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Insilico Medicine explores use of 3CL protease inhibitor for COVID-19 treatment

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The candidate is intended to be used for the treatment of SARS-CoV-2 and its variants, along with other coronaviruses



Insilico Medicine, a China & US-based clinical-stage end-to-end artificial intelligence (AI)-driven drug discovery company, has announced its nomination of a novel preclinical candidate (PCC) targeting 3C-like (3CL) protease for the treatment of COVID-19.

Insilico's PCC is an orally available 3CL protease inhibitor with a novel structure generated using Insilico's AI platform. The compound can be efficiently prepared with a two-step synthesis from commercial starting materials.

In preclinical studies, it demonstrated a favorable profile with good *in vivo* efficacy at low doses and its observed efficacy is independent of co-administration with CYP3A4/Pgp inhibitor (e.g. Ritonavir).

It also showed broad-spectrum antiviral activities, not only for SARS-CoV-2 and its variants, but also for other types of coronaviruses that cause diseases including severe acute respiratory syndrome (SARS) and Middle East respiratory syndrome (MERS).

Insilico initially trained its end-to-end AI platform to combat the pandemic early in the outbreak based on knowledge of the virus' structure and properties developed from the SARS outbreak in 2003. Empowered by its AI platform, the company narrowed and identified the 3CL target in early 2020 and then published its first set of novel compound structures designed using its small molecule generation platform Chemistry42 in February 2020.