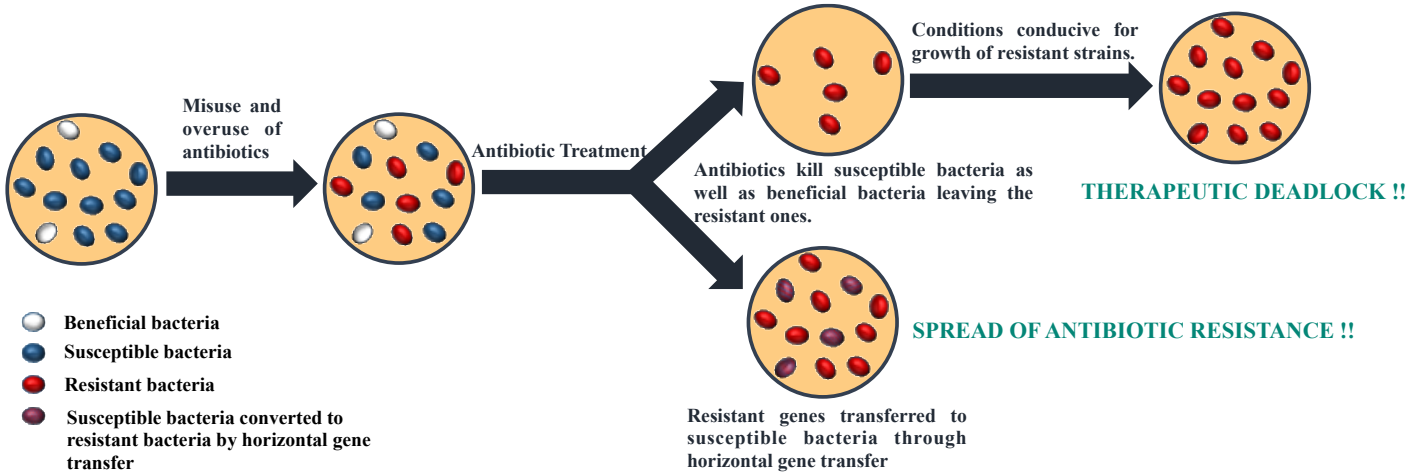
Theoretical insight into the structure and functioning of Defensin family of proteins: An all-atom Molecular Dynamics simulation study (DBT, India)

Sandip Paul
Department of Chemistry, IIT Guwahati

Antibiotic Resistance: A Health Concern of the Modern Society

Cause of Antibiotic Resistance :



Project Summary:

Sugarcane Defensin 5 (SD5) exhibits complex conformational dynamics involving all the components of its secondary structure that influences its membrane recognition and binding affinity. Evidence suggests its selectivity to fungal phospholipid glucosylcerebroside CMH, forming membrane disruption complex but the exact mechanism of such complex formation, the thermodynamics and its inhibition is yet unexplored and is an area of active research. In this project we would like to study the molecular level insights into temperature and osmolyte-induced stress on SD5 protein. Then, we extend our study towards the interaction of defensin proteins with membrane lipids in order to gain an insight into membrane permeabilization property of the proteins. We would also like to examine the mode of interaction that dictates the mechanism of membrane disruption. Finally, we would like to explore the self-assembly of human defensing (HD6) proteins.