Abstract

Hearing is one of our uniquely robust and subtle sensory mechanism that is tightly controlled under the mechanical forces generated by sound-waves. Ca+2 ions play significant role in hearing. It provides the structural rigidity to the molecular constructs, cadherin proteins at tip-links, directly involved in hearing. Objective of this work is to understand the role of Ca+2 ions that serve as structural determinant for cadherins in silico. We performed molecular dynamics simulations using GROMACS (GROningen MAchine for Chemical Simulations), VMD, UCSF Chimera (an Extensible Molecular Modelling System) to understand the dynamics of cadherins with Ca+2 ions. The system was well energy-minimized and equilibrated in NVT ensemble and NPT ensemble. We estimated the structural rigidity of proteins, using RMSD, structure overlay and tensor calculations and identified different conformations of cadherins at different Ca+2 ions concentrations. As prelude, the concepts of statistical mechanics and classical mechanics that is used in MD simulations, are also discussed.