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IIT Varanasi to re-purpose approved drugs for COVID-19 treatment

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The research group of Prof. Vikash Kumar Dubey is working on developing new drug candidates against SARS-CoV-2



The Science and Engineering Research Board has approved support for research at IIT (BHU) Varanasi to identify lead compound(s) from available and approved drugs for fast-track anti-SARS-CoV-2 drug molecule.

The research group of Prof. Vikash Kumar Dubey is working on developing new drug candidates against SARS-CoV-2 by exploring DrugBank (DrugBank is a database of FDA approved drug compounds).

This database will be used for searching drug against SARS-CoV-2) database compounds as an inhibitor of SARS-CoV-2 main protease, a key enzyme required for SARS-CoV-2 assembly and multiplication. They will be carrying out extensive computational and experimental studies to identify an inhibitor of SARS-CoV-2 main protease.

Taking advantage of available crystal structure of the SARS-CoV-2 main protease, a structure-based inhibitor design will be done by the researchers from the available FDA approved drugs compounds in the DrugBank database.

Subsequently, experimental validation of the designed inhibitor(s) on recombinant SARS-CoV-2 Mpro Protein will be carried out. Various inhibitor parameters will be calculated to establish the effectiveness of the inhibition of the SARS-CoV-2 Mpro enzyme function.

As the enzyme SARS-CoV-2 Mpro, is key for processing and polyprotein for virus assembly, the inhibition of this key protein can have an anti-viral effect. As most of DrugBank database compounds are characterized in terms of pharmacokinetics and toxicity, the identified molecule could be brought to the market rapidly.