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

Students' Annual Seminar

Computational perspective of Antimicrobial action of short-chain β-peptides

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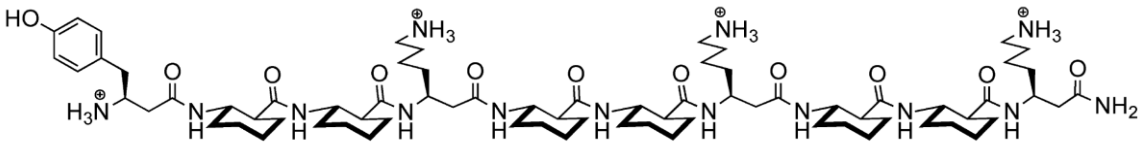
Anti-microbial peptides play a crucial role in innate-immune response. They act as the primary line of host defence against several kinds of microbes. Peptides made of β-aminoacids are observed to not only highly mimic the antimicrobial property of natural antimicrobial peptides, but are more potent than their natural counterparts because of stable helical amphiphilic structure which made β-peptides better alternative. These antimicrobial peptides are observed to cause cell death of different microbes like Gram negative and Gram positive bacteria, E.coli etc by disrupting the membrane leading to leakage of cytoplasm of cell. But the mechanism of how the membrane gets disrupted remains to be illusive.

Using a 10 residue short β-peptide with the sequence βY-(ACHC-ACHC-βK)$_3$ as our model system(figure below), we perform several μs long simulations to get a glimpse of the antimicrobial action of β-peptides from computational perspective on a bacterial mimetic membrane containing 128 lipids with 3:1 ratio of POPE and POPG respectively.



The initial analysis revealed spontaneous insertion of peptide during 1:128 peptide:lipid ratio(P/L), whereas for 7:128 P/L disruption of membrane bi-layer has been observed which intern led to proliferation of water till half of the membrane bi-layer which is completely different from former computational observations of natural occurring antimicrobial peptides. Comparative study between the above mentioned peptide with its non-globally amphiphilic counterpart revealed decreased peptide-membrane interactions in case of non-GA peptide for 1:128 and 7:128 P/L concentrations.

Friday, Apr 26th 2019

3:00 PM (Tea/Coffee at 1:30 PM)

Seminar Hall, TIFR-H