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

# Internal Seminar

## Atomistic Insight of AMA1-RON2 Interaction Through Molecular Simulation

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Malaria remains a major challenge to global healthcare and is one of the leading causes of morbidity and mortality. Of the six plasmodium species which are pathogenic to humans, Plasmodium falciparum is the most common. The invasion of malarial merozoites into erythrocytes is a complex process, which is achieved through formation of a moving junction (MJ) between the apicomplexan parasite and the host cell. The MJ contains two key parasite components- the surface protein Apical Membrane Antigen 1 (AMA1) and its receptor, the Rhoptry Neck Protein (RON) complex, which is targeted to the host cell membrane during invasion. In particular, RON2, a trans-membrane component of the RON complex, interacts directly with AMA1. Understanding the AMA1-RON2 complex from structural perspective is crucial due to its immense therapeutic potential. Molecular Mechanics Poisson-Boltzmann Surface Area (MMPBSA) method is typically based on molecular dynamics simulations of the receptor–ligand complex and is therefore intermediate in both accuracy and computational effort between empirical scoring and strict alchemical perturbation methods. The current talk will emphasise on key results pertaining to the energetics of AMA1-RON2 complex using MMPBSA method. One of important components of AMA1-RON2 recognition is the role played by domain II (DII) loop of AMA1. The role of DII loop of AMA1 has so far been remained elusive. All the crystal structures solved so far could not locate the electron density of the DII loop due to its highly flexible nature. We have conducted micro second level molecular simulations to understand the dynamics of DII loop. In this talk I will present few preliminary but crucial results from these efforts.

***Wednesday, May 2nd 2018***

***2:30 PM (Tea/Coffee at 2:00 PM)***

***Seminar Hall, TIFR-H***