



ICTS Colloquium

Title : Mechanism of SARS-cov-2 main protease activation

Speaker : Shreyas Kaptan (Free University of Berlin, Germany)

Date : Monday, 1st March 2021

Time : 03:00 pm (IST)

Abstract : Covid-19 is an ongoing health emergency. The leading candidates to combat its causative agent, the SARS-cov-2 virus are vaccines and drugs. The viral main protease (Mpro) is a dimeric enzyme required for the maturation of the virus particles after successful infection of the host cells. Dimerization of its monomers is believed to activate the enzyme leading to efficient catalysis of the viral polypeptides. We use Molecular dynamics simulations (MD) and Machine Learning (ML) in concert as a computational microscope to shed light on the mechanism of dimerization of the main protease and create a pathway for developing drug based strategies to stop the virus in its tracks.

Venue : Please click on the link to join the meeting.

<https://zoom.us/j/94661404956?pwd=SnBMNmE2RW1uN2xtTEJEK2ZuZlFBOT09>

Meeting ID: 946 6140 4956

Passcode: 629869