Tata Institute of Fundamental Research
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Internal Seminar

Atomistic Insight into intrinsic AMA1-RON2 Interactions from Molecular Dynamics Simulations

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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 invading 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 transmembrane 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. One of the 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 molecular simulations to understand the dynamics of DII loop. Besides the dynamics of DII loop, it is equally pertinent to understand the internal dynamics of RON2 itself in water which is currently being investigated thoroughly. To this end, in this talk I will present important results obtained from these efforts.

Wednesday, Apr 24th 2019

11:30 AM (Tea/Coffee at 11:00 AM)

Seminar Hall, TIFR-H