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Review of AI/ML applications in medicines lifecycle (2024)

Horizon Scanning Short Report

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1. Introduction

This report highlights examples of current uses and potential applications of Artificial Intelligence (AI) and Machine Learning (ML) technologies in the medicine lifecycle and highlights possible regulatory opportunities and challenges stated by the developers in the research publications. This exercise is not a comprehensive and systematic review of all AI/ML uses but includes examples of applications relevant for EMA future activities.

2. Methods

2.1. Search Strategy and Sources

For this review the OECD AI definition has been used: *"AI system is a machine-based system designed to operate with varying levels of autonomy and that may exhibit adaptiveness after deployment and that, for explicit or implicit objectives, infers, from the input it receives, how to generate outputs such as predictions, content, recommendations, or decisions that can influence physical or virtual environment".*

The EMA's Horizon Scanning tool, TRIP (Topics, Relationships, Impact assessment, Proposal generation) has been used to search for AI/ML related info items between January and November 2024.

Information items from peer-reviewed journals, preprints, and clinical trials were curated by a team of curators from TRS-INO.

Other relevant information sources, e.g. reports from FDA and WHO as well as EU-funded projects were also included in this report, as a complement.

2.1.1. Inclusion and exclusion criteria

Publications were selected as relevant according to the following criteria:

- AI/ML technologies employed in the drug development and medicines lifecycle.
- Publications with results that may have impact in medicines approval and regulation.

Publications were not considered if they did not meet the following criteria:

- Articles unrelated to medicines development; or clinical practice-related studies for example, prescription guidance, differential diagnosis, prognosis.

3. AI/ML in medicines lifecycle

The application of AI/ML in medicines lifecycle promises significant benefits for the development of new medicines and related technologies but also raises concerns and challenges. Identified AI applications are presented by respective phases of drug development and lifecycle: 1. Drug discovery, 2. Non-clinical development, 3. Clinical trials, 4. Precision medicine, 5. Product information, 6. Manufacturing, and 7. Post-authorization. In this report are listed some examples of uses of AI in the medicines development and it is described some opportunities and challenges pointed by the developers.

3.1. Drug discovery

Drug discovery can be defined as the process of researching, identifying and developing new medicines.

AI technologies can be applied mainly to (examples in **Table 1**):

- drug target identification
- selection and prioritization of drugs
- screening and designing compounds
- drug repurposing

Table 1. Examples of current research of AI in Drug Discovery

- Docking, binding affinity, and compound-protein interactions prediction (1-6)
- Protein engineering, particularly in designing proteins with desired properties (7, 8)
- Mining and analysis of large multi-omics and other big datasets (9)
- Drug repurposing (10-15)

Approaches based on protein structure predictions, like the Nobel awarded Alphafold, have the potential to accelerate the early stages of drug discovery by providing reliable structural data at the touch of a button (4).

Structure and interaction prediction models are trained with experimental data, to achieve accurate sequence-to-function models (1-6).

When designing new proteins, AI is being employed to predict protein fitness landscapes, facilitating the design of proteins with enhanced properties using minimal experimental data (7, 8).

One very relevant use of AI technologies is the mining of big datasets, for example, to predict and identify new antimicrobial peptides, and accelerating the discovery of new antibiotics (9). AI tools are also being used to discover enzyme inhibitors (2), psychedelic molecules (4), adeno-associated virus (AAV) capsids with multiple desirable traits (16), antibacterial agents (8, 9), and identify efficient cytidine deaminases (9).

Drug repurposing is one of the fields where AI is showing to be more promising and useful. The AI models can integrate curated facts and evidence from various biomedical entities, such as symptoms, drugs, genes, and ortholog genes, to enhance the accuracy and relevance of its predictions, facilitating the decision-making process. Deep-learning models can predict drug response based on multi-omics data, drug descriptors, and drug fingerprints and facilitate the repurposing of drugs based on those responses (11, 13). Technologies that analyse drug-target interaction networks can also be used for drug repurposing (13). These models can rank drugs for potential new indications and contraindications (11), and there is an effort to make them more accessible to healthcare professionals (10, 11), so they can be easily integrated in the daily medical practice. The technology is being applied to identify drug candidates for rare diseases (10), and glioblastoma (12) for example, enabling the identification of new therapeutic applications for existing drugs, which can significantly shorten the development timeline and reduce costs.

Opportunities

- Reduction of the need for extensive experimental validation, saving both time and resources in the drug discovery process.
- Streamline the drug discovery process, making it faster and more efficient to identify potential drug candidates.

Challenges

- Data quality and availability: The data and how the data are applied have a significant impact on the quality and performance of ML models (17). ML can be conditioned by the scarcity of high-quality, labelled data for training models.
- Model interpretability and transparency: deep learning models can be seen as "black boxes", making it difficult to understand how predictions are made.
- Integration with existing systems: integrating AI models with existing drug discovery workflows and ensuring compatibility with current data formats and processes.

3.2. Non-clinical development

Non-clinical or pre-clinical development refers to the phase in medicines development that focuses on assessing the safety and efficacy of a candidate therapy before it is tested in humans.

In this phase of development, AI can be used to (examples in **Table 2**):

- Replace, Reduce, Refine (3Rs) the use of animals in medicine development
- improve efficacy and safety modelling
- modelling of pharmacokinetics and pharmacodynamics

Table 2. Examples of current research of AI in Non-clinical development

- Blood-brain barrier (BBB) penetration prediction (18)
- Pharmacokinetics (PK) prediction (19)
- Prediction of toxicity (20, 21)

Regarding pharmacokinetics and toxicity predictions, the models can be more focused on specific pharmacologic parameters like BBB penetration or can be more complex and designed to predict, analyse, and optimize the PK and toxicity profiles of small molecules, across several endpoints, including absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties (18, 19, 21).

The tool Toxometris.ai, has shown potential of AI-based risk assessments for predicting carcinogenicity in humans (22).

Opportunities

- AI provides probabilistic outputs that capture uncertainties in risk assessments, offering a better understanding of potential risks associated with medicines exposure.
- It can be used to improve the efficiency and accuracy of safety assessments, guiding the design of preclinical studies using in vivo models and reducing the need for laboratorial testing and *in vivo* animal toxicity testing (17, 19, 20).

Challenges

- Model interpretability and reliability: ensuring that AI models are interpretable and transparent for regulatory acceptance, as the 'black box' nature of generative AI tools can be an obstacle.
- Regarding the prediction of NOALs and LOAELs, the developers need to be cautious, as the endpoints defined can affect the prediction accuracy in specific models (17).
- Standardization: Developing standardized protocols for AI model development, validation, and application in toxicology is necessary (21), like the OECD framework for Quantitative Structure-Activity Relationship ((Q)SAR) Assessment, to ensure consistency and reliability across different studies and regulatory contexts.

3.3. Clinical trials

Clinical trials are research studies that involve human participants to evaluate the safety and effectiveness of new medical interventions, such as drugs, vaccines, or medical devices.

In clinical trials, AI can be implemented in (examples in **Table 3**):

- medical devices technologies
- *in vitro* diagnostics
- data collection
- analysis and inference
- patient stratification
- treatment assignment
- participant recruitment
- digital endpoints
- disease models and digital twins

Table 3. Examples of current research of AI in Clinical Trials

- Analyse qualitative data (23)
- Risk stratification (24)
- Participant recruitment (25)
- Benefit prediction (26)
- Virtual Human Twins (VHTs) (27-30)

AI is being used to analyse qualitative data from Patient-reported outcome (PRO) measures, enhancing the understanding of patient experiences (23). By integrating Thematic Analysis (TA) and Natural Language Processing (NLP), researchers can gain deeper insights into patient experiences and outcomes. Also, sentiment analysis techniques can analyse the emotional tones in patient narratives, revealing sentiments such as fear or anger.

Furthermore, models have been developed and validated to identify specific markers of risk of an event, combined with a decision tree to help identify patients at high risk, treatment group assignments and optimizing participant selection for clinical trials (24, 25).

Virtual Human Twins (VHTs) are virtual replicas of patients that can simulate real-world scenarios, preserving individual patient characteristics. TWIN-GPT is a large language model-based approach

designed to create digital twins for clinical trials (30). For example, the AI company Unlearn.AI developed a digital twin technology to simulate control groups in clinical trials, reducing the number of participants needed and accelerating trial timelines. Other examples include Sanofi digital trials initiative, that tests compounds in digital patients before progressing to clinical trials, and the European Virtual Human Twin (EDITH), funded by the European Commission, that will develop a simulation platform that will support the transition towards VHT modelling.

Opportunities

- Enhanced data analysis, that retrieves more accurate interpretation of PROs.
- Understanding the emotional responses of participants can guide the development of drugs that better address the psychological aspects of certain conditions.
- Enhancement of the efficiency and accuracy of participant recruitment.
- Improvement of treatment assignment.
- More accurate endpoints.

Challenges

- Data privacy: ensuring the privacy and security of patient data used by the AI system, in compliance with regulations such as GDPR.
- Model validation: rigorous validation of the AI models to ensure their reliability and accuracy. Ensure validation of the AI-analysed PROs.
- Ethical considerations: addressing ethical concerns related to the use of AI in patient selection, including transparency, accountability, and potential biases in the AI models.

3.4. Precision medicine

AI/ML can be used to individualise treatment in relation to factors such as disease characteristics, patient genotype, wide-band biomarker panels and clinical parameters.

AI can be used for treatment optimisation (examples in **Table 4**) via:

- posology adjustment or treatment combinations for each patient
- the identification of novel biomarkers for individualised therapy

Table 4. Examples of current research of AI in Precision Medicine

- AI-based personalized treatment (iRITUX Trial), (31)
- Response/efficacy prediction (29, 32)
- Identify drug-gene pairs/ pharmacometric models (27, 33)
- Identify novel gene and protein biomarkers (28, 34)

AI algorithms can create and propose personalized treatment options, for example, the iRITUX trial will compare the efficacy of AI-based personalized treatment protocol in Membranous Nephropathy. Machine-learning-based Clinical Decision Support Systems (CDSS) can recommend individualized treatment regimens, facilitating the selection of personalized treatment regimens, like drug combinations (31).

AI is also being used to analyse clinical data to predict outcomes, for example inhibitor development in children with hemophilia A, improving patient management and treatment outcomes (29).

AI is being used to analyse large datasets to identify gene signatures predictive of treatment response, mainly for oncology treatments (28).

AI-predicted pharmacogenes can be integrated into pharmacometric models to hypothesise dose adjustments, aiming to improve treatment outcomes for malaria and tuberculosis (27). Web applications with ML to match genetic alterations with potential drug candidates, can aid clinicians in making informed treatment decisions (33). They generate decision trees that support the healthcare professionals taking decisions. These technologies can be very useful but also raise some ethical questions, concerning responsibility for medical malpractice (35).

Opportunities

- Guide personalized treatment decisions, improving patient outcomes management by identifying those who would benefit most from the therapy.
- The AI suggestions can also be used for drug repurposing.

Challenges

- Data quality and availability: the effectiveness of the Clinical Decision Support Systems (CDSS) depends on the quality and completeness of the data used to train the ML models.
- Integration with clinical practice: implementing the CDSS in routine clinical practice requires adequate digital infrastructure and training for healthcare providers.
- Acceptance by clinicians: in some cases, clinicians may be hesitant to adopt recommendations generated by AI.
- Data privacy: maintaining patient data privacy and complying with regulations such as GDPR and local data protection laws.
- Model validation: rigorous validation of AI models to ensure their reliability and accuracy in clinical settings.
- Regulatory approval: Ensuring the biomarker's clinical validity and utility through rigorous regulatory approval processes.

3.5. Product information

Product information refers to the officially approved documentation that provides essential details about a medication to ensure its safe and effective use. This information typically includes Summary of Product Characteristics (SmPC) outlining the drug's indications, dosage, contraindications, and side effects; package leaflet; and labelling. FDA developed a framework designed to improve drug labelling analysis processes using AI tools (36).

Opportunities

- AI can significantly speed up the process of reviewing large volumes of documents, and generating drug labelling documents, reducing the time and resources required.
- By leveraging AI, the accuracy of information extraction and document generation can be improved, minimizing human errors.
- AI ensures consistency in the language and format of regulatory documents, which is crucial for compliance and clarity.

Challenges

- Transparency and explainability: to build trust and confidence, reviewers need transparent outputs with traceable evidence from reliable sources. Linking the model's output to the original text can help address concerns about the model's trustworthiness.
- Data security: regulatory data is often sensitive and cannot be processed through public AI tools due to confidentiality and privacy concerns. Therefore, a localised solution is necessary to handle such data securely.

3.6. Manufacturing

Manufacturing involves a series of controlled chemical and biological processes, according to the Good Manufacturing Processes, to ensure that the medicines meet strict safety, efficacy, and quality standards. In this phase, AI can be used, for example (examples in **Table 5**):

- for model design
- performance assessment
- lifecycle management
- process design and scale up
- process optimization
- in-process quality control
- batch release

Table 5. Current research of AI in Manufacturing

- Predicting solubility and bioavailability (37)
- Quality control of pluripotent stem cells (38, 39)

The use of ML can lead to the development of more effective drug formulations with enhanced solubility and bioavailability, improving therapeutic outcomes, and reducing the need for laboratorial validations (37).

Regarding advanced therapy medicinal products (ATMPs), ML models can predict the optimal conditions for generating specific cell types, improving the efficiency and consistency of regenerative treatments. AI has been instrumental in refining induced Pluripotent Stem Cells (iPSC) classification, monitoring cell functionality, and conducting genetic analysis to ensure quality standards (38, 39). For example, it is possible to accurately classify pluripotent and differentiated cells and predict their potential to become specialized 2D cells and 3D organoids (39).

Opportunities

- Validation processes are more efficient and cost-effective compared to traditional experimental methods.
- Optimized development of cell-based therapies.
- Improvement of quality control.

Challenges

- Implementation: integrating these tools into existing workflows and ensuring their accuracy and reliability remains a challenge.
- Standardization and quality control: there is a need for standardized methods and markers to assess the quality and pluripotency of iPSCs. The lack of standardisation can lead to variability in results and hinder the reproducibility of studies.

3.7. Post-authorization phase

Post-authorization refers to the period after a medicine has received regulatory approval and is available on the market. During this phase, ongoing monitoring and evaluation of the drug's safety and effectiveness continues through pharmacovigilance. In this phase examples of AI use are (examples in **Table 6**):

- prediction of adverse drug reactions (ADRs)
- safety signal detection
- adverse event detection
- extraction/processing of adverse event report

Table 6. Current research in AI in post-authorization phase

- Automatic signal detection from Electronic Health Records (EHRs) (40, 41)
- Risk association predictions (42)

ML can be used to predict and map ADRs using EHRs, and other sources to detect safety signals (40, 41). The use of ML algorithms to predict ADRs can significantly enhance drug safety by identifying potential risks early in the post-authorization phase. For example, FDA's Sentinel Initiative uses AI to monitor the safety of approved drugs by analysing EHRs and insurance claims data.

Opportunities

- Improved signal detection and risk assessment capabilities.
- Better processing and analysis of large amounts of data.

Challenges

- Data security: ensuring patient data privacy while using EHRs for ML models is crucial.
- Bias mitigation and continuous monitoring: training AI systems with diverse datasets representing different demographics is necessary to avoid biases that could impact patient safety. Continuous monitoring of AI systems is needed to identify and mitigate any undesired outcomes early on, including regular updates and validation of AI models.

- Collaboration: Collaboration among AI developers, healthcare providers, and regulatory bodies is necessary to create responsible AI systems that can be effectively integrated into pharmacovigilance practices.

4. EU funding

The European Commission has launched a call for proposals on advancing the adoption of AI in health under the EU4Health Programme (deadline for application is 22 January 2025).

Multiple EU-funded projects are exploring the applications of AI to development of medicines (source: EU Funded projects | EU Funding & Tenders Portal). Relevant examples include:

Drug repurposing

- DREAMS: AI-based identification of targets, repurposable medicines and new entities for the treatment of rare neuromuscular disorders.

Pre-clinical development

- QUANTUM-TOX: application of AI to develop computational toxicology and improve in silico toxicity predictions

Manufacturing

- AIDPATH: application of AI to the decentralised production of advanced therapies in hospitals

Clinical trials

- BRAINTEASER: integration of large clinical datasets with novel personal and environmental data collected using low-cost sensors and apps from patients with amyotrophic lateral sclerosis and multiple sclerosis.

Precision medicine

- Histotype Px: application of AI to digital pathology for the stratification of colorectal cancer patients into low, intermediate, or high risk prior to chemotherapy;
- PHIRE: Photoacoustic imaging and AI-based theranostic approach for cancer;
- OPTIMA: first interoperable and GDPR compliant European real-world oncology data and evidence generation platform that aims to strengthen shared decision-making based on innovative data and AI-driven technology and tools;
- AI4LUNGS: AI-based tools and computational models to improve patient stratification optimising diagnosis and treatment of infectious and non-infectious respiratory diseases.

5. Discussion

This report highlights current uses and potential applications of Artificial Intelligence (AI) and Machine Learning (ML) technologies in the medicine lifecycle and highlights possible regulatory opportunities and challenges.

AI is being used and further developed and explored during all phases of the medicine lifecycle, including 'Drug discovery', 'Non-clinical development', 'Clinical trials', 'Precision medicine', 'Product information', 'Manufacturing', and 'Post-authorization'.

Main opportunities include faster drug screening, which reduces the time and cost associated with experimental screening. Even more, in phase I studies, AI-discovered drugs show a better success rate (43).

Predictive models using ML algorithms can also be extensively explored and trained to create predictions to be used in all medicine's development phases like toxicity and safety, pharmacokinetic properties, outcome assessment, pharmacogenetic studies, clinical decision support, cell therapy quality control, and even detect signals/ADRs.

Regarding Natural Language Processing, one of the most common uses is in the analysis of PROs and EHRs. This can further be used to better assess treatment efficacy or help in patient recruitment for clinical trials.

Real World Evidence (RWE) and big data analyses are gaining so much relevance. To produce more accurate and reliable insights, AI and ML tools are essential to mine and analyse these big datasets.

AI/ML implementation in the medicine's lifecycle is of high relevance to increase efficacy and success rates, but there are some challenges that need to be addressed.

The initial investment in AI technologies and the resources required for comprehensive data analysis can be substantial (44). Inequity of access can be a barrier to innovation, as academic researchers often lack access to advanced graphics processing units necessary for training large language models and other AI applications. This contrasts with big industry researchers who have more substantial budgets and resources (45).

Navigating the regulatory landscape for repurposed drugs is also pointed as challenging. Even though these drugs have known safety profiles, demonstrating their efficacy for new indications requires rigorous testing and compliance with regulatory standards (44).

Data protection and data privacy is one of the main challenges stated in several studies, that can be addressed using for example, synthetic data, created using AI technologies, that preserves the overall patterns and relationships found in the original patient's data. This approach ensures that individual identities are not exposed, effectively reducing the risk of re-identification (46). The biggest limitation to the adoption of synthetic data concerns whether the data that are computer-generated, genuinely preserve privacy. If there is a risk of being able to re-identify real individuals from a synthetic dataset, the advantages of synthetic data are compromised (46).

Biased data can lead to incorrect risk assessments. So, addressing biases in the data used to train AI models is essential to ensure fair and accurate predictions.

Another limitation is the quality and quantity of training data to feed these models and improve predictions. For this, federated learning (FL) has emerged as a solution, enabling training across hospitals without direct data sharing, creating a multi-centre cohort (47).

For ML methods, best practice recommendations are emerging, and their adoption is inconsistent (48). Also, adherence to well-established best practice recommendations from traditional biostatistics literature is still inadequate (48).

AI is a great opportunity to improve processes in regulatory agencies but there is the need to adapt frameworks and processes to accommodate the use of AI in internal processes. This includes implementing AI tools, updating guidelines and ensuring that regulatory staff are trained to evaluate AI-driven assessments (21).

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