



## **ICTS Seminar**

Title : Allosteric Regulation of the AMPA Receptor-Channel

Speaker : Shreyas Kaptan (Frei University, Berlin)

Date : Wednesday, 27<sup>th</sup> November 2019

Time : 3:00 PM

Venue : Emmy Noether Seminar Room, ICTS Campus, Bangalore

Abstract : AMPA receptors (AMPAR) are ionotropic channel-receptor proteins

responsible for synaptic transmission and maintenance of neural plasticity. Neurotransmission by these tetrameric proteins is exceptionally fast and happens at a sub-millisecond level. Ligand binding at a distal exoplasmic domain of AMPAR controls the ion channel domain in the transmembrane region. We use techniques of molecular dynamics (MD) simulations and Markov state models (MSMs) to decipher the mechanistic details of molecular processes that participate in the information transfer from the ligand binding domain (LBD) to a gate located in the exoplasmic end of the ion channel. We demonstrate the allostericity of the regulation in the computer simulations. We use Zn bridging experiments to validate the predictions of the in-silico models. Additionally, we calculate the kinetics of the channel gating with the computational MSMs and confirm them with single channel electrophysiology experiments.

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