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ADSORPTION OF TRP-CAGE MINI PROTEIN ON A GRAPHENE SURFACE: A MOLECULAR SIMULATION APPROACH

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Examination of protein adsorption to solid surfaces with molecular dynamic simulations will yield many different aspects of innovations in the field of biochemistry. In contrast to computational simulations, laboratory experiments for protein adsorption on solid surfaces are rather expensive and time-consuming. Therefore, a computational approach is preferred, and protein adsorption to solid surfaces remains a challenge to chemists due to its highly complex behaviour. This research was primarily focused on trp-cage mini protein (PDB ID: 1L2Y) adsorption on a graphene solid surface. Molecular dynamic simulations were conducted using GROMACS software, and the Kirkwood-Buff derived force field (KBFF20) was incorporated. Four simulations were conducted: the original protein near the solid surface, the protein rotated by 180° around a horizontal axis, and the protein adsorption on the solid surface having +0.1*e* or -0.1*e* partial charge on each atom in the graphene layer. Adsorption was explained by the change of distance between the centre-of-masses (COMs) of protein and the graphene surface along the vertical axis. The diffusion coefficient was used to indicate the rate of adsorption of the protein. The first and second simulations concluded that the protein was stable near the COM distances of 0.732 nm and 0.760 nm starting from 1 nm away from the graphene surface. The calculated average one-dimensional diffusion coefficients along the vertical axis were 1.914 (±0.008) × 10^{-4} nm^2 ns^{-1} and 1.248 (±0.009) × 10^{-4} nm^2 ns^{-1} for simulations one and two, respectively. For other simulations, overall adsorptions of the protein were not indicated. The study concludes that protein adsorption depends on the number of hydrophobic and hydrophilic residues exposed to the solid surface, and the more hydrophobic residues it has, the higher tendency for the protein to adsorb onto the non-polarized surface.

Keywords: Graphene, Molecular Dynamics, Protein Adsorption, Surface Science