PRESS RELEASE

Pharma's AlphaGo Moment:
AI System Has Designed New Drug in Just 21 Days

DEEP LEARNING ENABLES RAPID IDENTIFICATION OF POTENT DDR1 KINASE INHIBITORS
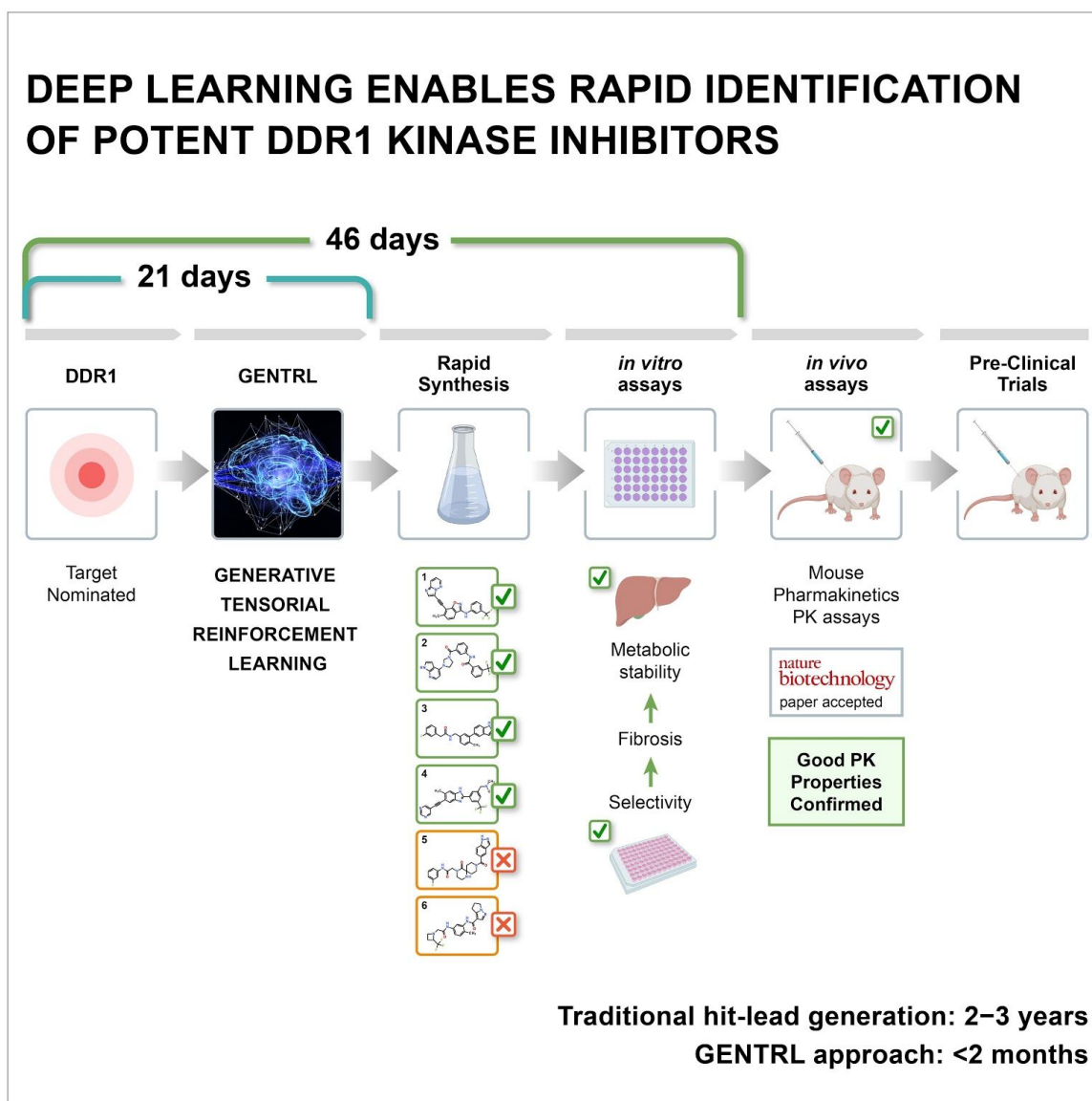
September 3, 2019, London, UK: Deep Knowledge Analytics acknowledges the new ground-breaking achievement of Insilico Medicine, which succeeded to design, synthesize and validate a novel drug candidate end-to-end in just 46 days, which is 15 times faster compared to what it typically takes even for the top pharma corporations capable to conduct the most efficient R&D process, as described in a new scientific paper published in the peer-reviewed journal *Nature Biotechnology*. There is a high probability that this achievement will become a true game-changer for the entire pharmaceutical industry.

"Zhavoronkov et al. show that AI techniques can be used to guide our search for good drug molecules in the vastness of chemical space, one of the key challenges in drug discovery today. The work provides compelling evidence that AI can learn from historical datasets to generate novel molecular compounds with drug-like properties, and helps clarify how AI can be used to improve the speed of drug development." **said Mark DePristo, former Head of Genomics at Google Brain, Co-founder and CEO, BigHat Biosciences.**

This accomplishment is the culmination of Insilico Medicine's efforts in pioneering the use of cutting-edge techniques in AI and Deep Learning (specifically, the combination of Generative Adversarial Networks and Reinforcement Learning) for drug discovery and biomarker development, which began more than 2 years ago. Insilico Medicine was the first to utilize Generative Adversarial Networks (GANs) to generate novel molecules in 2016, and since then have spent two years developing the theoretical base for the combined use of GANs and RL, documented in 15+ papers and 80+ conference presentations. Now, for the first time, these efforts have been utilized to design a novel DDR1 kinase inhibitor from scratch in just 21 days, and then to synthesize and preclinically validate the new drug in just 25 days (46 days end-to-end).

The company screens potential drug candidates using GANs. These specialized algorithms create synthetic datasets that are indistinguishable from real datasets by having two neural networks compete against each other. One neural network generates the data and the other compares it to a real data set in iterative cycles so that the degree of error in the synthetic data set is gradually decreased. Rather than using trial and error when looking for molecular leads, requests are made to the network to generate specific leads and leads are generated on demand.
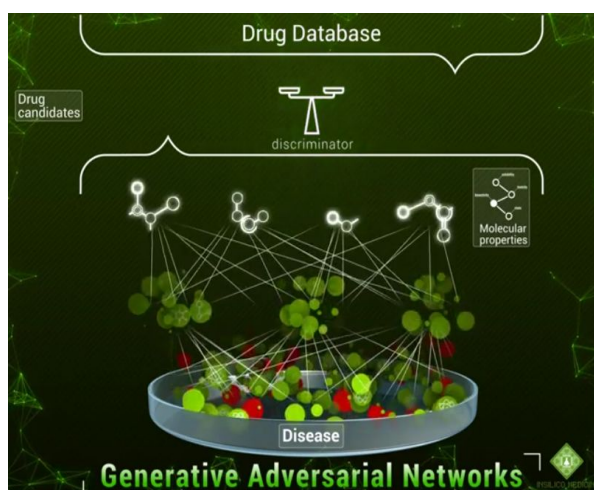
"This is an important demonstration of the power of AI, using a GAN approach, to markedly accelerate the design and experimental validation of a new molecule, no less one targeting fibrosis, a major unmet medical need." **said Dr. Eric Topol, Executive Vice-President of Scripps Research and Founder and Director of the Scripps Research Translational Institute** (Eric Topol has no relationship with the company in question nor its authors).

Furthermore, the use of AI in drug discovery has the power to do more than just accelerate drug development timelines. It also has the potential to vastly increase efficiency and decrease preclinical failure rates by discovering drugs in an intelligent and focused manner, designing particular molecular properties according to the specifics of a given disease target, rather than trying to discover them using a blind, random, trial-and-error method.

What is also striking is the fact that this new GAN-RL approach represents less than 1% of Insilico Medicine's lead generation pipeline, and that they are hard at work to ensure that the

fruits of their labour are as accessible as possible for other researchers to build on their own progress, and to expedite the industry-wide penetration of AI in pharma, drug development and clinical translation.

"When Deep Knowledge Ventures chose to provide Insilico Medicine's initial funding round in 2014, we did so because we saw their potential to increase Quality-Adjusted Life Years (QALY) for the betterment of humanity as a whole. Since then they have been the first to use cutting edge deep learning techniques like Generative Adversarial Networks to design novel drug candidates from scratch with specified molecular properties in 2016, and in 2018 to succeed in designing, synthesizing and validating a new drug end to end in less than 2 months. I am also thrilled by the fact that this article visualizes what Insilico Medicine has been making in their R&D already back in 2017 and submitted for publication in 2018. I would not be surprised to find out that since then they have made even greater progress in applying next-generation AI techniques for drug design, which might be publicly disclosed in 2020" **said Dmitry Kaminskiy, General Partner of Deep Knowledge Ventures.**

This can be thought of as **Pharma's AlphaGo Moment**, when the potential for AI to radically transform the current operating procedures and business models in the Pharma industry becomes tangibly obvious to the public. In the case of the AI industry in general, this was when the AI-company DeepMind (acquired by Google for $500M) succeeded to develop the first computer program capable of beating a professional human world champion in the game "Go". This recent achievement by Insilico Medicine may very well be the Pharma industry's analogous, totally game-changing moment - the first time a drug was designed by AI from scratch and validated not in years, but in days.

Reference to the paper:
Web link: https://www.nature.com/articles/s41587-019-0224-x

About Deep Knowledge Analytics
The Pharma Division of Deep Knowledge Analytics is the leading analytical agency specifically focused on deep intelligence of the pharma industry and the AI for Drug Discovery sector, and a specialized department of Deep Knowledge Analytics, a DeepTech-focused analytical company focusing on advanced industry analytics on the topics of Artificial Intelligence, GovTech, Blockchain, FinTech, Invest-Tech and Frontier Technologies. Its proprietary and open-access reports have been covered by top-tier tech, business and finance media including *Forbes, Financial Times, The Guardian, The Telegraph*, and acknowledged by many other authoritative entities such as *MIT Technology Review*.