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Identification of herbal drug-like inhibitors against SARS-CoV-2 main protease.

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Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV 2) began as an epidemic outbreak in Wuhan, China, in December 2019. With the absence of definitive anti-viral therapy to address the exponential increase in the infected, the need of the hour is to find the soft spots that can be targeted to curb the spread and control its progression in the human population.

The study's objective is to identify the molecules that can arrest the virus proliferation by inhibiting SARS-CoV-2 Main Protease (MPro). It is the crucial enzyme that processes all other SARS proteins to become functional through proteolytic processing. Using docking and MD simulation studies, we have identified many herbal inhibitors to be tested for their efficacy using in-vitro studies to address this issue. Since an active MPro is required to screen them, we expressed the protein and conducted its purification using affinity and gel filtration chromatography. The protein was found to be ~ 34kDa which was confirmed using SDS-PAGE and Western blotting through hybridization with MPro specific antibodies. To ensure the functionality of the purified protein, the biochemical assays were optimized and performed on the enzyme using different parameters of pH (8.0), temperature (37°C), enzyme (0.1µM), and substrate (1µg/µL) concentration. Having optimized the activity profile of MPro and identifying its inhibitors, our further strategy is to screen the inhibitors identified. The screened molecules will be tested for binding with the enzyme using biophysical parameters, including X-ray crystallography, and validation in SARS-CoV-2 culture to inhibit the viral replication.

Biography

Aditya is a doctoral candidate at Shiv Nadar University and has a keen interest in protein biochemistry. Before starting his work on SARS-CoV-2, he undertook and contributed to projects on the Zika virus (to identify lead molecules against the NS2B-NS3 complex), Leishmania donovani (to develop a cell-free assay to test Dipeptidylcarboxypeptidase activity), and Hepatitis-E virus (to test the effect of critical mutations on cysteine protease activity).

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