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Robust AI-driven Cancer Drug Development

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AI can accelerate the discovery of new anti-cancer drug molecules and the synthesis of more desirable drug molecules



In the recent past, many companies across the globe have increased their research and development efforts for anti-cancer drugs. Although the understanding of cancer mechanisms has advanced over the years, the process of cancer drug discovery continues to offer multiple challenges. It is especially difficult to design anti-cancer drugs due to factors such as undruggable targets, chemoresistance in oncology, metastasis, and tumour heterogeneity, to name a few. Thus, it calls for more effective anti-cancer drug design strategies to reduce the cost of drug development and the time required for clinical trials.

Artificial intelligence (AI) is being leveraged to address these challenges and increasingly explored by researchers in academia and the biotech industry to improve the anti-cancer drug design process. For instance, AI is being used to integrate data from multiple sources to help with anti-drug target identification, predicting druggability of anti-cancer drug targets, screening of anti-cancer drug hit compounds, de novo design of anti-cancer drugs, etc.

Researchers are using AlphaFold, an AI-powered protein structure database, to create a drug that could potentially treat hepatocellular carcinoma (HCC), or liver cancer. Another AI-driven cancer drug discovery engine called CancerOmicsNet can predict how a specific cancer would respond to a specific drug. Researchers are also applying AlphaFold to Pharma.AI platform to uncover a novel target for cancer and develop a “novel hit molecule” that could bind to that target without aid.

To quote a few examples, Australia-based QIMR Berghofer has recently partnered with Korean company Syntekabio to use their AI and high performance computing to accelerate potential new treatments for cancer and chronic inflammation. Likewise, University of Sydney and Pharos Therapeutics, the Australian subsidiary of Korean pharma company Pharos iBio are using AI to identify promising compounds for rapid development into treatments for cancer.

Swiss biopharma firm Debiopharm and ThinkingNodeLife.ai (TNL), a trailblazer in AI Digital Cells Lab in the US, are advancing the development of a cutting-edge cancer drug. ThinkingNodeLife.ai stands as the first AI Digital Cells Lab at scale generating any human digital cell clones within hours, with its Generative Distributed Reasoning AI (GDR-AI) that employs Distributed Reasoning AI instead of statistical correlation to generate causal reasoning models.

Then there is US-based biotech startup Absci recently signing a $247 million partnership with British pharma company AstraZeneca to focus on expediting the discovery of novel cancer treatments with the help of generative AI technology.

Another recent development that strengthens the association between AI and cancer treatment is the designing of an AI algorithm referred to as Substrate PHosphosite-based Inference for Network of KinaseS (SPINKS) by a group of scientists in the US. The algorithm offers applications to precision cancer medicine, giving oncologists a new tool to battle this fatal disease.

Scientists in the US and Europe are also utilising AI to identify dual-purpose target candidates for the treatment of cancer and ageing. In fact, this collaborative study is the first to show the feasibility of AI-driven approaches to identify potential dual-purpose targets for anti-ageing and anti-cancer treatment, and clearly demonstrates the value of such tools in addressing the complex challenges at the interface between ageing and carcinogenesis.

AI can undoubtedly accelerate the discovery of new anti-cancer drug molecules and the synthesis of more desirable drug molecules. While AI is proving to be a powerful driving force for human cancer research and treatment in the future, it will offer some limitations too.

Over the coming years, we must ensure that we have solid data foundations and tight circles of model validation to leverage our data resources. Moreover, in the drug development process, predicting the underlying logic behind a model is critical to designing the right drug molecules. Interpretable AI models will be the new development direction, and the close combination of data and computation will be a feature of AI-assisted cancer drug development.

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