ABSTRACT

The interaction of biological systems with synthetic materials, particularly through plasma protein adsorption, is important to understand. Human Serum Albumin (HSA), the main plasma protein (±60%, 66.5 kDa), plays a role in maintaining osmotic pressure and as a drug receptor. Polyurethane (PU), a polymer widely used in everyday life, is known to be potentially toxic and relevant in microplastic studies. PU can enter the body through the respiratory and digestive systems, potentially disrupting the structure and function of HSA. This study combines in-silico methods through Molecular Docking and Molecular Dynamic on various PU monomers and temperatures of 305–315 K and in-vitro through testing the concentration of dispersed PU at the same temperature using UV–Vis, fluorescence, and FTIR. The results show that the HSA...PU complex (2 and 5 monomers) forms a stable interaction with negative interaction energy and moderate–weak hydrogen bonds. The longer the PU chain and the higher the temperature, the lower the binding free energy (ΔG_{Bind}), accompanied by a decrease in the HSA helical structure. Fluorescence confirmed static quenching with spontaneous interactions dominated by electrostatic forces, consistent with ΔG_{Bind} and van't Hoff calculations. UV–Vis and FTIR analyses indicated changes in the secondary structure and microenvironment of HSA that could potentially disrupt its physiological function.

Keywords: Human Serum Albumin (HSA), Polyurethane (PU), Interactions, in-silico and in-vitro