New AI technology sheds light on drug development

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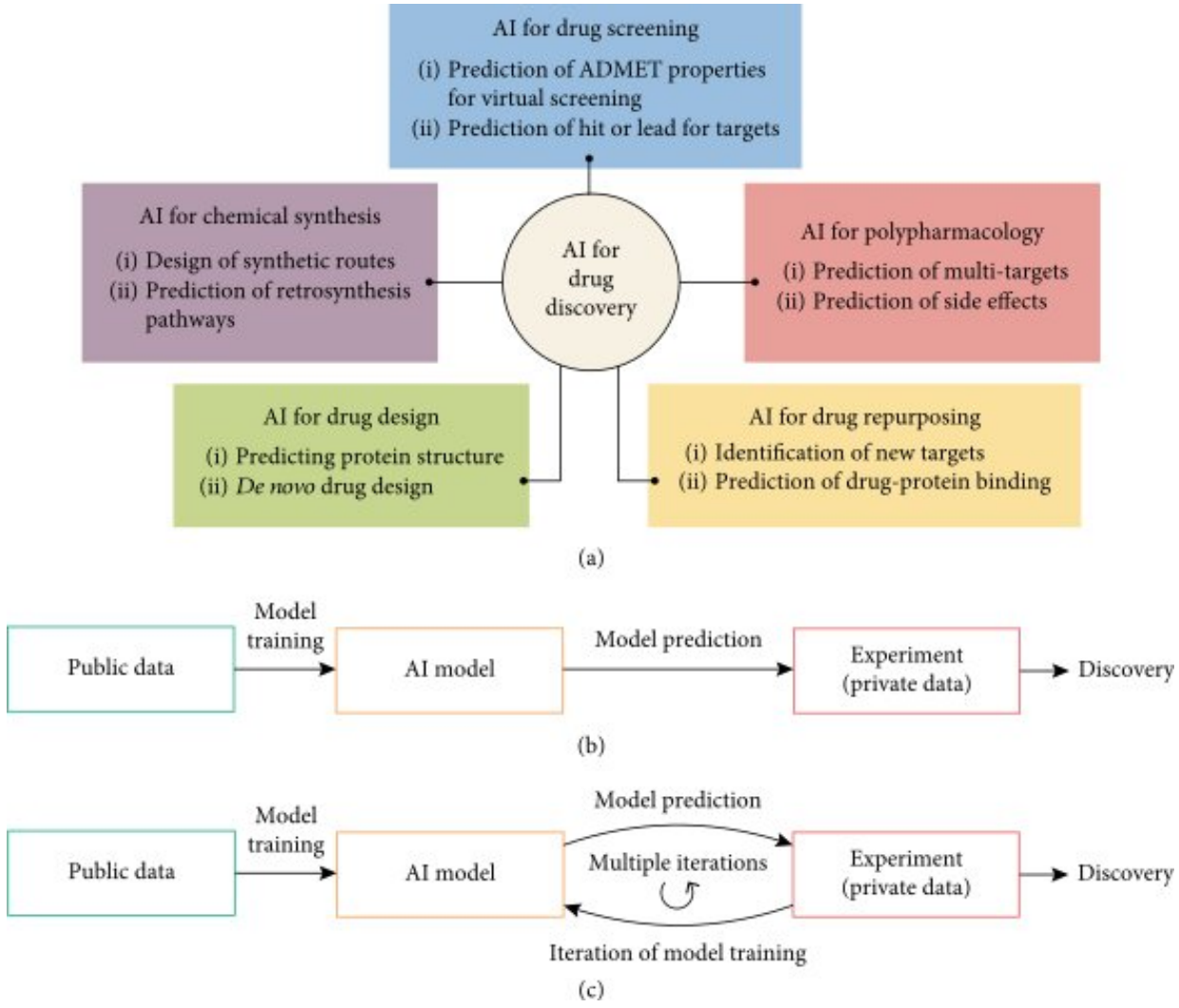

AI for drug development. (a) AI can be used for drug development in different ways, including drug screening, polypharmacology, drug repurposing, chemical synthesis, and drug design [6]; ADMET: absorption, distribution, metabolism,

elimination, toxicity. (b) Illustration of the traditional paradigm of AI-based drug development where AI and data generation are connected in a linear way. (c) Illustration of an active learning paradigm of AI-based drug development where AI and data generation form an iterative feedback loop. Credit: DOI: 10.34133/2022/9816939

Will artificial intelligence (AI) change the traditional trial–and–error drug development process and become a revolutionary force in the pharmaceutical sector? Active learning and interpretable AI are the two critical paradigms that lead to the positive answer, according to a perspective article recently published in *Health Data Science*.

"Promising progress has been made in using AI for drug design recently. However, we are still far from certain that these early results could be translated to more effective drugs with a high success rate," said co-author Jianzhu Ma, Ph.D., a specialist and associate professor of artificial intelligence at Peking University. "How to harness the value of data is the key to building successful AI for drug development."

The authors pointed out that the major limitation of conventional AI-aided drug development is its linear paradigm. Without continuous feedback from the downstream experimental results, the preceding step of AI model prediction is only "educated guesses." While a subdomain of AI, active learning, creates an interactive feedback loop between the AI modeling and the downstream experimental evaluation, potentially increasing the overall outcome.

In addition, the "black box" behind the conventional AI models hurdles scientists' accessibility to the hypothesis and logic that the algorithm uses for data mining. However, the internal rationale behind a prediction in the drug development process is crucial for designing a correct molecule.

Therefore, the authors suggested that "the AI model should unveil how it reaches a particular prediction., based on which training molecules." According to the authors, explainable AI is an active direction in the machine learning community.

"The next decade's AI-based drug development will feature the tight integration of data and computation, where interpretable AI and experimental biology form an active-learning loop and inform each other with feedback," Ma said. "It will iteratively improve the workflow and generate interpretable insights that scientists can monitor, analyze, and understand for every stage in drug development."

More information: Yunan Luo et al, Next Decade's AI-Based Drug Development Features Tight Integration of Data and Computation, *Health Data Science* (2022). DOI: 10.34133/2022/9816939

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