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The Key to a Precision Medicine Future: AI Plus Human Ingenuity

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Artificial intelligence (AI) is being used to find new promising targets and design new molecules to treat diseases. It is also being applied in the optimisation of the clinical trial process – analysing data to predict outcomes to help prevent timely and costly late-stage failures, and producing health digital twins to speed up trials, and precision public health. It's very possible to imagine a data-driven, streamlined, precision medicine future merging the best of human and machine intelligence to manage our individual health in ways we never previously imagined.

Artificial intelligence (AI) is accelerating precision medicine, giving us the ability to analyse complex data sets and find patterns that can tell us how genes are linked to diseases, and how diseases are linked to biological processes. AI can process reams of existing scientific data and uncover new biomarkers for disease, new targets for therapeutics, and even design new drug-like molecules to treat disease. And we're still in the early stages of what this technology can do.

Generative Adversarial Networks (GANs) – machine learning models that create new images, video, and text from existing data – were first proposed in 2014 by a young scientist named Ian Goodfellow, currently with DeepMind. He and other scientists discovered that technology can be utilised to generate new images based on specific generation conditions. Now, this technology has exploded, bringing with it breakthroughs that have lately dominated headlines – from Microsoft's new Copilot for Office, to Bing's AI chatbot, to image- and art-generating tools like DALL-E and Midjourney.

Generative AI is an amazing tool that is quickly evolving to transform the way we create, work, and discover. What is often misunderstood, however, is the essential role that humans play in advancing these technologies. That's particularly true in AI drug discovery, where we are working with diverse and complex datasets and an untold number of potential interactions and biological responses. Back in 2016, Insilico Medicine's founder and CEO, Alex Zhavoronkov, PhD, was one of a few pioneers

to realise the potential of generative AI in drug discovery. He published the first peer-reviewed paper in the emerging field of “generative chemistry” on applying GANs to generate novel small molecules against cancer.

In order to continue to evolve generative AI to a place where it can accurately assess, diagnose, and provide individualised treatments for patients, there are three essential elements that are needed: highly sophisticated AI and machine learning algorithms; robust and accurate data; and human scientific expertise.

Too often, discussions around AI focus on how machines will be used to replace humans, when in fact the technology serves as a tool to automate and accelerate key parts of the process in order to improve speed, cost, and accuracy.

AI is very good at finding hidden connections in large quantities of data around diseases, genes, and clinical trials that human scientists might miss. Once those connections are discovered, however, it’s up to human scientists to produce and test the compounds and provide the feedback that improves the data and ultimately strengthens the predictive accuracy of these AI systems which are themselves designed by computer scientists.

Insilico Medicine’s Chemistry42 generative AI drug design system, for instance, relies on a library of millions of small molecules, many of which have known properties, combined with in vitro and in vivo data. Over 40 generative AI algorithms embedded in the platform were trained on this data to design completely novel molecules. Through the process of active learning, these molecules are optimised for key features such as novelty, diversity, affinity, metabolic stability, synthetic accessibility and ADME features, among others. Think of it as launching over 40 intelligent Voyager probes into the chemical space in order to find new previously unexplored chemical galaxies – and the most promising small molecule “stars” within them. Ultimately, generated individual molecules need to be synthesised and further assessed and tested, and this work is done by medicinal chemists.

This ongoing human-to-machine feedback loop is essential as we move toward a precision medicine future. We will need to build on the expertise of scientists from both big pharma and small biotech companies with their research and development capabilities and on rapidly evolving tech innovation happening in AI drug discovery biotechs which are continually improving and adapting their platforms. This even includes incorporating conversational large language model functionality into the platform, as Insilico Medicine has recently done by introducing ChatPandaGPT.

AI is already being used to find new promising targets and design new molecules to treat diseases, as has been shown by a number of AI-driven biotech companies in the field, including Insilico Medicine, with our programmes in idiopathic pulmonary fibrosis, cancer, and COVID-19. By advancing the field of AI-powered drug discovery, Insilico Medicine is aiming to extend healthy productive longevity for everyone, Alex Zhavoronkov has even pledged his entire wealth into this field.

AI is also being applied in the optimisation of the clinical trial process – analysing data to predict outcomes to help prevent timely and costly late-stage failures, and producing health digital twins to speed up trials, reduce costs, provide additional patient insights, and precision public health. It’s very possible to imagine a data-driven, streamlined, precision medicine future merging the best of human and machine intelligence to manage our individual health in ways we never previously imagined.

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