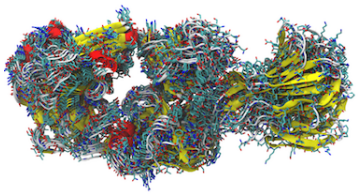

IV ASBioSim – Advanced School on Biomolecular Simulation: Protein Engineering with Rosetta, from fundamental principles to tutorials

05 to 10/May, 2019, Recife/PE, Brazil

Flip to Enter: Initial Steps of BP-100/Membrane Interaction

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Abstract:

BP100 is a short antimicrobial peptide and can also act as a molecule-carrier into cells. Like with other antimicrobial peptides, the precise mechanism of membrane disruption is not fully understood. Here we use computer simulations to understand, at molecular level, the initial interaction between BP100 and zwitterionic/negatively charged model membranes.

In agreement with experimental results, our simulations showed BP100 folded into an alpha helix when in contact with negatively charged membranes. BP100 binding induced the aggregation of negatively charged lipids on mixed membranes composed of zwitterionic and anionic lipids. The peptide in alpha-helix conformation initially interacts with the membrane via electrostatic interactions between the negatively charged lipids and the positively charged residues of the peptide. At that point the peptide flips, burying the hydrophobic residues into the bilayer highlighting the importance of the hydrophobic effect contribution to the initial interaction of cationic antimicrobial peptides with membranes.