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

Internal Seminar

Computer simulation of antimicrobial peptides in action

Namita Dube

TIFR-Hyderabad

The self-assembly of simple units into complex structures is a fascinating example of emergent phenomena. One such example is the self-assembled peptide nanofibers which can form biomimetic hydrogels at physiological pH and ionic strength, through non-covalent and reversible interactions. Inspired by natural antimicrobial peptides, a class of cationic amphiphilic self-assembled peptides (CASPs) that self-assemble into thixotropic nanofibrous hydrogels was designed by Sarkar et al. These constructs employ amphiphilicity and high terminal charge density to disrupt bacterial membranes. I used μs-timescale coarse-grained simulation to elucidate the interaction between this peptide and bacterial membranes. I demonstrate that the membranes stiffen, contract, and buckle after binding to peptide nanofibers, allowing disruption of the osmotic equilibrium between the intracellular and extracellular fluid. My studies suggest that self-assembled peptide nanofibrils can be general membrane-disrupting antimicrobial agents. Another interesting example is the self-assembly of a class of helical β-peptide molecules known as AAKG(bY-(ACHC-ACHC-bK)$_3$). The additional carbon atom on the backbone of a β-amino acid can be used to incorporate cyclic groups along the backbone, which imparts significant stability to helical structures. Through, my study I was able to develop the coarse-grained martini force field parameterization to effectively study the molecular mechanism of disruption of these β-peptide. My study suggests that these molecules self-assemble and interacts with the membrane to form pore thus, disrupting the bacterial membrane. This will further be used to study different systems such as non-globular antimicrobial peptides and nylon based polymers.

Monday, Aug 19th 2019

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

Seminar Hall, TIFR-H