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IIT Roorkee discovers three anti-viral molecules for treating COVID-19

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To quickly direct the development of new anti-viral therapy against SARS-CoV-2 and its emerging variants



A team of researchers at Indian Institute of Technology Roorkee (IIT Roorkee) has identified anti-viral molecules that can be used effectively to treat COVID-19 infections. The researchers identified three such anti-viral molecules through drug repurposing, computational and anti-viral experimental studies.

The COVID-19 pandemic spurred both computational and experimental studies all over the world to understand the structure and nature of SARS-COV-2 viral proteins and develop vaccines and cures for it. One important branch of study is structure-function studies to unravel the atomic structures of the virus and its proteins that constitute the virus.

The IIT Roorkee team is executing protein structure-based drug-repurposing research on SARS-CoV2 molecules for clinical evaluation and eventual use as anti-viral therapeutics.

The team used the Protein Data Bank to target and identify drug molecules for the COVID-19 virus. They focused on discovering molecules that acted on a specific part of the viral proteins called the nucleotide-binding pockets (NBPs). As the name suggests, the NBP binds to the nucleotides – the building blocks of RNA and DNA – and help in the replication of the virus. NBP-targeting drugs are known and used for viral diseases such as HIV, hepatitis B, hepatitis C, and herpes, among others.

Six NBPs were identified using the atomic structures available in the Protein Data Bank. The team used a novel approach of multi-targeting various virus-specific proteins using one drug, instead of targeting only one virus-specific protein. This novel multi-targeting approach is expected to be therapeutically highly effective and is less likely to result in resistant variant strains.