

WuXi AppTec, Insilico unite to integrate AI with Drug Discovery

12 June 2018 | News

WuXi AppTec and Insilico Medicine establish a close strategic collaboration to integrate next-generation artificial intelligence with drug discovery



Insilico Medicine, a Baltimore-based next-generation artificial intelligence company specialized in the application of deep learning for target identification, drug discovery and aging research, announced that it has entered into a collaboration agreement with WuXi AppTec, a leading global pharmaceutical and medical device open-access capability and technology platform company.

Under the terms of the agreement, the companies will perform series of experiments, where many novel molecules discovered using Insilico Medicine's generative adversarial networks (GAN) and reinforcement learning (RL)-based drug discovery pipelines will be tested at WuXi AppTec.

The companies set a series of milestones to apply next-generation AI to discover the ideal pre-clinical candidates for novel and challenging biological targets, including orphan targets with no known crystal structure and no known ligands.

"More than 90% of the molecules discovered the traditional techniques and tested in mice fail in human clinical trials. Our goal at Insilico Medicine is to develop advanced end-to-end AI solutions to discover the optimal pre-clinical candidates," said Alex Zhavoronkov, PhD, founder and CEO of Insilico Medicine. "Our collaboration with WuXi AppTec enables us to focus on artificial intelligence without the need to invest in the expensive laboratory infrastructure. It also enables us to collaborate with some of the world's brightest medicinal chemists and biologists to optimize the drug development process."

Since 2016, Insilico Medicine published multiple research papers, demonstrating the capabilities of GANs and RL systems for de novo generation of diverse molecules with the desired molecular properties, and preliminary experimental validation uncovered the most promising research directions.

The new research collaboration with WuXi AppTec will enable the company to perform the rapid experimental validation of the molecules discovered using AI and generate the valuable data to advance its AI research.

Dr. Tao Guo, Vice President, Head of International Discovery Service Unit of WuXi AppTec said, "The compounds generated by Insilico Medicine's innovative approaches to artificial intelligence have the potential to shorten cycle times and improve the quality of pre-clinical candidates."