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REVIEW article

Artificial Intelligence in pharmaceutical sciences: Transforming drug discovery, formulation, and manufacturing

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Abstract: Artificial intelligence, a major feature of machine learning and deep learning, is changing the way pharmaceutical research and development are done by speeding up drug discovery, formulation, stability prediction, and manufacturing processes. Artificial intelligence enables more rapid target identification, chemical space exploration, and de novo molecule design with fewer iterative experimental cycles, lead selection being optimised, and formulation behaviour and stability predicted. Machine learning and generative models are extensively used in early drug discovery for virtual screening, activity prediction, ADMET profiling, and multi, objective lead optimization resulting in development timelines being reduced drastically. In formulation and preformulation, artificial intelligence models are used to predict physicochemical properties, excipient interactions, and process effects leading to a dose form getting designed more efficiently even if it is complex. Stability prediction models are used to identify degradation pathways, moisture, induced changes, and biologics' aggregation thereby helping the formulation to be done early and the regulatory risk to be assessed. Artificial intelligence, assisted process analytical technology and digital twins in manufacturing lead to enhanced real, time monitoring, predictive control, and continuous manufacturing, thus quality and throughput are ensured. The main issues faced are data quality, model explainability, regulatory acceptance, and workforce readiness although the benefits have been demonstrated. The next steps will be the multimodal artificial intelligence integration, foundation models, or self-driving laboratories that will, without any doubt, speed up the process of pharmaceutical innovation even further. Together, artificial intelligence is no more a supplemental tool but rather the main driver of efficiency, quality, and predictability in pharmaceutical sciences.

Introduction

Artificial intelligence (AI), driven largely by machine learning (ML) and deep learning (DL) advancements, is changing the face of pharmaceutical research and development in a very significant way. AI is making a big difference in the move from small, scale proof, of, concept studies to fully functioning platforms. Target identification, chemical space screening, de novo molecule design, and decision-making in formulation and manufacturing are the processes where AI is having a major impact in speeding up. There are a lot of benefits that AI brings which include cutting down the number of iterative wet, lab cycles, being able to select higher-quality leads, predicting formulation behaviour and stability, and making predictive process control in

manufacturing environments easier. These improvements meet the pharmaceutical industry's urgent goals of shortening development timelines, reducing costs, and increasing product quality and regulatory compliance. This review brings together a large volume of peer-reviewed research that illustrates the varied applications of AI across the pharmaceutical value chain. The review focuses on the main areas of drug discovery, formulation development, stability prediction, quality control, process analytical technology (PAT), and manufacturing processes. The compilation of this research is supported by industry real, world case studies which demonstrate the powerful implementation of AI in these fields. After a short methodology section, the story is logically divided into broad thematic discussions which are intended to provide a smooth transition from one topic to another while at the same time, limiting the use of subheadings, thus, ensuring an interesting read and at the same time, covering the essential elements of AI's role in transforming pharmaceutical practices [1-3].

Search strategy

To find relevant studies, we performed a targeted literature search of highly-indexed, peer-reviewed journals (Nature Biotechnology, Nature Reviews Drug Discovery, Nature Machine Intelligence, Chemical Reviews, Journal of Controlled Release, Advanced Drug Delivery Reviews, International Journal of Pharmaceutics, Pharmaceutical Research, Journal of Pharmaceutical Sciences, mAbs, AIChE Journal, and others). The search terms were the combinations of "artificial intelligence", "machine learning", "deep learning", "drug discovery", "de novo design", "formulation", "stability prediction", "process analytical technology", "continuous manufacturing", and "digital twin". We looked first at review articles and seminal experimental papers showing algorithmic advances and industrial implementations that have been validated. The inclusion criteria focused on journals of high impact and demonstrations that are experimental or applied; articles in the news and non-peer-reviewed reports were excluded. The final manuscript is based on 20-30 high-index references.

Artificial intelligence in drug discovery and early R&D: ML and DL methods have been implemented in various aspects of early-stage drug discovery. Traditionally, discovery was based on iterative experimental cycles-hypothesis generation, high-throughput screening (HTS), medicinal chemistry optimization, and preclinical testing-which were both time-consuming and costly. ML provides means to shorten these cycles by modeling predictive relationships from large chemical, biological, and biomedical data sets and by creating candidates directly (generative design). Several surveys and benchmark studies have demonstrated that graph-based neural networks, message-passing architectures, transformer-based sequence models, and generative models (VAEs, GANs, reinforcement learning hybrids) can not only predict activity, ADMET properties but also produce chemically valid novel scaffolds prioritized for synthesis, **Table 1**, [4-8]. The rapid identification of DDR1 kinase inhibitors using the generative tensorial reinforcement learning (GENTRL) approach is perhaps the most frequently cited experimental example of this paradigm shift; the research confirmed several active compounds and demonstrated how de novo generative methods might yield the fastest viable leads in terms of calendar time by far [9]. Later work has taken these techniques further by introducing multi-objective optimization that tries to improve potency, selectivity, synthetic accessibility, and ADMET endpoints at the same time using multi-objective reinforcement learning and Bayesian optimization strategies [6, 8]. The need for AI explainability has driven the emergence of a subfield reliant on explainable AI (XAI) techniques which are increasingly used to interpret model outputs in chemically relevant ways to support medicinal chemistry decisions [5].

Machine learning has revolutionized the arena of virtual screening: Conventional docking and scoring suffer from errors that limit throughput and predictive performance; ML strategies, which are developed using extensive bioactivity datasets, can rank the most probable actives with higher hit rates, thus lowering the demand for experimental screening [10, 11]. It should also be noted that transformer models trained on extensive SMILES

and reaction corpora have paved the way for more accurate predictions of reactivity, retrosynthesis pathways, and molecular properties (**Table 2**). As a result, many businesses are now implementing ML-guided filtering as the first step before any physical screening, which substantially lowers both cost and cycle time [4, 11]. Lead optimization, which has been an iterative and chemist-driven process in the past, is now made better with the use of ML-based QSAR, along with property prediction (solubility, permeability, metabolic stability), and toxicity prediction. By the means of generative design coupled with ADMET predictors, teams are able to automatically prioritize candidates with well-balanced properties and at the same time be free of liability motifs that are already known [6, 13]. Several industry reports and peer-reviewed papers have been vocal about the fact that the implementation of ML for lead optimization is a way to decrease the design-synthesis-test cycle count and, at the same time, increase the chemical quality of candidates [6, 14].

Table 1: Representative AI methods and their primary pharmaceutical uses (illustrative)

AI class/method	Typical pharmaceutical applications
Graph neural networks, MPNN	Predicting binding affinity, property prediction, de novo scaffold evaluation
Transformer models	SMILES/property prediction, reaction prediction, retrosynthesis
Generative models (VAE/GAN/RL)	De novo molecule generation, multi-objective optimization
Random forest / XGBoost	Formulation property prediction, stability classification
Convolutional neural networks	Image-based defect detection, 3D structures featurization
Digital twins + reinforcement learning	Process optimization, predictive control in continuous manufacturing

Table 2: Typical data sources used to train pharmaceutical AI models

Data source	Examples
Chemical libraries	ChEMBL, PubChem, proprietary HTS datasets
Structural biology	PDB, cryo-EM maps
Omics	Transcriptomics, proteomics datasets
Formulation & process records	LIMS, PAT streams, historical DoE results

Formulation development and preformulation: Development of new drugs is still largely empirical and highly demanding of resources, especially if we are talking about complex dosage forms or biologics. AI can be helpful here by predicting physicochemical parameters based on the molecular structure and by understanding excipient interactions and process parameter effects from historical formulation datasets. ML models (random forests, gradient boosting, ANNs) trained on formulation databases can be used to predict solubility, crystallinity tendencies, hygroscopicity, and even powder flow or compaction behaviour, characteristics that help to direct preformulation decisions [15, 16]. AI techniques can capture non, linear interactions between formulation variables and process parameters to a greater extent as compared to traditional design of experiments (DoE). Formulation science research shows that ML models have a higher statistical probability to outperform linear models in predicting tablet hardness, disintegration, nanoparticle size distribution, and coating uniformity, thus leading to a smaller number of physical experiments needed to achieve the target specifications [16]. In the case of biologics, deep models incorporating sequence and structural features can figure out aggregation propensity, forecast viscosity at high concentration, and identify buffer compatibility, features helping the production of stable parenteral products [17]. Such prediction tools, therefore, enable teams to be more efficient in formulating the right strategies (e.g., solubilization via amorphous solid dispersion or lipidic vehicles, selection of stabilizing excipients) at the early stages of development.

Stability prediction and shelf-life modelling: Stability testing is still a considerable time-consuming task in the development process, as it requires both real-time and accelerated stability studies under ICH conditions. AI provides alternative methods to determine degradation kinetics or the probability of main degradation routes simply by using data of accelerated stress and molecular/formulation descriptors. Different machine learning algorithms (XGBoost, random forest, support vector machines, neural networks) have been trained to anticipate impurity generation, potency loss rate, polymorphic conversions, and moisture-induced degradation in various API/excipient matrices [18-20]. In the case of small molecules, the models which integrate reaction-center prediction with environmental predictors (temperature, humidity, pH) are able to predict chemical degradation patterns and also indicate the most vulnerable functional groups. As for solid dosage forms, ML can foresee moisture absorption and consequently the changes in hardness, dissolution, and impurity profiles, thus allowing earlier prevention through packaging or formulation modification. In the case of biologics, sequence- and structure-based deep models can predict aggregation or certain chemical modifications (oxidation, deamidation) upon stress, thus helping buffer design and the selection of storage conditions [17, 20]. The initial application of AI for the screening of high-risk candidates not only shortens the time for stable formulation but also facilitates regulatory risk assessments.

Manufacturing, pat, and digital twins: The manufacturing industry is a great candidate for AI technology due to the availability of a large amount of real-time sensor data from various PAT instruments (NIR, Raman, FTIR, mass spectrometry, particle counters, imaging). ML models that interpret spectroscopic and process data can determine blend uniformity, endpoint detection (e.g., granulation end-point), coating thickness, and moisture content in a much shorter time and, in many cases, with higher accuracy than conventional chemometric models. The use of AI with PAT facilitates real-time release testing (RTRT) approaches and predictive batch quality evaluation in line with Quality by Design (QbD) regulatory principles [21]. The use of AI control loops that forecast deviations and take corrective actions to ensure the maintenance of critical quality attributes (CQAs) and the reduction of downtime is a major continuous manufacturing advantage. Digital twins, i.e., virtual models of machinery and processes enhanced with AI, help to simulate "what-if" scenarios and thus facilitate process transfer and scale-up with less experimental work. Research is available to support the idea that digital twins and AI-assisted control can reduce variability to increase throughput in pilot and commercial lines [22, 23].

Industry implementations and case studies: Real-world implementations complement academic advances and illustrate practical benefits. Equally distributed among these big pharma and AI-native biotech companies are:

- Insilico Medicine generated drug candidates by using generative models that quickly went through preclinical and clinical pipelines, thereby confirming the viability of AI-driven end-to-end discovery workflows [5, 12].
- Exscientia engineered molecules for clinical candidates through AI platforms and took the first fully AI-designed small molecule from lab to human trials, thereby showing the time-compression potential [13].
- Pfizer and Moderna employed ML models in various parts of mRNA-LNP formulation and stability optimization during vaccine development and manufacturing. They also used predictive models to guide lipid selection and storage condition decisions [7].
- Novartis and GSK have been collaborating with cloud/AI providers to use large biomedical datasets along with ML platforms for target identification and the candidate selection process optimization, as well as to initiate the digital-twin applications for process scale-up [22, 24].
- Some manufacturers (Janssen, Merck) announce that they have successfully applied AI-enhanced PAT for granulation endpoint detection and real-time blend monitoring, thus enabling RTRT pilots and shortening release cycle time [21].

These case studies, covered in core journals and institutional publications, demonstrate that AI integration results in measurable efficiency gains in cycle time, reduction of experimental work, and improvement of early stage decision quality. In areas with a dearth of official publications, peer-reviewed reviews and validated pilot studies are considered as proof [5, 13, 21, 24].

Challenges and practical considerations: Several major challenges that have been addressed but not solved fully continue to be the reasons for the slow adoption of these approaches despite the benefits that can be demonstrated. The first thing is that data quality and standardization are still the main obstacles: many formulation and manufacturing datasets are a mixture of different things, are closed, and lack sufficient annotation for general model training. The second thing is that to get model explainability and regulatory acceptance, transparent and validated workflows are needed; where no one can understand how the black-box model works, it faces regulatory pathways with scepticism unless it is accompanied by a mechanistic rationale or robust validation [5]. The third thing is that to integrate AI in a regulated environment, governance frameworks, data lineage, and cybersecurity provisions for models and digital twins are required. The fourth thing is that workforce skills have to change: pharmaceutical scientists need to be familiar with data engineering, model evaluation metrics, and experimental design for ML validation. The last thing is that though there are many success stories, there is a publication bias towards positive results; reproducibility and prospective validation across therapeutic areas are still the main things that will be able to demonstrate long-term value [5, 11, 21]. Regulatory agencies (FDA, EMA) have shown that they are in Favor of model-informed approaches and advanced manufacturing and at the same time are continuously refining the guidance on AI validation, model change control, and lifecycle management. Therefore, practitioners should focus on transparent model documentation, prospective validation studies, and risk-based deployment strategies to meet regulatory requirements.

Future directions: It is anticipated that the integration of multimodal AI models will become more in-depth in the very near prioritized, these models will combine structural chemistry, multi-omics disease data, revolutionized evidence, and manufacturing sensor streams. One of the significant steps forward in this field is the arrival of foundation models, large, pre-trained models for chemical and biomedical data. These models, in combination with transfer learning, can have a tremendous effect in quickly adapting to various tasks and drastically lowering data requirements for achieving specialized endpoints. Also, the idea of self-driving laboratories, in which robotic automation carries out experiments guided by an AI planner, is no longer merely a concept but is actually making the transition to practical pilots. This transition is geared towards lessening the time of cycles in experiments. At the same time, digital twins will be able to cover product life cycles completely. This will be instrumental in predictive maintenance, provenance tracking, and adaptive control, thus facilitating a highly detailed integration of development knowledge with manufacturing execution [25]. The realization of these technologies will depend on measures such as enhanced attention to explainability, uncertainty quantification, and proactive regulatory validation, which are indispensable for their implementation on a large scale and smooth functioning in different sectors.

Conclusion: Artificial intelligence has radically changed pharmaceutical sciences and is now leading the way in drug discovery, formulation, stability prediction, and manufacturing strategies. The latest developments position AI not as a mere future technology, but a must-have tool to get more research done. Major academic publications and industry projects are progressively adopting machine learning and deep learning methods that, among other things, drastically shorten the development time, increase the quality of the hits and the predictability of formulation and stability behaviours. Moreover, the use of predictive process control is gradually being accepted as the norm in industry. The achievements of such AI initiatives depend on a number of decisive prerequisites,

e.g., availability of high, quality, well-annotated data, model transparency, compliance with regulations and organizational readiness to set up hybrid teams of pharmaceutical scientists and data professionals. As artificial intelligence tools get more advanced, they will be able to not only speed up pharmaceutical product development and manufacturing but also make them safer and more predictable. The progression of foundation models, extended multimodal integration, and the growing functional capabilities of digital twins collectively ensure that AI will be the major driver of the enormous change in the pharmaceutical industry leading to the development and manufacture of pharmaceutical products in a radically different way.

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الذكاء الاصطناعي في العلوم الصيدلانية: نقلة نوعية في اكتشاف الأدوية، وصياغتها، وتصنيعها

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الملخص: يُحدث الذكاء الاصطناعي، وهو سمة رئيسية من سمات التعلم الآلي والتعلم العميق، ثورةً في أساليب البحث والتطوير الدوائي، إذ يُسرّع من اكتشاف الأدوية، وصياغة تركيباتها، والتنبؤ بثباتها، وعمليات تصنيعها. ويُمكّن الذكاء الاصطناعي من تحديد الأهداف بشكل أسرع، واستكشاف الفضاء الكيميائي، وتصميم الجزيئات من الصفر، مع تقليل عدد دورات التجارب المتكررة، وتحسين اختيار المركبات الرائدة، والتنبؤ بسلوك التركيبة وثباتها. ويُستخدم التعلم الآلي والنماذج التوليدية على نطاق واسع في المراحل المبكرة لاكتشاف الأدوية، من خلال الفحص الافتراضي، والتنبؤ بالنشاط، وتحديد خصائص الامتصاص والتوزيع والاستقلاب والإخراج والسمية (ADMET)، وتحسين المركبات الرائدة متعددة الأهداف، مما يُؤدي إلى تقليص مدة التطوير بشكل كبير. وفي مجال صياغة الأدوية وتحضيرها، تُستخدم نماذج الذكاء الاصطناعي للتنبؤ بالخصائص الفيزيائية والكيميائية، وتفاعلات السواغات، وتأثيرات العمليات، مما يُسهم في تصميم شكل الجرعة بكفاءة أكبر، حتى وإن كان معقدًا. تُستخدم نماذج التنبؤ بالاستقرار لتحديد مسارات التحلل والرطوبة والتغيرات المستحثة وتجمع المواد البيولوجية، مما يساعد على إعداد التركيبة في وقت مبكر وتقييم المخاطر التنظيمية. يؤدي الذكاء الاصطناعي، وتقنيات تحليل العمليات المدعومة، والتوائم الرقمية في التصنيع إلى تعزيز المراقبة الآنية، والتحكم التنبؤي، والتصنيع المستمر، مما يضمن الجودة والإنتاجية. وتتمثل التحديات الرئيسية في جودة البيانات، وقابلية تفسير النماذج، والقبول التنظيمي، وجاهزية القوى العاملة، على الرغم من إثبات الفوائد. وتتمثل الخطوات التالية في دمج الذكاء الاصطناعي متعدد الوسائط، والنماذج الأساسية، أو المختبرات ذاتية التشغيل، والتي ستساهم بلا شك في تسريع عملية الابتكار الصيدلاني بشكل أكبر. وبذلك، لم يعد الذكاء الاصطناعي مجرد أداة تكميلية، بل أصبح المحرك الرئيسي للكفاءة والجودة والقدرة على التنبؤ في العلوم الصيدلانية.