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β-lactoglobulin as a platform for designing biologically active carriers – experimental and computational studies

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β-lactoglobulin (LGB) is known as one of the most interesting transport proteins. In particular, it can serve as a carrier for hydrophobic molecules, through the binding of potential ligands at the active site located in the β-barrel [1]. According to previous studies, the binding of ligands to LGB is strongly dependent on the pH of the solution due to the conformational changes of LGB known as the Tanford transition [2]. In the presented study, the interactions and binding behavior of anesthetic tetracaine (TET) to LGB were investigated under varying environmental conditions (pH, ionic strength, concentration, LGB-TET complex molar ratio). The Laser Doppler Velocimetry (LDV), the UV-Vis spectroscopy, and the Circular Dichroism (CD) were utilized to determine the physicochemical properties of LGB and LGB-TET complex in a sodium chloride solution. Electrophoretic mobility measurements showed that the zeta potential of the LGB became more positive upon interactions with TET due to electrostatic forces of the amino group present in the TET structure. The finding suggested the formation of LGB-TET complexes and the binding of ligand molecules on the protein surface. Based on UV-vis spectra the binding constant (K-UV) of the LGB-TET complex was calculated, while CD spectra showed that interactions with the ligand did not change the secondary structure of LGB molecules. Quartz Crystal Microbalance with Dissipation Monitoring (QCM-D) measurements presented that the molar ratio of LGB to TET is equal to 1:13 confirming the binding of TET not only to β-barrel but also on the LGB surface. What is more, QCM-D performed under varying environmental conditions allowed determining the optimized conditions for LGB-TET complex formation. Implementation of molecular docking enabled estimation of the binding position of the TET. The method suggested that interactions between the protein and ligand were possible with the most likely binding site with the hydrophobic cavity located in β-barrel [3].

References:

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