

## **Internal Seminar**

### **Protein engineering for antimalarial research and electrochemical catalysis**

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Widespread resistance of *Plasmodium falciparum*, a deadly malaria parasite, against front line antimalarials warrants immediate alternatives to contain the outbreak of drug resistant malaria. Two parasite proteins, Apical Membrane Antigen 1 (AMA1) and Rhoptry Neck protein 2 (RON2), are known to be crucial for erythrocyte invasion of blood stage parasite. Unnatural D-peptide/protein based inhibitors have huge potential as therapeutics due to their high protease resistance and low immunogenicity. We are utilizing a unique combination of chemical protein synthesis and 'Mirror-Image Phage Display' to find suitable D-protein inhibitors for both pfAMA1 and pfRON2. In this talk, I will describe challenges associated with the chemical synthesis and folding of pfAMA1-domain-1. In addition, a strategy of hybridizing *P. falciparum* specific R1 and pfRON2 to generate a more potent parasite inhibitor will be described. Molecular dynamics (MD) simulations coupled with molecular mechanics/Poisson-Boltzmann surface area (MM/PBSA) calculations were utilized for choosing the fragments from each parent peptides for designing the hybrid peptide. This hybrid peptide exhibited a spectacular 100 fold increase in growth inhibition of *P. falciparum* compared to its parent peptides.

I will also describe a novel strategy of protein functionalization on carbon nanotubes (CNTs) to design effective catalysts for electrochemical Hydrogen Evolution Reaction (HER). In recent years, there has been an increasing interest in designing economically viable metal free carbon based catalysts for water splitting. The roles of protein denaturation, overall nitrogen content in proteins, presence of residues that favours electron transport, as well as the importance of their covalent connectivity with the CNTs will be explained. HER characteristics of these catalysts have been systematically established with different metal free peptides and proteins. A mechanistic insight of the observed phenomena will also be discussed in this talk.

***Wednesday, Oct 16<sup>th</sup> 2019***

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

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