## Drug repositioning to fast-track drug discovery against COVID-19: THSTI's team efforts

Scientists at Faridabad based institute, Translational Health Science and Technology Institute (THSTI) have been working on repositioning drugs to act against SARS-CoV2. Dr. Shailendra Asthana and his team at DBT's THSTI used molecular dynamics (MD) simulations to find out a computational model of the drug binding site. They used the model for virtual screening to facilitate the rapid identification of potent molecules. They findings on identification of potential molecules against COVID-19 main protease through the structure-guided virtual screening approach have been published in the *Journal of Biomolecule Structure and Dynamics*. The findings may provide an opportunity to explore these compounds for anti COVID-19 therapeutics.



Hydroxychloroquine, Remdesivir, and others are not new but in news almost every day now. Why? SARS-CoV2, the virus that causes COVID-19 has allowed the scientists, clinicians and governments very little time to respond. On the stake are billions of lives. This very little time is strategically being used for developing rapid tests, vaccines which otherwise take 5 to 15 or more years, and drugs. Usually, developing a new drug for a disease too takes about 10 years, but drug repositioning is an approach that finds a new purpose for a drug by tailoring its composition, dosage to cure a different disease than it was originally meant for. Case in point are hydroxychloroquine, an anti-malarial drug and remdesivir, originally developed against hepatitis C among the most mentioned.

Link: https://doi.org/10.1080/07391102.2020.1768151