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Protocol 2: MD simulation with Gromacs

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ABSTRACT

Structural stability of the docked complexes was monitored using MD simulation with Gromacs 2020.5 (RRID:SCR_014565). The protein topology was created using Gromos96 force field and the PRODRG server was utilized to create the topology of the ligand. The docked complexes were solvated using 'Simple Point Charge' (SPC) water model in a cuboidal box with adequate size to accommodate the complete complex at the center.The modeled systems were neutralized using required number of counter ions (Na+ / Cl-). The undesirable contacts and steric conflicts were then removed from the neutralized systems using steepest descent followed by conjugate gradient methods for 50,000 steps each. The NVT ensemble used to maintain constant number of atoms, volume, and temperature, further NPT ensemble was used to maintain constant pressure. NVT and NPTensembles were used to maintain temperature. The temperature and pressure were set constant at 300K and 1 bar respectively, during the equilibration of 1ns. Further, followed by 1ns of equilibration, unrestrained MD simulation was performed for a period of 100ns in solvent. The Particle Mesh Ewald (PME) method was used to handle coulomb electrostatic interactions, while the LINear Constraint Solver (LINCS)s algorithmwas used to limit H-bonds. Using a cut-off value of 14 Å, the non-bonded contacts were trimmed. The trajectories generated were analyzed using some of the inbuild gromacs tools like '*gmx rms,' 'gmx rmsf,' 'gmx hbond,' 'gmx gyrate,' 'gmx sasa,*' etc. and other additional packages for specific analysis wherever required. Conformational changes at the secondary structural level were monitored by using Dictionary of Protein Secondary Structure (DSSP) software (RRID:SCR_002725).

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