

The Promise of AI and Agentic AI in Reimaging Pharmaceutical Research



Agentic AI is building on the promise of AI in almost every industry, and pharma is no exception. Unlike traditional AI, which typically handles one task at a time, agentic AI systems coordinate across various roles, functions and datasets to complete tasks without human intervention. Agentic AI acts as an operations manager, anticipating, adjusting and executing tasks proactively. It is not being used as a complete substitute for traditional research methods. Instead, it is being used as a powerful helping hand, speeding up the incredibly time-consuming background work and making it accessible to experienced researchers.

EXPLAINABLE ARTIFICIAL INTELLIGENCE (XAI) AND DATA PROCESSING

One of the most powerful functions of AI, data processing capabilities, involves benefits as well as risks. Artificial intelligence has been applied to data analysis working

on several different disease functions, including cancer, Alzheimer's disease, new antibiotics and drugs to combat COVID-19 (Blanco-González et al., 2023). AI greatly speeds up the time required to identify promising approaches across an incredible volume of data. However, as AI models are based on and trained with existing data, any biases or inaccuracies in this data affect the accuracy of predictions and decisions. In healthcare industries, biases related to race, sex or socioeconomic status can impact patient outcomes. Validating training datasets is crucial to producing reliable results at every stage.

When evaluating processes and results, transparency may become an issue. Many AI systems are considered "black boxes" because their decision-making process is not clearly displayed and explained. This raises concerns about how decisions are made and undermines trust in AI systems. The entire process ultimately needs to

be understood by both industry decision-makers and regulatory authorities. AI applications in drug discovery must adhere to the requirements of agencies like the Food and Drug Administration (FDA) and the European Medicines Agency. Any part in the process that is not completely and easily transparent risks violating regulations for applicable agencies (Kokudeva et al., 2024).

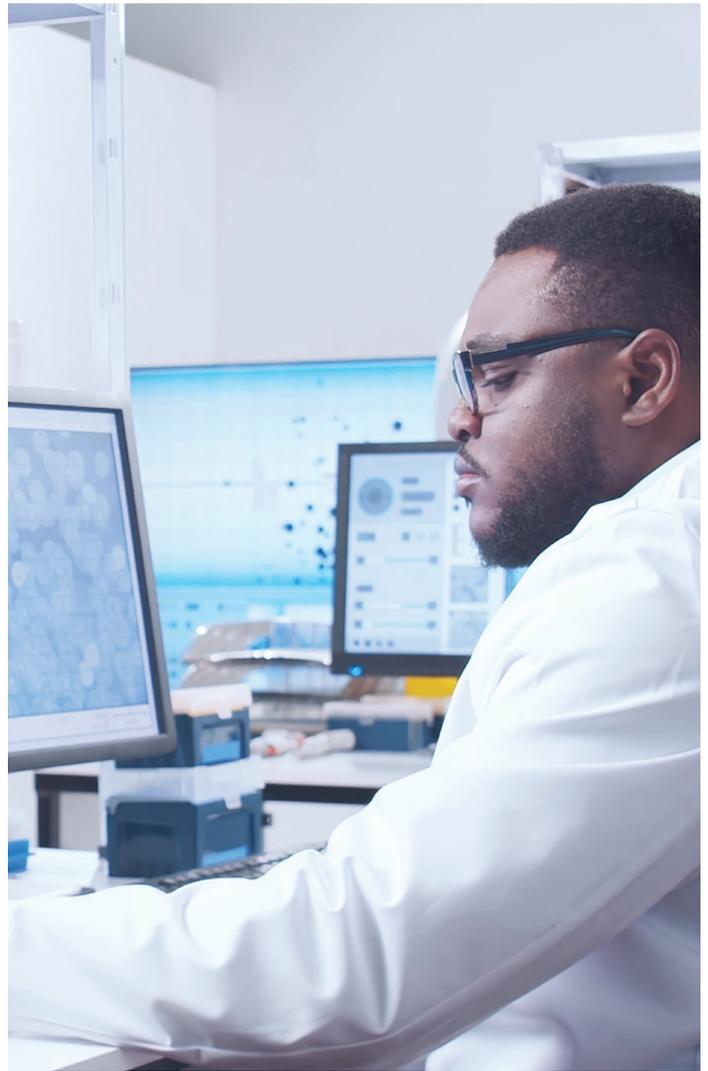
To mitigate this issue, it's important for the industry to integrate explainable artificial intelligence (XAI), which provides a framework for research and regulation. XAI uses prediction accuracy, traceability and decision understanding. Prediction accuracy involves comparing the results of simulations to the training data, to confirm that they come to compatible conclusions. Traceability restricts ways that decisions can be made into a narrower set of choices, and decision understanding works by educating involved team members on how AI works (IBM, n.d.). Using explainable artificial intelligence (XAI) leads to confidence and ultimately trust in the conclusions.

AGENTIC AI AND INNOVATIONS IN TESTING

In addition to utilizing existing datasets, AI can lead to potentially more ethical drug development. Animal testing has been a necessary part of drug development for over a century, but it has always come with some controversy. Currently there is significant industry pressure to move away from conventional animal studies. In July 2025 the National Institutes of Health announced that new funding programs require that non-animal testing methods are incorporated into the study design (Knapp, 2025). AI, with its ability to process vast amounts of data and simulate complex biological interactions, is being increasingly used to model drug interactions with the human body.

This shift is further supported by legislative changes, such as the FDA Modernization 2.0 Act, which allows for alternative testing methods that do not involve animals. The act encourages the use of AI and organoids—tiny, lab-grown versions of human organs—to predict how drugs will behave in humans. These organoids are more accurate representations of humans than animal subjects, and they also have the promise of being more time and cost effective than traditional animal testing.

This promise is not without limitations—more work needs to be done on replicating systemic effects outside of a



single organ. In fact, Najat Khan, Chief R&D Officer at Recursion, estimates that we only understand 10%-15% of basic biologic processes (Labroots, 2025).

The complex and slow process of drug development has a failure rate as high as 90%, with a \$3.5 billion investment and 10 years to market, so there is definite room for improvement (Feldman, 2025). With thoughtful, transparent implementation of an AI-human hybrid model, agentic AI can result in positive changes to the development process, leading to better population health and commercial success.

Sources:

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