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Insilico Medicine discovers industry first preclinical drug candidate using AI

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Preclinical Candidate for Idiopathic Pulmonary Fibrosis with both novel drug target and novel molecule discovered by artificial intelligence

China based Insilico Medicine has demonstrated a breakthrough in Artificial Intelligence ("AI") and drug discovery — linking together generative chemistry and biology for the first time — to discover a novel preclinical candidate addressing idiopathic pulmonary fibrosis **("IPF")** and be validated with multiple human cell and animal model experiments. Often found implicated in a wide range of diseases and multiple organs such as lung, liver and kidney, IPF addresses a very broad medical need that affects hundreds of thousands of individuals worldwide.

Researchers have successfully linked both biology and chemistry and nominated the preclinical candidate for a novel target, with the intention of taking it into human clinical trials, which is orders of magnitude more complex and more risky problem to solve.

The preclinical candidate is a first-in-class novel small molecule inhibitor of a novel biological target with unprecedented mechanism of action (MOA). It demonstrated experimentally great in vitro and in vivo efficacy in preclinical studies for idiopathic pulmonary fibrosis, and good safety profile in the 14-day repeated mouse dose range-finding study.

To nominate a preclinical candidate, Insilico Medicine started with a set of 20 completely novel targets discovered by AI for fibrosis and narrowed down the target to specifically address IPF. Subsequently, Insilico generated a set of novel compounds to selectively inhibit the novel target.

The molecules had to be selective, bioavailable, metabolically stable, capable of oral administration, safe, and have many other properties of a good drug. The company also predicted high-probability of success of the phase 2 clinical trial outcome in IPF.

The molecules were first generated using Insilico's Chemistry42 system, powered by NVIDIA V100 Tensor Core GPUs, that adopts Structure-based Drug Design (SBDD) generative chemistry approach, tested in human cell and animal models.

Subsequently, the molecules were re-designed using the Ligand-based Drug Design (LBDD) to optimize for additional properties, and then tested in human cells and animal models.

After a review by a large team of internal and external veteran drug developers specializing in fibrosis, a preclinical candidate was nominated, and IND-enabling experiments started.

Insilico's AI-discovered and validated preclinical candidate for IPF achieves several multiple industry firsts in the fields of biotechnology and drug discovery.