

University of Washington Researchers Create AI Platform FOR PREDICTING PROTEIN FOLDING

► **Trend Watch:** AI Partnerships and Open-Source Data Advance Drug Development



The lab of David Baker at the University of Washington's Institute for Protein Design has released its application to solve one of the toughest problems in the life sciences: how to quickly and accurately predict the folding of a protein computationally. The findings, building on work performed by the Google-owned company DeepMind last fall, were published in the July 15, 2021, edition of *Science* the same day DeepMind released its approach in *Nature*. The applications of both teams should provide an accelerant for research across the life sciences, from basic science to drug development.

Historically, predicting the folding of even a small protein has taken immense computing power with mainly incremental results. Drug companies and researchers have relied on laborious experimental methods to determine the structure of proteins, such as critical drug targets. Last fall, DeepMind stunned the field with its application at a biennial competition of computational and structural biologists. The method relied on a deep learning network to predict structures.

Though DeepMind did not release details at the time, computational chemist Minkyung Baek, Ph.D., in the Baker lab and her colleagues began to work on a similar approach. The researchers worked with a larger team, including scientists at institutions in Victoria, B.C., South Africa, and the United Kingdom. In the study, the researchers predicted the structure of hundreds of proteins, including many that were previously only poorly understood.

The new application is called Rose TTAfold. Like DeepMind's AlphaFold2, it uses AI's ability to

discern patterns in vast databases. When given a new protein to model, Rose TTAfold proceeds along multiple "tracks." Rose TTAfold can predict a structure in as little as 10 minutes on a gaming computer, according to the lab.

Rose TTAfold is a "three-track" neural network, meaning it simultaneously considers patterns in protein sequences, how a protein's amino acids interact with one another, and a protein's possible three-dimensional structure. In this architecture, one-, two-, and three-dimensional information flows back and forth, allowing the network to collectively reason about the relationship between a protein's chemical parts and its folded structure.

According to *Science*, DeepMind's application is more accurate, but Rose TTAfold performs nearly as well, and also better predicts some aspects of protein structure. In addition, while DeepMind's application has been run on single proteins, Rose TTAfold can predict how proteins fit together in complexes, molecular machines that do much of the work in the body.

The group released its computer code on the web, so others can improve on it. As a result of the group's work, progress should now be swift.

"In just the last month, over 4,500 proteins have been submitted to our new web server, and we have made the Rose TTAfold code available through the GitHub website. We hope this new tool will continue to benefit the entire research community," Dr. Baek says. "I am delighted that the scientific community is already using the Rose TTAfold server to solve outstanding biological problems."

AI and Big Data Will Continue to DISRUPT PHARMACEUTICAL SECTOR

The COVID-19 pandemic has given businesses an unprecedented opportunity to implement technology-fueled changes to the way they operate. AI and big data/analytics have been identified by healthcare industry professionals as the top technologies that will transform pharmaceutical drug discovery and development processes, as well as marketing and sales, according to a survey by GlobalData, a leading data and analytics company.

AI and big data will play a major role in optimizing pharmaceutical drug discovery and development process, as indicated by 24% and 25% of global healthcare industry professionals, respectively. At least 23% of the surveyed healthcare industry professionals confirmed that their companies were currently using AI to enhance drug discovery and development processes with 28% expecting to continue to implement/start using this technology in the next two years. Also, 27% of survey respondents believed that big data/analytics would play a major role in optimizing marketing and sales.

More than 30% of global healthcare industry professionals were currently using big data/analytics in marketing and sales process and expected to use it in the next two years. The implementation of AI in sales and marketing is believed to reach a bigger uptake in the next few years, up by 4% from a current use rate of 18%.

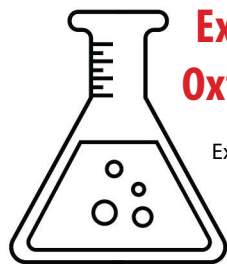
Abbott Receives FDA Clearance for OCT IMAGING WITH AI



Abbott has received U.S. FDA clearance for its latest optical coherence tomography (OCT) imaging platform powered by the company's new Ultrreon Software.

This innovative imaging software combines OCT with AI to provide physicians an enhanced, comprehensive view of coronary blood flow and blockages to assist physician decision-making and provide the best pathway for treatment.

"Abbott's new Ultrreon Software for OCT allows physicians to guide stents with precision," says Ziad Ali, M.D., D.Phil, director of the DeMatteis Cardiovascular Institute at St. Francis Hospital and Heart Center in New York. "These types of innovative technologies are instrumental in providing the best care for our patients."



Exscientia Builds Automated Laboratories in Oxford TO EXPAND PIPELINE

Exscientia is opening a 21,000-square-foot expansion of its facilities at Oxford Science Park, U.K., increasing capacity for its technology teams as well as significantly expanding its laboratory-based experimental capabilities in structural biology, biophysics, and high-content pharmacology.

In parallel, Exscientia is building a new 26,000-square-foot robotic laboratory at nearby Milton Park, Oxfordshire, U.K., focused on the automation of chemistry and biology to accelerate drug discovery. This will take Exscientia toward its goal of drugs designed by AI and made by robots.

"Exscientia has grown significantly in 2021,

driven by new partnerships with leading pharma and biotech companies, as well as by our in-house drug discovery work," says David Hallet, Ph.D., chief operating officer of Exscientia. "Our pipeline includes more than 25 active research programs across therapeutic areas, with a focus on immunology and oncology. To meet this expanded growth, we have added more than 100 employees to date in 2021 and are excited to continue this growth as we seek to add more world-class scientists and technologists to our team."

The company currently has more than 170 people, roughly split between technologists and drug discovery scientists, with a united goal of finding smarter and faster ways to discover and develop new drugs.

Insilico Medicine's AI Engines Identify Another NEW DRUG CANDIDATE

In February 2021, Insilico Medicine demonstrated its AI programs could identify a new disease target, design a new drug, and prepare it for clinical trials, all within 18 months at a total price tag of less than \$3 million when its AI system identified a novel drug target and novel compound to treat idiopathic pulmonary fibrosis, which is another fibrotic disease affecting patients worldwide with high unmet medical needs.

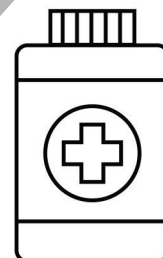
Its latest preclinical drug candidate is aimed at kidney fibrosis, the tissue scarring that's a hallmark of chronic kidney disease and can lead to losses in renal function, a condition affecting millions of people worldwide. The preclinical candidate has the desirable pharmacological properties and pharmacokinetic profile, and demonstrated highly promising results in in vitro and in vivo preclinical studies. Insilico Medicine is working to advance this program to clinical trials and plans to complete the IND-enabling studies in 2022.

In other news, Insilico Medicine and Usynova have announced a strategic partnership to combine the advantages of Insilico Medicine's AI-powered drug discovery platform with Usynova's experience in the small molecule innovative drug development to accelerate the development of small molecule innovative drugs, with a view to jointly address significant unmet medical needs and tackle novel and challenging targets in cancer and autoimmune diseases.

Usynova is an innovative enterprise, the founding team members of which come from multinational pharmaceutical enterprises and domestic CRO-leading companies and possess rich experience in drug R&D. Focusing on the two major areas of autoimmune diseases and cancer, the enterprise has built platforms for small molecule chemical drugs and biomacromolecule drugs, developed several pipeline products at different R&D stages, and carried out two clinical trials.

"China is on the path to becoming the source of truly innovative medicines for the world. We are very pleased to partner with Usynova to discover novel biomedicines utilizing the latest advances in next-generation artificial intelligence," says Alex Zhavoronkov, Ph.D., CEO of Insilico Medicine.

"We hope to effectively improve the efficiency and accuracy of small molecule drug R&D," says Hu Tao, Ph.D., CEO of Usynova. "The combination of innovative drug companies and AI platforms will definitely change the traditional R&D model."



Ono Enters AI Research COLLABORATION WITH HEALX

Japanese drug major Ono Pharmaceutical has entered into a research collaboration agreement with Cambridge, U.K.-based Healx, an AI-driven biopharmaceutical company, to jointly discover and develop novel, efficacious treatment drugs for diseases with unmet medical needs.

Under the accord, Healx will use Healnet, the core of Healx's AI drug discovery platform, to identify potential indications for Ono's proprietary assets. Ono will select diseases from Healx's therapeutic recommendations and conduct verification studies on Ono's compound assets for selected diseases. Ono retains exclusive rights to develop and commercialize compounds for the indications

selected through this collaboration worldwide, and in return, will pay Healx an undisclosed research fee during the collaboration period, as well as development and sales milestones.

"We extremely appreciate Healx's AI technology, Healnet, for discovering new therapies that meet unmet medical needs in rare diseases," says Toichi Takino, a member of the board, senior executive officer and executive director, discovery and research at Ono, adding: "By combining the profiling data of new drug candidates and Healx's AI technology, we expect to increase efficiency of finding clinical indications with high prediction accuracy and identifying new drug candidates."

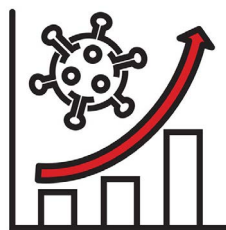
AI In Pharma Global Market Report 2021: COVID-19 GROWTH AND CHANGE

According to The Business Research Company's global AI in pharma market report 2021, to bring a new drug to the market takes on average 10 to 15 years, and half of this time is consumed during the clinical trial phases of the drug development cycle. Using AI models and analytics tools can accelerate the clinical trial phases, perception of diseases, identify suitable cases and key investigators to inform site selection, and support novel clinical study designs.

The global AI in pharma market is expected to grow from \$910 million in 2020 to \$1.27 billion in 2021 at a compound annual growth rate (CAGR) of 39%. The growth is mainly due to companies resuming their operations and adapting to the new normal while recovering from the impact of

COVID-19, which had earlier led to restrictive containment measures involving social distancing, remote working, and the closure of commercial activities that resulted in operational challenges. The market is expected to reach \$5.94 billion in 2025 at a CAGR of 47%.

The Business Research Company's report titled AI In Pharma Global Market Report 2021: COVID-19 Growth and Change covers major AI in pharma companies, AI in pharma market share by company, AI in pharma manufacturers, AI in pharma market size, and AI in pharma market forecasts. The report also covers the global AI in pharma market and its segments.



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