Profiling AI-derived Janus Kinase (JAK) Inhibitors for COVID-19 Treatment

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Website
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Industry
Biotechnology

Location
Hong Kong, China

Employee count
51-100

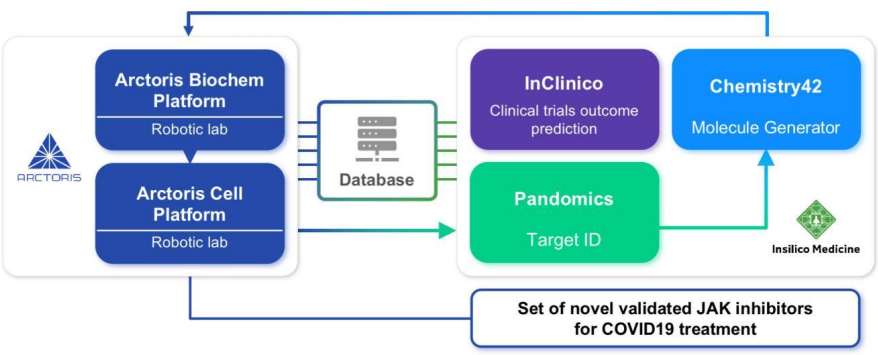
Overview

Insilico Medicine is one of the world's leading Artificial Intelligence companies. Since 2014 Insilico Medicine focuses on generative models, reinforcement learning, and other state-of-the-art machine learning techniques for the generation of new molecular structures with the specified parameters, generation of synthetic biological data, target identification, and prediction of clinical trial outcomes.

Insilico Medicine pioneered the applications of AI solutions in drug discovery, developing an impressive pipeline of therapeutic programs in cancer, fibrosis, anti-infectives, immunology, and longevity/ senescence.

Challenges & Objectives

After the onset of the COVID-19 pandemic, Insilico Medicine rapidly embarked on an ambitious project to design and synthesize inhibitors against four Janus kinase (JAK) family members JAK1, JAK2, JAK3 and TYK2 that could serve to treat severely sick COVID-19 patients. They looked for a partner that could offer compound profiling at superior speed and quality.



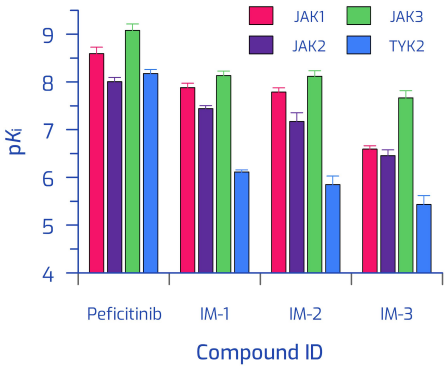
Working with Arctoris, Insilico Medicine was able to receive full kinetic IC50 profiling data of a set of inhibitors in less than 24 hours.

"Arctoris brings a new scale to the drug discovery process that complements our unique AI platform - leading to increased speed and improved chance of success for our pipeline assets."

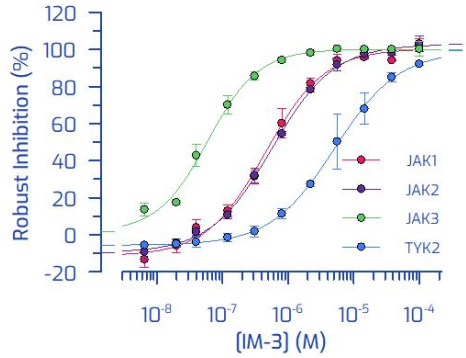
- Alex Aliper PhD, Insilico Medicine, President

Action & Results

Insilico Medicine identified novel small molecule JAK inhibitors using its generative chemistry platform, with Arctoris rapidly evaluating the biological activity on its next-generation robotic platform in Oxford, UK. In a closed design-synthesise-test loop, the partners arrived at highly promising new molecules at a fraction of the time required by other industry players, providing unprecedented prospects for new drug discovery successes. Now entering in vivo studies, JAK inhibitor study profiled a set of potent inhibitors that can help patients by modulating the life-threatening cytokine storm caused by COVID-19.



Benchmarking of three selected Insilico Medicine molecules (IM-1, IM-2, IM-3) against a clinical stage inhibitor (Peficitinib). The machine learning-generated compounds were developed and tested with unparalleled speed, exhibiting competitive potencies & selectivity profiles.



Full biochemical IC50 profile for IM-3, showing log-scale selectivity differentiation for the inhibitor against the JAK family members, with a clear binding preference for JAK3 over JAK1/2 and TYK2.

Value

The partnership with Arctoris enabled Insilico Medicine to combine its unique strengths in AI-guided drug discovery for target identification and generative chemistry with the benefits of a robotic platform for rapid generation of high-quality cell-based, molecular and biochemical data. The partnership propels Insilico Medicine's abilities to discover and validate novel molecules faster.

Further collaborations will focus on joint drug discovery projects in oncology and longevity, areas of particular interest to both Arctoris and Insilico Medicine, with their mission to eliminate age-related disease and promote healthy longevity.