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Molecular dynamics simulation (Protein-Ligand)

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Hossein Tarrahimofrad[1], Amir Meimandipour[1], Sareh Arjmand[2], Mohammadtaghi Beigi Nassiri[3], Ehsan Jahangirian[1], Hossein Tavana[4], Javad Zamani[1], Somayyeh Rahimnahal[1], Saeed Aminzadeh[1]

[1]Bioprocess engineering group, Institute of Industrial and Environmental Biotechnology, National Institute of Genetic Engineering a nd Biotechnology (NIGEB), Tehran, Iran;

[2]Protein Research Center, Shahid Beheshti University, G. C., Tehran, Iran;

[3]Department of Animal Science and Food Technology, Agriculture Science and Natural Resources University Khouzestan, Ahwaz, Ir an;

[4]Department of Biomedical Engineering, The University of Akron, Akron, OH 44325, USA

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Hossein Tarrahimofrad

ABSTRACT

The prepared protein and protein-ligand complexes (protease-SDS and protease-tween complexes) were used in MD simulation, performed using GROMACS v 4.6.5 with CHARMM36 all-atom force field. The CGenFF server (https://cgenff.umaryland.edu/) provides topologies and parameters of ligands compatible with the CHARMM36 all-atoms force field. Protein and protein-ligand complexes were soaked in a cubic box of water molecules, and the charges on the protein were neutralized by the addition of Na^+ and Cl^- ions. The energy of the system was minimised using the steepest descent algorithm to eliminate bad contact and clashes. The NVT and NPT ensembles were used during the equilibration to achieve the desired temperature (373.15 K for protease and 300 K for protease-ligand complex) and pressure (1 bar) for 100 ps and restraint forces of 1000 kJ/mol. Finally, 40 ns MD run were performed in triplicate after releasing all restraints. All bonds were constrained by the LINCS algorithm.

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