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

Seminar

Multiscale computational methodologies to accurately model complex biological assemblies of relevance to HIV-1 lifecycle and Ice-binding Proteins

Arpa Hudait

University of Chicago, IL

Recent advances in computational methodologies allow us to accurately model biomolecular assemblies in coarse-grained resolution, accessing length and time scales far beyond that of atomistic simulations. At the heart of this approach is systematically deriving coarse-grained (CG) models from experimental structures and their underlying atomic-scale interactions, known as "bottom-up" coarse-graining. My particular contribution in this field is to develop an "integrated hierarchical coarse-graining protocol" for biological assemblies and the associated computational implementation. Using this approach, I developed CG models of massive biological assemblies such as the HIV-1 virus and Nuclear Pore Complex (NPC). Using these CG models, I performed simulations of the entry of the HIV-1 virus into the Nuclear Pore Complex to infect the host cell and how Lenacapavir (the only antiviral drug approved for clinical usage) averts infection. Finally, I will also briefly discuss how the difference in the size of ice-binding proteins accounts for their distinct functions: promoting or preventing ice growth.

Tuesday, Nov 5th 2024

16:00 Hrs (Tea / Coffee 15:45 Hrs)

Auditorium, TIFR-H