**Tata Institute of Fundamental Research**
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

# Seminar

## Atom-by-atom Growth of de novo ligands around a given receptor: application to a few systems

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### IISER, Pune

In this talk, I am going to discuss a de novo atom-by-atom generation of ligands around a given protein surface. This is a general method that uses Monte Carlo optimisation of the ligand (currently based on classical interaction). With this method, one can target any biological receptor and come up with new binders. We have applied this to RBD (receptor binding domain) of spike protein of SARS-COV-2 virus and then validated our approach with all-atom enhanced sampling techniques like well-tempered metadynamics. We also have shown a possible method of repurposing of the existing drug molecules for the current target. We are also applying this method to various other systems and simultaneously modifying it to get better drug molecules for a known receptor.

***Tuesday, April 5th 2022***

***04:00 PM***

***Auditorium, TIFR-H***