Abstract

The binding interactions between new Schiff base palladium(II) complex and two transporter proteins, human serum albumin (HSA) and β-lactoglobulin (βLG) were studied by spectroscopic and computational methods. Fluorescence spectroscopy results revealed the strong quenching of intrinsic fluorescence of both HSA and βLG due to interaction with Pd(II) complex by a static quenching mechanism. The Pd(II) complex interacted with studied proteins with moderate binding affinity (K_b = 1.01×10^4 M^{-1} for HSA and 6.60×10^3 M^{-1} for βLG at 303 K). The thermodynamic parameters revealed the contribution of hydrogen bond and Van der Waals interactions but, the role of hydrophobic interactions was not negligible due to imine group in structure of complex and obtained small positive ΔS° values in both systems. UV–Visible and FT-IR measurements indicated that the binding of Pd(II) complex to HSA and βLG may induce conformational and micro-environmental changes of these proteins. Moreover, a powerful chemometrics method, Multivariate Curve Resolution- Alternating Least Square (MCR-ALS), was used for resolution of measured complex spectra. The spectra of UV–Vis and fluorescence in two different titration modes were augmented in order to estimate the stoichiometry of interactions and spectral information regardless of spectral overlapping of components. The docking studies indicate the Pd(II) complex binds to residues located in the subdomain IB of HSA and site II of βLG.

Keyword: Pd(II) complex, β-lactoglobulin, Human serum albumin, ADMET, Molecular docking, MCR-ALS.

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