“Molecular Dynamics Simulation on an Engineered T4 Lysozyme Protein for Potential Nano-Biotechnological Applications”

Hadeer A. Elhabashy[1], S. M. ElSheikh[1], Ahmed S. Moussa [2], Mohammad S. Yousef[3,4]

1 Department of Physics, The American University in Cairo, Cairo, Egypt.
2 Faculty of Computers and Information, Cairo University, Cairo, Egypt.
3 Biophysics Department, Cairo University, Cairo, Egypt.
4 Department of Physics, Southern Illinois University Edwardsville, Illinois, USA.

The idea of developing a Bio-molecular mechanical device has attracted the attention of many research groups due to its promising Nano and Bio-technological applications such as flow-control valves, switches and bio-sensors. T4 Lysozyme protein is an enzyme, which has been extensively studied. This protein provides a wealth of information regarding the structure function relationship of proteins at atomic resolution. An engineered variant of T4 Lysozyme has been reported to trigger a large scale translocation of an engineered helix (~ 2nm), upon the addition of an external ligand. The design was based on the duplication of a surface helix, followed by manipulating the stability of an adjacent loop, which caused the duplicated helix to switch between two conformations. The purpose of this study is to investigate the dynamics of the engineered motion for potential Nano and Biotechnological applications. Many wild type and mutant static crystal structures of T4 Lysozyme have been shown to display a range of about 50 degrees in hinge bending motion between the N- and C-terminal domains of the protein, indicating intrinsic flexibility. Our Molecular dynamics simulations detect similar motion in the engineered protein, within 100 nanosecond time scale. A preliminary mathematical model (solvent free) describing the hinge bending motion and the impact force is constructed. However, in the nanosecond time scale, the engineered triggered motion (the helical translocation) was partially detected only when bond constraints were significantly relaxed.