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IIT-R works on structure based potential antivirals against SARS-CoV2

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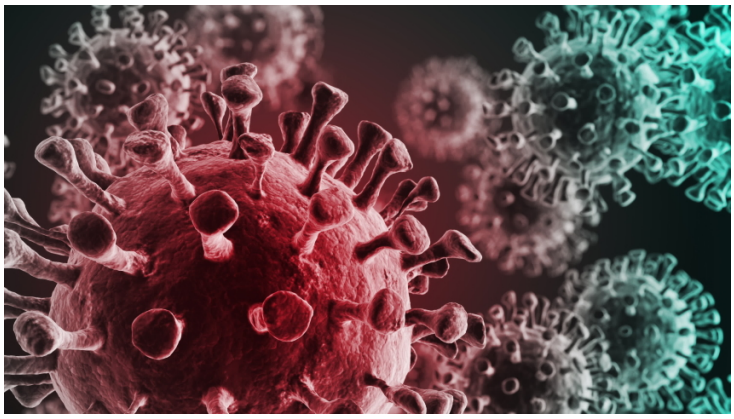
A computer-based high throughput virtual screening approach will be used to identify antiviral molecules



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. ShaillyTomar 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.