DST-SERB supports study for identification of structure-based potential antivirals against COVID 19

The Science and Engineering Research Board (SERB) under Department of Science & Technology (DST) has recently supported a proposed study by Prof. Pravindra Kumar from IIT- Roorkee for identification of structure-based potential antivirals against SARS-CoV2.

The study to be funded under Intensification of Research in High Priority areas (IRHPA) will search for small molecule inhibitors targeting some of the most important viral replication enzymes. These enzymes are viral proteases (papain-like protease & 3CLprotease), RNA dependent RNA polymerase (nsp12), and the Methyltransferase or MTase (nsp14). Viral proteases, which are enzymes encoded by the genetic material (DNA or RNA) of viral pathogens, catalyze the cleavage of specific peptide bonds in cellular proteins.

In this study, a computer-based high throughput virtual screening approach will be used to identify antiviral molecules from different compound libraries that will be experimentally validated for antiviral potential. The collaborators Dr. Shailly Tomar from IIT Roorkee and Dr. Gaurav Sharma from Indian Veterinary Research Institute (IVRI), Bareilly, will help in experimental testing and evaluation of the antiviral efficacy of the identified antiviral molecules against SARS-CoV-2 virus.

As a preliminary work, the investigators have already performed the *in silico* work by high-throughput virtual screening approach to examine the binding affinity of FDA approved drugs targeting the viral protease Mpro.

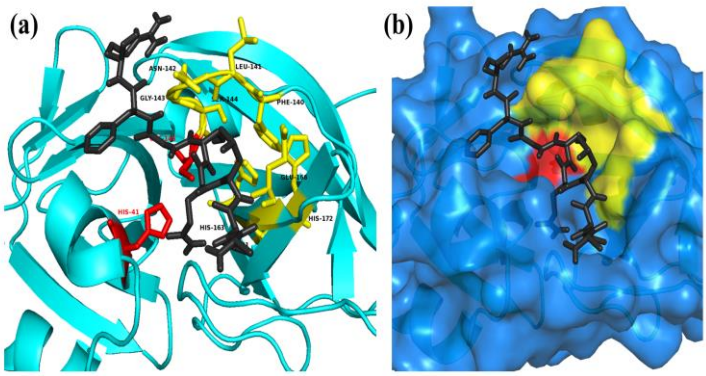

Figure: Three-dimensional structure focusing on the Mpro active site. The substrate peptide (black color) is shown to bound at the active site.

"The hunt for new drugs, including repurposed drug candidates, is getting a boost by *in silico* approaches, which allude to identifying the potential antiviral molecules based on computer simulation of their molecular structures. This approach is expected to be much faster and accurate in selection of potential drugs and vaccines for experimental and clinical testing.", said Prof Ashutosh Sharma, Secretary, DST.

SARS- CoV-2 is the etiological agent responsible for the global COVID-19 pandemic with high morbidity and mortality. Across the globe, the R&D activities by various agencies were initiated towards the identification of clinically effective vaccine or specific antiviral drugs or drug repurposing strategies to combat the COVID-19 infections either in the form of prevention or treatment.

Using structure-based approach for drug repurposing, this study would pave the way to identify the molecules that bind to Mpro active site, and their potential can be used as antiviral molecules against COVID-19.

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