery process. Following this, organic synthesis of drug molecules is carried out. Following high throughput screening in the main test, the manufactured drug molecules or collected drug compounds undergo successful Structure Activity Relationship (SAR) analysis, counter screening, and bioavailability evaluation in secondary assays. The induction and deduction stages are interchanged in the drug development process. The automation of specific portions of the inductive-deductive cycle decreases the unpredictability and inaccuracy; hence, enhances the efficacy of the drug discovery process. Manufacturers of chemicals and pharmaceuticals use deep learning software, such as "NVIDIA DGX-(Mak and Pichika, 2019)," to analyze and extract multiple patents and genetic data-based scientific science knowledge. The entirety of the information accessible for the growth of scientific study cannot be operated by humans. In order to identify the relationships between the substances and provide novel therapeutic molecules, AI supercomputers are able to receive and analyze the data (Agatonovic-Kustrin and Beresford, 2000; Lakdawala *et al.*, 2018). The usage of chemical space is one of the applications of AI in the drug development process (Mak and Pichika, 2019; Lakdawala *et al.*, 2018). Since it is possible to

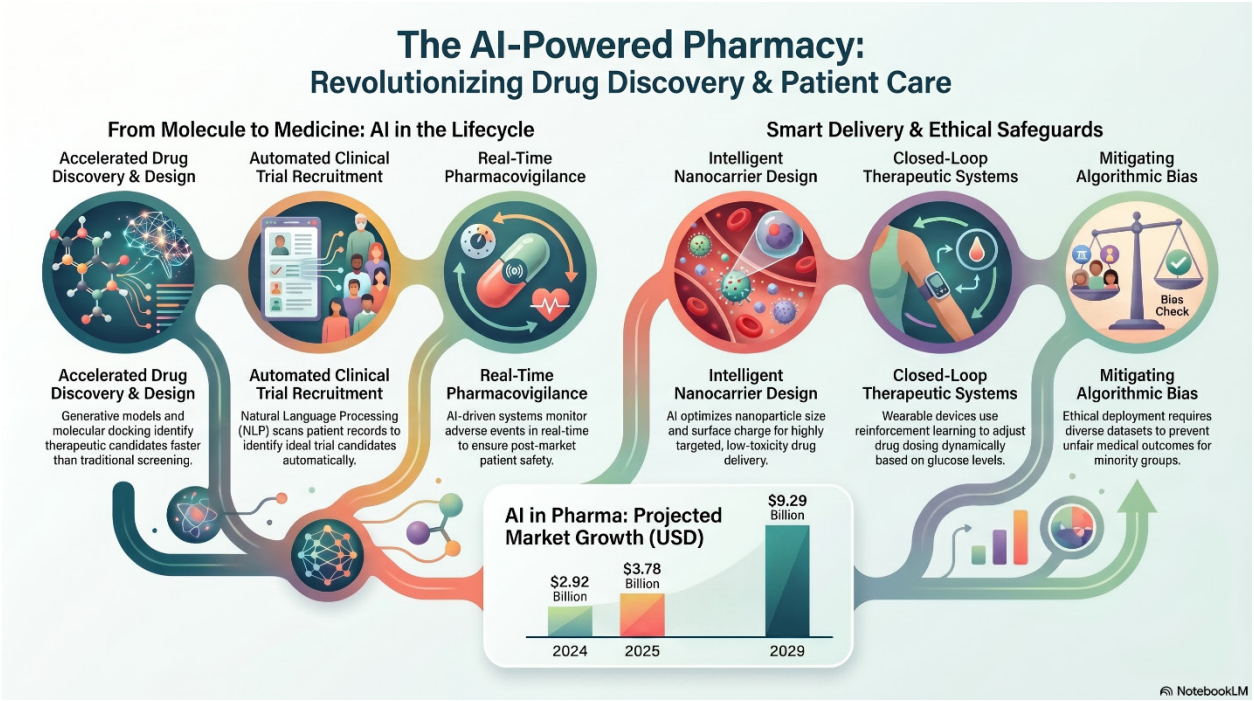


Figure 1: AI Innovations in Pharmacy.

computationally list the required compounds, the chemical space really provides the phase for the identification of novel molecules (Reymond *et al.*, 2010). In addition, the machine learning and associated prediction techniques also aid for the identifications of target-specific effective compounds (Ferrero *et al.*, 2017). The most difficult aspect of the entire procedure is choosing a successful new medication molecule from a vast number of pharmacologically active chemical entities (Katsila *et al.*, 2016). The goal of benevolent AI is to process fewer molecules with far greater certainty on their activity. In this sense, de novo design requires knowledge of organic chemistry for the synthesis of in silico molecules and virtual screening modeling, which serve as substitutes for numerous biochemical and biological tests to assess toxicity profiles and efficiency (Yuan *et al.*, 2011; Merk *et al.*, 2018; Blaschke *et al.*, 2018; Gupta *et al.*, 2018).

The creation of novel active compounds without the assistance of reference molecules is the goal of de novo design in drug development (Merk *et al.*, 2018). Lastly, novel compounds with potential activities against the target-setting of illnesses or disorders can be found thanks to active learning algorithms. Together with the readily available data on small molecule modulator probes or structural biology characteristics, a number of *in silico* techniques for profile selection, such as ligand-based design approaches or molecular structure-based design approaches, may be used (Ferrero *et al.*, 2017). The next generation of AI is being obtained by *in silico* molecules. There are various proposals and software solutions available for it. This design is not effective in drug development; but it is connected to the production of components featuring difficulties in synthesis (Mak and Pichika, 2019).

Drug compounds can be designed using Generative Adversarial Networks (GANs). The technique can use the text representation to create photo-realistic images Kadurin *et al.* (2017). used GAN in a study to recommend drugs with anticancer properties (Kadurin *et al.*, 2017) This technology also allows for the generation of new data or imagination based on existing data. AI of the future is independent of learning from huge data sets. All issues that were previously challenging to resolve may be handled by the new AI technology (Silver *et al.*, 2017). This innovative technology aids scientists and researchers in identifying and choosing potential chemical compounds based on their safety, effectiveness, and ability to select people for clinical trials (Mak and Pichika, 2019; Fleming, 2018). AI can prioritize compounds for therapeutic delivery based on their ease of synthesis or usefulness. Proven instruments for optimal synthetic techniques (Lakdawala *et al.*, 2018).

Table 2 provides a summary of key AI-based technologies for drug development.

AI approaches in polypharmacology

Today, the 'one-disease-multiple-targets' idea is preferred over the 'one-disease-one-targets' model for better understanding of pathological processes in numerous illnesses at the molecular level. Polypharmacology refers to the phenomena of treating a single illness using several targets (Prescott *et al.*, 2006). Various databases, such as PubChem, KEGG, ChEMBL, ZINC, STITCH, Ligand Expo, PDB, Drug Bank, Supertarget, and Binding DB,

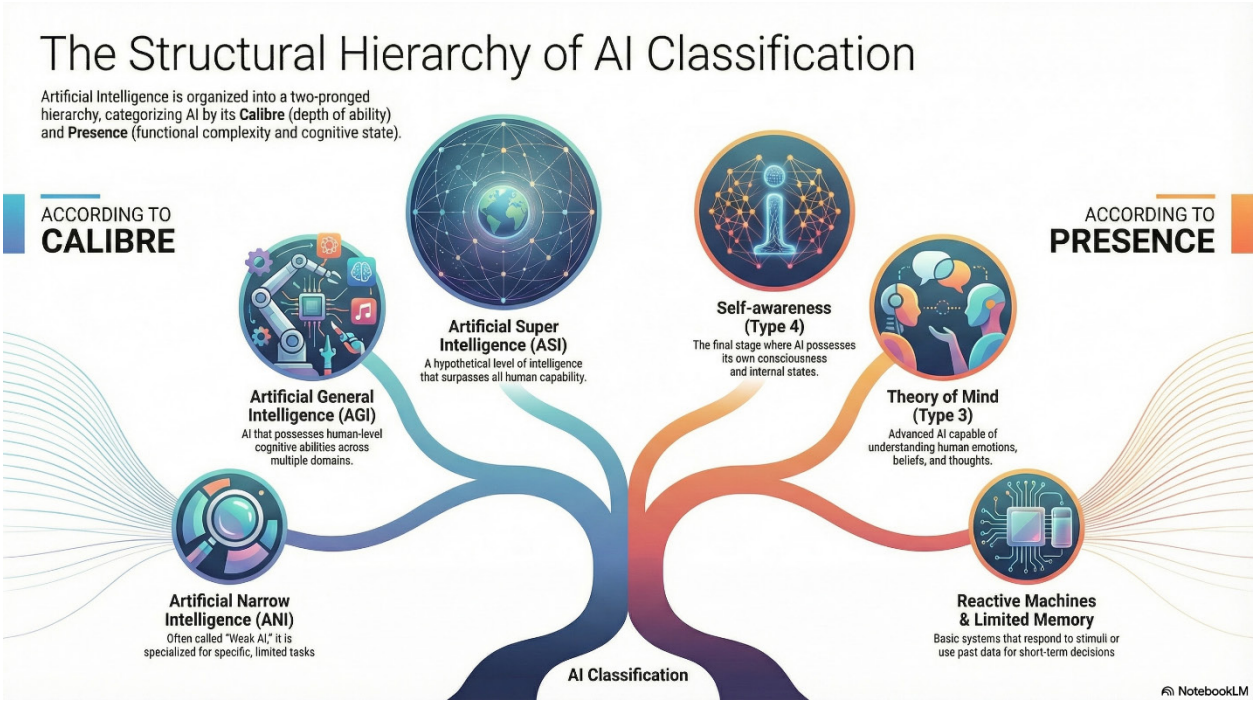


Figure 2: Classification of AI.

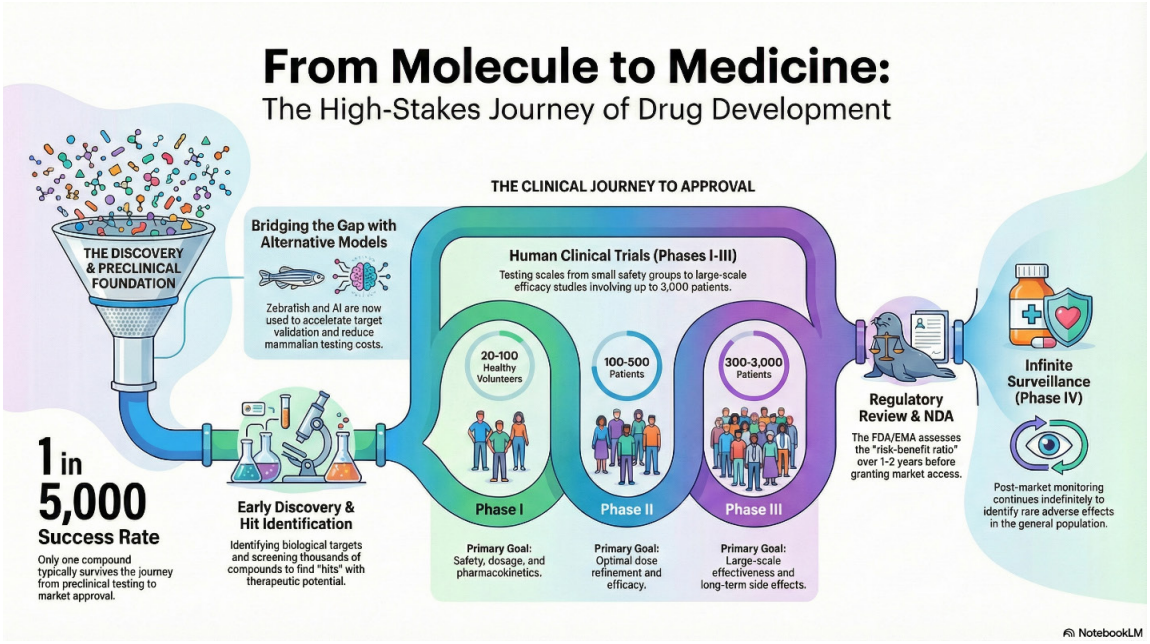


Figure 3: AI In Drug Discovery Process.

Table 1: Shows some current studies on the application of artificial intelligence in the development of medication delivery systems.

Drug Delivery System	AI / Modeling Approach Used	Key Application	References
Ibuprofen sustained-release tablets	Adaptive neural-fuzzy inference system	Sustained release optimization	Rebouh *et al.* (2019)
Pellet-containing tablets	ANN	Tablet performance prediction	Huang *et al.* (2015)
Liposomes (ultrasonic release)	ANN	Controlled release	Moussa *et al.* (2017)
Doxycycline-HPβCD complex	RSM, ANN, SVM	Formulation optimization	Wang *et al.* (2013)
Oral disintegrating tablets	ANN, DNN	Disintegration prediction	Han *et al.* (2018)
Agar nanospheres of bupropion	GA, ANN, RSM	Nano-delivery optimization	Zaki *et al.* (2015)
Pilocarpine HCl nano-liposomes	RSM, ANN	Ophthalmic delivery	Zhao *et al.* (2018)
Rosiglitazone maleate floating tablets	ANN	Gastro-retentive delivery	Güler *et al.* (2017)
Nifedipine osmotic tablets	GI simulation, ANN	Controlled release	Ilić *et al.* (2014)
Diclofenac sodium gelatin nanoparticles	CCD, ANN	Nanoparticle optimization	Koletti *et al.* (2020)
Ciprofloxacin bone implants	QbD, factorial design	Implant optimization	Nayak *et al.* (2011)
Alginate-PVP microbeads of diclofenac	CCD, RSM	Controlled release	Nayak *et al.* (2011)
Timolol nanoliposomes	ANN, MLR	Ocular delivery	León Blanco *et al.* (2018)
Transferosomal gel (insulin)	Factorial design, RSM	Transdermal delivery	Malakar *et al.* (2012)
Besifloxacin HCl liposomal gel	Factorial design, RSM	Topical delivery	Bhattacharjee *et al.* (2020)
Transferosomal gel (risperidone)	CCD, RSM	Transdermal delivery	Das *et al.* (2017)
Prednisone pellet system	Box-Behnken, ANN	Multiparticulate delivery	Manda *et al.* (2019)
Mesalamine matrix tablets	ANN, MLP	Colon targeting	Khan *et al.* (2020)
Voriconazole lipid carriers	Box-Behnken, QbD	Topical delivery	Waghule *et al.* (2019)
Metformin HCl mucoadhesive beads	Factorial design, RSM	Oral delivery	Nayak and Pal (2013)

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

Tool Name	Application Area	AI / ML Model	Input Data Types	Key Features
AlphaFold 2	Protein structure prediction	Deep Learning (Transformer-based)	Amino acid sequences, MSA, BFD	Accurate 3D protein structure prediction
AlphaFold 3	Biomolecular complex prediction	Pairformer + diffusion model	Protein, DNA, RNA, ligands, ions	Predicts protein-ligand complexes
ChemicalX	Drug-drug interaction scoring	Deep Learning (MR-GNN, DeepDDI)	SMILES, fingerprints, molecular graphs	Unified drug-pair scoring framework
ODDT	Virtual screening	RF, SVM, Neural Networks	PDB, SDF, SMILES	CADD and docking tools
DeepTox	Toxicity prediction	Deep Neural Network	HTS data, molecular fragments	Winner of Tox21 challenge
Chemputer	Automated synthesis	Pathfinding algorithms	XDL, hardware graphs	Autonomous synthesis and purification
ORGANIC	Molecular generation	GAN	SMILES	Inverse molecular design
Hit Dexter	Assay interference prediction	Machine Learning	Small molecules	Detects non-specific assay responses
REINVENT	*De novo* drug design	RNN + Reinforcement Learning	SMILES	Generates novel molecules

provide valuable information on crystal structure, chemical features, biological properties, molecular pathways, binding affinities, disease concerns, and drug targets. AI can aid in the discovery of databases for polypharmacological compounds and agents.

Future Directions / Research Gaps

AI technologies are expected to operate independently of learning from massive datasets. Advanced generative models, such as Generative Adversarial Networks (GANs), will increasingly be used to generate novel pharmaceutical compounds with desired molecular properties *in silico*, resolving synthesis issues that were previously challenging. Further research is needed to bridge the gap between AI-designed chemical spaces and optimal, highly predictable *in vivo* synthetic outcomes.

CONCLUSION

In recent years, there has been a growing interest in using AI technology to analyze and interpret important pharmacy fields such as drug discovery, polypharmacology, and hospital pharmacy. AI technology mimics human decision-making and problem-solving abilities. Automated procedures and databases, together with AI-based analysis, have proven beneficial. AI allows for faster and more cost-effective formulation and analysis of hypotheses, methods, and associated aspects.

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ABBREVIATIONS

AI: Artificial Intelligence; **AGI:** Artificial General Intelligence; **ANI:** Artificial Narrow Intelligence; **ANN:** Artificial Neural Network; **ASI:** Artificial Super Intelligence; **BFD:** Big Fantastic Database; **CADD:** Computer-Aided Drug Design; **CCD:** Central Composite Design; **CT:** Computed Tomography; **DNN:** Deep Neural Network; **ECG:** Electrocardiogram; **ECHO:** Echocardiogram; **GA:** Genetic Algorithm; **GAN:** Generative Adversarial Network; **GI:** Gastrointestinal; **HPβCD:** Hydroxypropyl-β-cyclodextrin; **HTS:** High-Throughput Screening; **ML:** Machine Learning; **MLP:** Multilayer Perceptron; **MLR:** Multiple Linear Regression; MR-**GNN:** Multiresolution Graph Neural Network; **MSA:** Multiple Sequence Alignment; **PDB:** Protein Data Bank; **PVP:** Polyvinylpyrrolidone; **QbD:** Quality by Design; **QSAR:** Quantitative Structure-Activity Relationship; **QSPR:** Quantitative Structure-Property Relationship; **RF:** Random Forest; **RNN:** Recurrent Neural Network; **RSM:** Response Surface Methodology; **SAR:** Structure Activity Relationship; **SDF:** Structure Data File; **SMILES:** Simplified Molecular Input Line Entry System; **SVM:** Support Vector Machine; **XDL:** Chemical Description Language.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

AUTHOR CONTRIBUTIONS

Atul Sharma: Conceptualization, literature search, data collection, manuscript drafting, and preparation of figures and tables.

Sonika Rattan: Supervision, critical review of the literature, manuscript editing, and intellectual input.

Nitika Sharma: Literature review, data analysis, manuscript revision, and reference management.

Sharad: Manuscript review, editing, validation of scientific content, and final approval of the manuscript.

SUMMARY

AI technology has transitioned from hype to hope in the pharmaceutical industry, offering highly beneficial statistical and computer intelligence models. It streamlines hospital pharmacy operations, enhances drug delivery system design through Artificial Neural Networks, and accelerates drug discovery by evaluating vast chemical spaces and polypharmacological targets.

REFERENCES

Agatonovic-Kustrin, S., & Beresford, R. (2000). Basic concepts of artificial neural network (ANN) modeling and its application in pharmaceutical research. *Journal of Pharmaceutical and Biomedical Analysis, 22*(5), 717-727. https://doi.org/10.1016/S0731-7085(99)00272-1

Bhattacharjee, A., Das, P. J., Dey, S., Nayak, A. K., Roy, P. K., *et al.* (2020). Development and optimization of Besifloxacin hydrochloride loaded liposomal gel prepared by thin film hydration method using 32 full factorial design. *Colloids and Surfaces. Part A: Physicochemical and Engineering Aspects, 585*, 124071. https://doi.org/10.1016/j.colsurfa.2019.124071

Bishop, C. M. (2012). Model-based machine learning. *Philosophical Transactions. Series A, Mathematical, Physical, and Engineering Sciences, 371*(1984), 20120222. https://doi.org/10.1098/rsta.2012.0222

Blaschke, T., Olivecrona, M., Engkvist, O., Bajorath, J., & Chen, H. (2018). Application of Generative Autoencoder in de nov Molecular Design. *Molecular Informatics, 37*(1-2), 201700123.

Cherkasov, A., Hilpert, K., Jenssen, H., Fjell, C. D., Waldbrook, M., *et al.* (2009). Use of artificial intelligence in the design of small peptide antibiotics effective against a broad spectrum of highly antibiotic-resistant superbugs. *ACS Chemical Biology, 4*(1), 65-74. https://doi.org/10.1021/cb800240j

Das, B., Sen, S. O., Maji, R., Nayak, A. K., & Sen, K. K. (2017). Transferosomal gel for transdermal delivery of risperidone: Formulation optimization and *ex vivo* permeation. *Journal of Drug Delivery Science and Technology, 38*, 59-71. https://doi.org/10.1016/j.jddst.2017.01.006

Dasta, J. F. (1992). Application of artificial intelligence to pharmacy and medicine. *Hospital Pharmacy, 27*(4), 319-322.

Duch, W., Setiono, R., & Zurada, J. M. (2004). Computational intelligence methods for rule-based data understanding. *Proceedings of the IEEE, 92*(5), 771-805. https://doi.org/10.1109/JPROC.2004.826605

Ferrero, E., Dunham, I., & Sanseau, P. (2017). *In silico* prediction of novel therapeutic targets using gene-disease association data. *Journal of Translational Medicine, 15*(1), 182. https://doi.org/10.1186/s12967-017-1285-6

Fleming, N. (2018). How artificial intelligence is changing drug discovery. *Nature, 557*(7707), S55-S57. https://doi.org/10.1038/d41586-018-05267-x

Gobburu, J. V., & Chen, E. P. (1996). Artificial neural networks as a novel approach to integrated pharmacokinetic-pharmacodynamic analysis. *Journal of Pharmaceutical Sciences, 85*(5), 505-510. https://doi.org/10.1021/js950433d

Güler, G. K., & Eroğlu, H. (2017). Development and formulation of floating tablet formulation containing rosiglitazone maleate using artificial neural network. *Journal of Drug Delivery Science and Technology, 29*, 385-397.

Gupta, A., Müller, A. T., Huisman, B. J. H., Fuchs, J. A., Schneider, P., & Schneider, G. (2018). Generative recurrent networks for de novo drug design. *Molecular Informatics, 37*(1-2), 1700111. https://doi.org/10.1002/minf.201700111

Han, R., Yang, Y., Li, X., & Ouyang, D. (2018). Predicting oral disintegrating tablet formulations by neural network techniques. *Asian Journal of Pharmaceutical Sciences, 13*(4), 336-342. https://doi.org/10.1016/j.ajps.2018.01.003

Hassanzadeh, P., Atyabi, F., & Dinarvand, R. (2019). The significance of artificial intelligence in drug delivery system design. *Advanced Drug Delivery Reviews, 151-152*, 169-190. https://doi.org/10.1016/j.addr.2019.05.001

Huang, Y., Yao, Q., Zhu, C., Zhang, X., Qin, L., *et al.* (2015). Comparison of novel granulated pellet-containing tablets and traditional pellet-containing tablets by artificial neural networks. *Pharmaceutical Development and Technology, 20*(6), 670-675. https://doi.org/10.3109/10837450.2014.910809

Ilić, M., Đuriš, J., Kovačević, I., Ibrić, S., & Parojčić, J. (2014). *In vitro-in silico-in vivo* drug absorption model development based on mechanistic gastrointestinal simulation and artificial neural networks: Nifedipine osmotic release tablets case study. *European Journal of Pharmaceutical Sciences, 62*, 212-218. https://doi.org/10.1016/j.ejps.2014.05.030

Jiang, F., Jiang, Y., Zhi, H., Dong, Y., Li, H., Ma, S., *et al.* (2017). Artificial intelligence in healthcare: Past, present and future. *Stroke and Vascular Neurology, 2*(4), 230-243. https://doi.org/10.1136/svn-2017-000101

Kadurin, A., Nikolenko, S., Khrabrov, K., Aliper, A., & Zhavoronkov, A. (2017). druGAN: An advanced generative adversarial autoencoder model for de novo generation of new molecules with desired molecular properties *in silico*. *Molecular Pharmaceutics, 14*(9), 3098-3104. https://doi.org/10.1021/acs.molpharmaceut.7b00346

Katsila, T., Spyroulias, G. A., Patrinos, G. P., & Matsoukas, M.-T. (2016). Computational approaches in target identification and drug discovery. *Computational and Structural Biotechnology Journal, 14*, 177-184. https://doi.org/10.1016/j.csbj.2016.04.004

Khan, A. M., Hanif, M., Bukhari, N. I., Shamim, R., Rasool, F., *et al.* (2020). Artificial neural network (ANN) approach to predict an optimized pH-dependent mesalamine matrix tablet. *Drug Design, Development and Therapy, 14*, 2435-2448. https://doi.org/10.2147/DDDT.S244016

Koletti, A. E., Tsarouchi, E., Kapourani, A., Kontogiannopoulos, K. N., Assimopoulou, A. N., & Barmpalexis, P. (2020). Gelatin nanoparticles for NSAID systemic administration: Quality by design and artificial neural networks implementation. *International Journal of Pharmacy, 578*, 1-14.

Lakdawala, A. S., Okafo, G., Baldoni, J., Palovich, M., Sikosek, T., & Sahni, V. (2018). Adapting drug discovery to artificial intelligence. *Drug target rev, 5(2),* 50-52.

León Blanco, J. M., González-R, P. L., Arroyo García, C. M., Cózar-Bernal, M. J., *et al.* (2018). Artificial neural networks as alternative tool for minimizing error predictions in manufacturing ultra deformable nanoliposome formulations. *Drug Development and Industrial Pharmacy, 44*(1), 135-143. https://doi.org/10.1080/03639045.2017.1386201

Ma, J., Sheridan, R. P., Liaw, A., Dahl, G. E., & Svetnik, V. (2015). Deep neural nets as a method for quantitative structure-activity relationships. *Journal of Chemical Information and Modeling, 55*(2), 263-274. https://doi.org/10.1021/ci500747n

Mak, K.-K., & Pichika, M. R. (2019). Artificial intelligence in drug development: Present status and future prospects. *Drug Discovery Today, 24*(3), 773-780. https://doi.org/10.1016/j.drudis.2018.11.014

Malakar, J., Sen, S. O., Nayak, A. K., & Sen, K. K. (2012). Formulation, optimization and evaluation of transferosomal gel for transdermal insulin delivery. *Saudi Pharmaceutical Journal, 20*(4), 355-363. https://doi.org/10.1016/j.jsps.2012.02.001

Manda, A., Walker, R. B., & Khamanga, S. M. M. (2019). An artificial neural network approach to predict the effects of formulation and process variables on prednisone release from a multipartite system. *Pharmaceutics, 11*(3), 109. https://doi.org/10.3390/pharmaceutics11030109

Manikiran, S. S., & Prasanthi, N. L. (2019). Artificial intelligence: Milestones and role in pharma and healthcare sector. *Pharma Times, 51*(1), 10-11.

Mayr, A., Klambauer, G., Unterthiner, T., & Hochreither, S. (2016). Deep Tox: Toxicity prediction using Deep Learning. *Frontiers in Environmental Science, 3*, 80.

Merk, D., Friedrich, L., Grisoni, F., & Schneider, G. (2018). De novo design of bioactive small molecules by artificial intelligence. *Molecular Informatics, 37*(1-2), 1700153. https://doi.org/10.1002/minf.201700153

Moussa, H. G., Husseini, G. A., Abel-Jabbar, N., & Ahmad, S. E. (2017). Use of model predictive control and artificial neural networks to optimize the ultrasonic release of a model drug from liposomes. *IEEE Transactions on Nanobioscience, 16*(3), 149-156. https://doi.org/10.1109/TNB.2017.2661322

Nayak, A. K., Das, B., & Maji, R. (2012). Calcium alginate/gum arabic beads containing glibenclamide: Development and *in vitro* characterization. *International Journal of Biological Macromolecules, 51*(5), 1070-1078. https://doi.org/10.1016/j.ijbiomac.2012.08.021

Nayak, A. K., Khatua, S., Hasnain, M. S., & Sen, K. K. (2011). Development of alginate-PVP K 30 microbeads for controlled diclofenac sodium delivery using central composite design. *DARU: Journal of Pharmaceutical Sciences, 19*(5), 356-366.

Nayak, A. K., Laha, B., & Sen, K. K. (2011). Development of hydroxyapatite-ciprofloxacin bone-implants using "Quality by design" >>Quality by Design<<. *Acta Pharmaceutica, 61*(1), 25-36. https://doi.org/10.2478/v10007-011-0002-x

Prescott, J. H., Lipka, S., Baldwin, S., Jr., Sheppard, N. F., Maloney, J. M., *et al.* (2006). Chronic, programmed polypeptide delivery from an implanted, multireservoir microchip device. *Nature Biotechnology, 24*(4), 437-438. https://doi.org/10.1038/nbt1199

Rebouh, S., Lefnaoui, S., Bouhedda, M., Yahoum, M. M., & Hanini, S. (2019). Neuro-fuzzy modeling of ibuprofen-sustained release from tablets based on different cellulose derivatives. *Drug Delivery and Translational Research, 9*(1), 162-177. https://doi.org/10.1007/s13346-018-00592-0

Reymond, J.-L., van Deursen, R. V., Blum, L. C., & Ruddigkeit, L. (2010). Chemical space as a source for new drugs. *MedChemComm, 1*(1), 30-38. https://doi.org/10.1039/c0md00020e

Russell, S., Dewey, D., & Tegmark, M. (2015). Research priorities for robust and beneficial artificial intelligence. *AI Magazine, 36*(4), 105-114. https://doi.org/10.1609/aimag.v36i4.2577

Sakiyama, Y. (2009). The use of machine learning and nonlinear statistical tools for ADME prediction. *Expert Opinion on Drug Metabolism and Toxicology, 5*(2), 149-169. https://doi.org/10.1517/17425250902753261

Silver, D., Schrittwieser, J., Simonyan, K., Antonoglou, I., Huang, A., *et al.* (2017). Mastering the game of Go without human knowledge. *Nature, 550*(7676), 354-359. https://doi.org/10.1038/nature24270

Waghule, T., Rapalli, V. K., Singhvi, G., Manchanda, P., Hans, N., *et al.* (2019). Voriconazole loaded nanostructured lipid carriers based topical delivery system: QbD based designing, characterization, *in vitro* and *ex vivo* evaluation. *Journal of Drug Delivery Science and Technology, 52*, 303-315. https://doi.org/10.1016/j.jddst.2019.04.026

Wang, Z., He, Z., Zhang, L., Zhang, H., Zhang, M., & Wen, X. (2013). Optimization of a doxycycline hydroxypropyl-β-cyclodextrin inclusion complex based on computational modeling. *Acta Pharmacologica Sinica B, 3*(2), 130-139.

Yuan, Y., Pei, J., & Lai, L. (2011). LigBuilder 2: A practical de novo drug design approach. *Journal of Chemical Information and Modeling, 51*(5), 1083-1091. https://doi.org/10.1021/ci100350u

Zaki, M. R., Varshosaz, J., & Fathi, M. (2015). Preparation of agar nanospheres: Comparison of response surface and artificial neural network modeling by a genetic algorithm approach. *Carbohydrate Polymers, 122*, 314-320. https://doi.org/10.1016/j.carbpol.2014.12.031

Zhang, Z.-H., Wang, Y., Wu, W.-F., Zhao, X., Sun, X.-C., & Wang, H.-Q. (2012). Development of glipizide push-pull osmotic pump controlled release tablets by using expert system and artificial neural network. *Yao Xue Xue Bao, 47*(12), 1687-1695.

Zhao, F., Lu, J., Jin, X., Wang, Z., Sun, Y., *et al.* (2018). Comparison of response surface methodology and artificial neural network to optimize novel ophthalmic flexible nano-liposomes: Characterization, evaluation, *in vivo* pharmacokinetics and molecular dynamics simulation. *Colloids and Surfaces. B, Biointerfaces, 172*, 288-297. https://doi.org/10.1016/j.colsurfb.2018.08.046

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