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In the field of inorganic Chemistry

A comparative study between two new Schiff base complexes. Synthesis, characterization, antioxidant activity and interaction with human serum albumin

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Abstract:

New Schiff base ligand N′- (3-(hydroxyimino) butan-2-ylidene) benzohydrazide (HIBYB);and its Zn(II) and Pd(II) complexes $[Zn(HIBYB)_2]Cl_2$ (A) and $[Pd(HIBYB)_2]Cl_2$ (B) were synthesized and characterized using elemental analysis (CHN) and spectroscopic methods including FT-IR, ^{1}HNMR, UV-Vis and TG. The antioxidant properties of the complexes and Schiff base ligand were investigated with the help of DPPH free radical and showed that complex B has more ability to inhibit the free radical. The interaction study of above complexes with human serum albumin (HSA) was done with the help of spectroscopic methods as well as molecular docking. Quenching of fluorescence by A and B was done through static mechanism. Binding constants (K_b) of complexes A and B with HSA at 310 K was, $2.69\times10^4 M^{-1}$ and $7.05\times10^4 M^{-1}$ respectively. During the interaction of complexes with HSA, the most important forces involved, were van der Waals interactions and hydrogen bonds. Considering that the quenching rate of tryptophan (Trp) was higher than that of tyrosine (Tyr), it can be concluded that Trp is closer to the Schiff complexes interaction sites than Tyr. Analysis of the CD spectra showed a decrease in the amount of α-helix and thus a decrease in protein stability in the presence of complexes. Molecular docking was used to predict that the Schiff base complexes are able to bind with HSA and to identify specific residues.

Keywords:

Schiff Base complexes, Human Serum Albumin, Antioxidant, Molecular Docking