Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Students' Annual Seminar

In-silico modelling and study of kinase inhibitors

Jaya Krishna Koneru

Kinase and their associated cell signalling pathways play a major role in many intercellular processes. Aberrant regulation of kinase can disrupt the dynamics of the processes resulting in several diseases like Alzheimers, Cancer etc. Although there are many kinase inhibitors available commercially, because of emergence of drug resistance mutations (gate-keeper residue mutations) at rapid pace in the kinases limits the usage of these inhibitors. So rational structure-based design of small molecule inhibitors which can by-pass the gate-keeper mutation and are effective over long-term treatments became challenging.

In this talk, I will describe the computational design of a series of kinase inhibitors which are both potent binders and also good candidates to circumvent drug resistance due to gate-keeper residue mutation. I have combined fragment-based drug design and novel enhanced sampling techniques of Molecular Dynamics simulation to efficiently screen a series of drugs, which might be of potential interest.

Monday, Mar 19th 2018

04:00 PM (Tea/Coffee at 03:30 PM)

Seminar Hall, TIFR-H