Special Report

Emerging Trends of Artificial Intelligence (AI) in Healthcare

Amalgamation of AI in Pharmaceutical Drug Development

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Artificial Intelligence (AI) in Pharmaceutical Product Life Cycle – An Overview

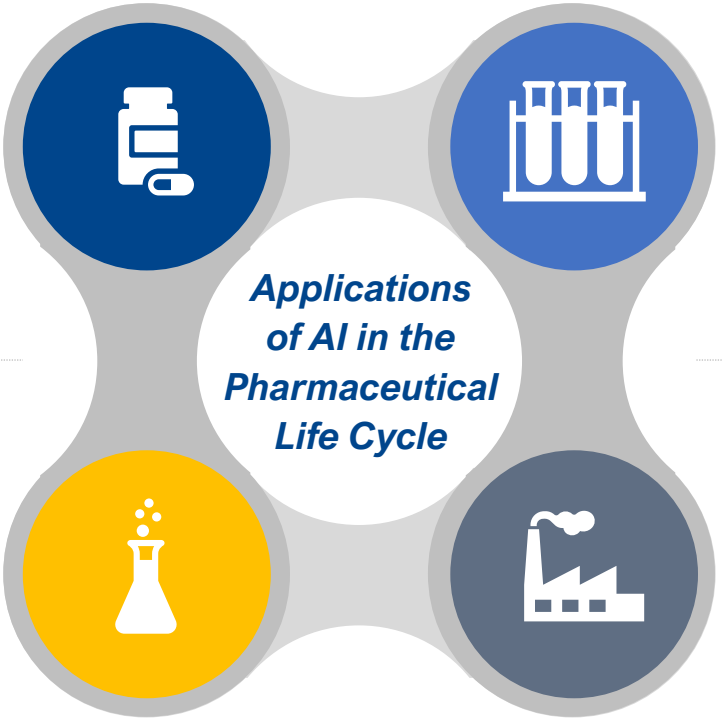
AI plays a crucial role in pharmaceutical product development, covering drug design, decision support, personalized therapy selection, clinical data management, and future drug development

Drug Discovery

- Design – Target protein structure prediction and Drug-protein interaction
- Screening – Bioactivity & toxicity prediction and Physiochemical property prediction

Pharmaceutical manufacturing

- Automated manufacturing
- Personalized manufacturing
- Correlating manufacturing errors to set parameters



Clinical Trial Design and Monitoring

- Design – Target protein structure prediction and Drug-protein interaction
- Screening – Bioactivity & toxicity prediction and Physiochemical property prediction

Product Development

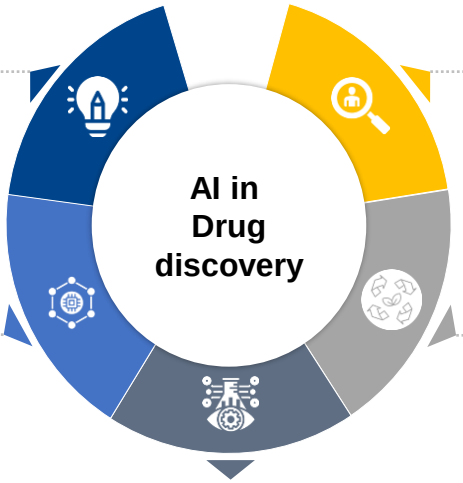
- Aid in deciding suitable excipients
- Monitoring & modifying development process
- Ensuring in-process specification compliance

AI holds immense importance in the pharmaceutical industry due to its ability to accelerate drug discovery and development processes, analyze vast datasets to identify potential drug candidates, optimize clinical trial design, and personalize treatment plans for patients based on their unique characteristics. These application represent a broader aspect of the pivotal role AI plays in the each of every stage of the Pharmaceutical Product Lifecycle

Source: *Secondary Research, Industry Analysis*

Applications of AI in Drug discovery

The vast chemical space allows for creation of many drug molecules, but without advanced tech, development is slow & expensive. AI can help by finding compounds, validating targets, & optimizing drug structures, for faster and more efficient output



AI in drug design	AI in polypharmacology	AI in chemical synthesis	AI in drug repurposing	AI in drug screening
▪ Predicting 3-D structure of target protein ▪ Predicting drug-protein interaction ▪ Determining drug activity ▪ De-novo drug designing	▪ Designing of bio-specific drug molecules ▪ Designing multi-target drug molecules	▪ Prediction of reaction yield ▪ Prediction of retrosynthesis pathways ▪ Developing insights into reaction mechanisms ▪ Designing of synthetic targeting routes	▪ Identification of therapeutic target ▪ Prediction of new therapeutic use	▪ Prediction of toxicity ▪ Prediction of bioactivity ▪ Prediction of physiochemical property ▪ Identification and classification of target cells

Source: *Secondary Research, Industry Analysis*

Applications of AI in Drug discovery – Drug Designing

AI aids in structure-based drug discovery by accurately predicting 3D protein structures, enabling design of drug molecules that selectively target disease-causing proteins & predict compound effects & safety considerations prior to synthesis or production

Prediction of the target protein structure

Correct target assignment is crucial in drug development for successful treatment. AI plays a vital role in predicting the 3D protein structure, allowing selective targeting of disease-related proteins, predicting compound effects, and safety considerations before synthesis or production

- AlphaFold, an AI tool based on DNNs, accurately predicted 25 out of 43 target protein structures by analyzing amino acid distances and peptide bond angles, showcasing its effectiveness in 3D protein structure prediction
- A study achieved 62.72% accuracy in predicting protein 2D structure using MATLAB with a nonlinear three-layered neural network (NN) toolbox. They employed supervised learning, backpropagation error algorithm, and NNs as learning algorithms and performance evaluators

Prediction of the drug target interactions

AI predicts drug-target interactions, enabling cost-effective drug repurposing and qualification for Phase II clinical trials, while avoiding polypharmacology. ML techniques like SVM, NN, logistic regression, and DL are used to forecast drug-disease associations through the "Guilt by association" approach. Platforms like PREDICT and SPACE employ logistic regression, considering various factors for effective drug repurposing

- DeepDTnet, a cellular network-based DL technology, is being developed & patented in the US to predict therapeutic application of topotecan, a topoisomerase inhibitor
- Unsupervised ML utilizes Self-organizing maps (SOMs) for drug repurposing, focusing on finding novel off-targets of drug molecules. SOMs employ a ligand-based approach, training the system on compounds with known biological activities and analyzing them
- Cyclica's Ligand Express, a cloud-based AI platform, uses proteome-screening to identify receptors interacting with a specific small molecule. This helps assess on-target and off-target interactions, providing insights into potential adverse drug effects

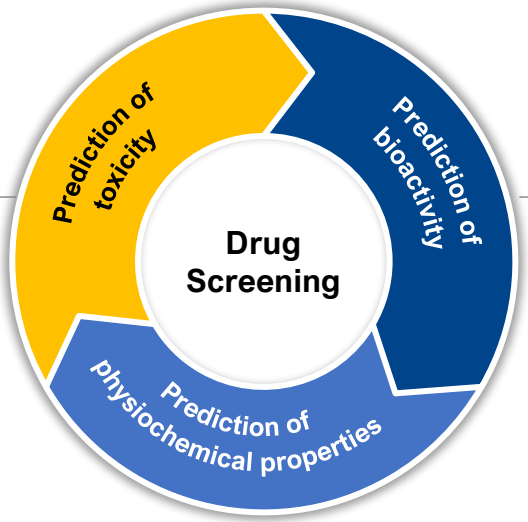
Source: *Secondary Research, Industry Analysis*

Applications of AI in Drug discovery – Drug Screening

Advanced algorithms in Virtual Screening (VS) enhance drug discovery by predicting synthesis feasibility, in vivo activity, and toxicity, potentially reducing the time and cost involved in drug development

Advanced AI methods leverage compound similarities or input features to predict drug toxicity, minimizing costs, while cell-based in vitro assays and animal studies are commonly conducted for toxicity assessment:

- TargeTox is an ML-based method using guilt-by-association principle with protein network data, combining properties to build a classifier for predicting drug toxicity risk
- PrOCTOR uses RF model, incorporating various properties to generate a 'PrOCTOR score' that predicts drug failure due to toxicity and identifies FDA-approved drugs linked to adverse events



AI methods predict drug-target interactions and binding affinity, assessing efficacy and toxicity through consideration of chemical moieties or similarities between the drug and its target:

- Web applications like ChemMapper & similarity ensemble approach (SEA) enable prediction of drug-target interactions
- ML and DL techniques, such as KronRLS, SimBoost, DeepDTA, and PADME, are employed to determine drug-target binding affinity (DTBA), without relying on 3D protein structure availability

AI-based tools effectively predict physicochemical properties crucial in drug design for informed decision-making on a drug's pharmacokinetics and receptor interactions:

- Neural networks, utilizing the ADMET predictor and ALGOPS program, enable prediction of lipophilicity and solubility for diverse compounds
- AI predicts compound acid dissociation constants using ANN-based models, graph kernels, and kernel ridge-based models. Cell lines like Madin-Darby canine kidney cells and human colon adenocarcinoma cells generate cellular permeability data with AI algorithms

Source: *Secondary Research, Industry Analysis*

AI in Clinical Trial Design

AI, utilizing digital medical data, can mitigate financial losses & failures in the pharmaceutical industry by addressing issues such as inappropriate patient selection, technical requirements shortages, & poor infrastructure during the lengthy clinical trial process

AI can aid in the early prediction of drug targets by analyzing patient-specific genome-exposome profiles, enabling the selection of suitable patients from a specific diseased population for recruitment in Phase II and III of clinical trials, ensuring a higher success rate and reducing the timeline dedicated to patient enrollment

Using predictive machine learning and other AI techniques, early prediction of lead molecules that have a higher likelihood of successfully passing clinical trials can be achieved, considering the specific patient population, thus aiding in preclinical discovery and selection of lead compounds before initiating clinical trials

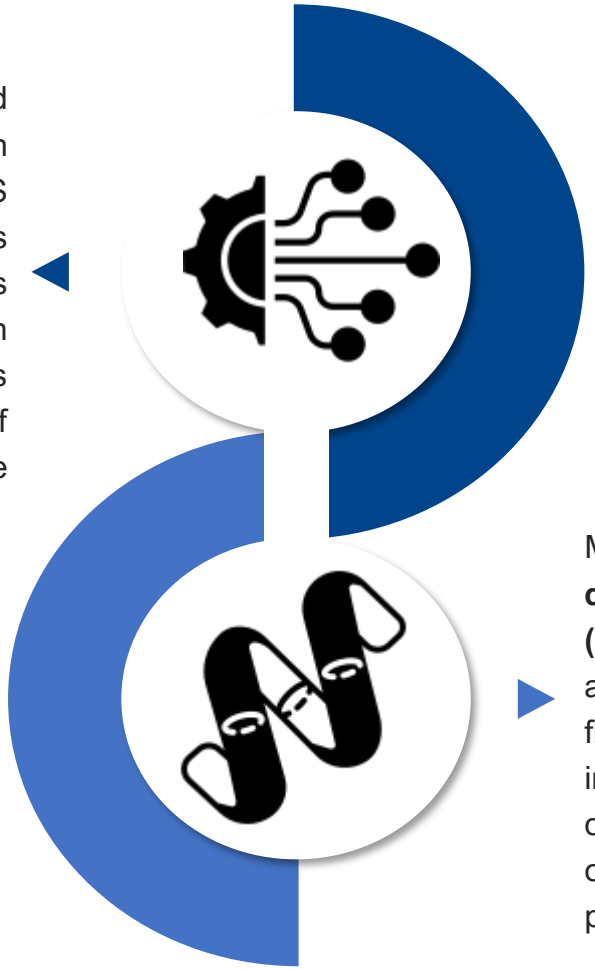
Close monitoring and assistance to patients in adhering to the clinical trial protocol can prevent dropouts, which contribute to 30% of trial failures, reducing the need for additional recruitment and saving time and resources

Source: *Secondary Research, Industry Analysis*

AI in Advancing Pharmaceutical Product Development

AI tools using Quantitative Structure-Property Relationship can tackle formulation challenges in drug design, by employing rule-based decision-support systems to select appropriate excipients based on the drug's properties & adapt processes accordingly

The **MODEL EXPERT SYSTEM (MES)** and **ANN (Artificial Neural Network)** both aid in hassle-free formulation development. MES utilizes input parameters to make decisions and recommendations, while ANN utilizes backpropagation learning to establish connections between formulation parameters and desired responses under the influence of a joint control module

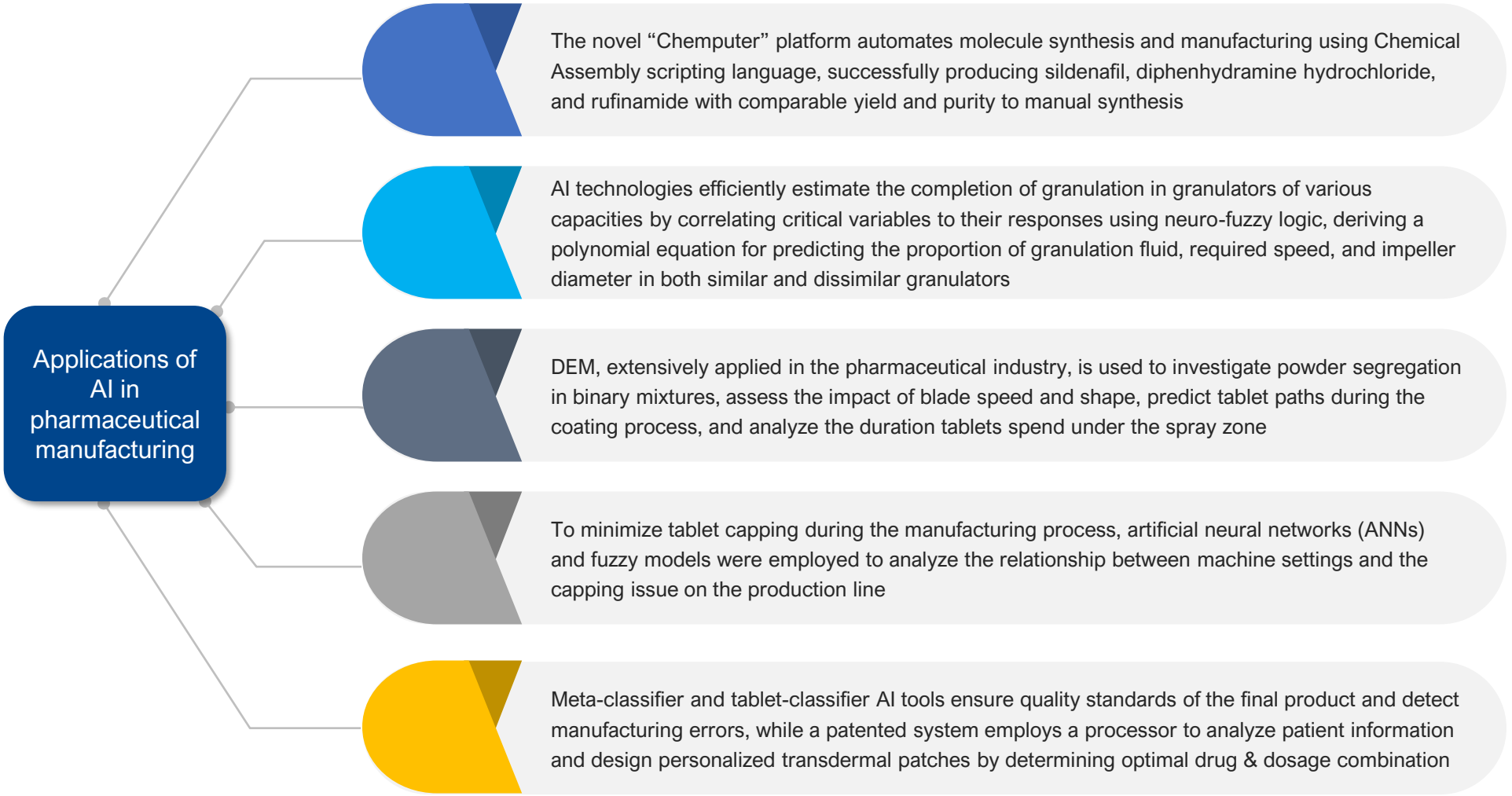


Mathematical tools like **computational fluid dynamics (CFD)**, **discrete element modeling (DEM)**, and the **Finite Element Method** analyze powder flow properties during die-filling and tablet compression, while CFD investigates how tablet geometry affects dissolution. Integrating AI with these models can greatly accelerate pharmaceutical production

Source: *Secondary Research, Industry Analysis*

AI in Simplifying Pharmaceutical Manufacturing

AI tools in modern manufacturing automate pharmaceutical operations by studying agitation & stress levels using CFD with Reynolds-Averaged Navier-Stokes solvers, while advanced simulations solve complex flow problems, enhancing efficiency & quality



Source: *Secondary Research, Industry Analysis*

Challenges To Drug Discovery With Traditional AI Methods & Strategies To Overcome Them (1/2)

Emerging AI tools like Human Protein Atlas and The Open Drug Delivery Platform show promise in overcoming data challenges, surpassing traditional methods in accurately evaluating the safety and efficacy of drug molecules by analyzing big data

Key Challenges		***Strategies to address them***
AI algorithms rely on substantial, high-quality data for accurate predictions. However, drug discovery data is often incomplete, inconsistent, or biased, leading to potentially unreliable results from AI algorithms	**Data Availability and Quality**	▪ Improving data quality and availability in drug discovery is crucial. Utilizing Data Commons, a centralized repository of open and freely shared data, expands access to diverse datasets, enhancing the accuracy and reliability of AI algorithms ▪ Examples include The Human Protein Atlas, The Cancer Genome Atlas, and The Drug Bank Database
Data complexity in drug development's AI poses challenges, making model training and deployment difficult due to intricate data, hampering pattern recognition and insights: ▪ Patient data, including health, treatment history, lifestyle, genetic data, and biometric measurements, involves alphanumeric and image formats like JPEG/JPG and DICOM. AI systems must be adaptable to diverse and complex data in drug development.	**Data Complexity**	Data visualization and Machine Learning effectively address data complexity: ▪ Data Visualization identifies hidden patterns, benefiting drug development by revealing potential drug targets, facilitating design, and optimizing the drug development process ▪ Machine Learning automates data analysis and drug discovery, freeing human resources for critical tasks like clinical trials

Source: *Secondary Research, Industry Analysis*

Challenges To Drug Discovery With Traditional AI Methods & Strategies To Overcome Them (2/2)

Initiatives such as the Drug Discovery Data Standard (D3S) by Pistoia Alliance and the Center for Drug Evaluation and Research Artificial Intelligence/Machine Learning Working Group by FDA is expected to solve the data challenges in drug development

Key Challenges		***Strategies to address them***
The industry should define a good dataset clearly, considering variations in data collection, coding, use of null or dummy data, and inconsistent documentation. Well-defined parameters enable study result reproduction, advancing research effectively by other groups	**Lack of Data Standards**	▪ Developing data standards in drug development is essential. The Pistoia Alliance is working on the Drug Discovery Data Standard (D3S) to define data structure, content, and guidelines for collection, storage, and analysis ▪ Open data sharing is crucial, enhancing AI algorithm accuracy and reliability. The Open Drug Discovery Platform (ODDP) facilitates data sharing and collaboration in drug discovery, promoting data standards with D3S support
Evolving regulatory frameworks for AI in drug development create ambiguity in applying existing regulations to AI-enabled processes, challenging compliance for drug developers. Regulatory bodies may lack expertise in evaluating AI's risks and benefits, further complicating compliance determination. Moreover, the lengthy and costly regulatory approval process for new drugs adds additional hurdles	**Regulations**	▪ The FDA has established the Center for Drug Evaluation and Research Artificial Intelligence/Machine Learning Working Group, developing recommendations to streamline approval for AI-enabled drugs ▪ The European Medicines Agency (EMA) has published scientific advice on AI in drug development, offering guidance on the risks and benefits of AI-enabled processes

Source: *Secondary Research, Industry Analysis*

Partnerships Between Pharmaceutical and AI-based Companies

Pharmaceutical companies have actively invested in and partnered with AI companies to create vital healthcare tools

Pharmaceutical organization	AI organization	Collaborative work
Pfizer	XtalPi	Use of quantum mechanics and ML algorithms with cloud computing architecture, to predict 3D structure of molecules, depict mechanical and chemical properties and understand binding interactions with protein receptors
NOVARTIS	IBM Watson	Use of ML, natural language processing, and cognitive reasoning technologies in immuno-oncology to find new drug targets, combination therapies, and patient selection strategies
janssen	BenevolentAI	BenevolentAI assumes exclusive rights to develop, manufacture, and commercialize Janssen's novel clinical-stage drug candidates, already used to provide clinical data in Phase IIb trials for Bavisant in Parkinson's disease patients
Takeda	Numerate	Design of small molecule modulators of ryanodine receptor 2 (RyR2),a target identified in cardiovascular diseases, using proprietary algorithm-driven drug discovery platform

Source: *Secondary Research, Industry Analysis*

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