Electronic Supplementary Material (ESI) for Dalton Transactions

Supplementary material for

Effect of substitution and planarity of the ligand on DNA/BSA interaction, free radical scavenging and cytotoxicity of diamagnetic Ni(II) complexes: A systematic investigation

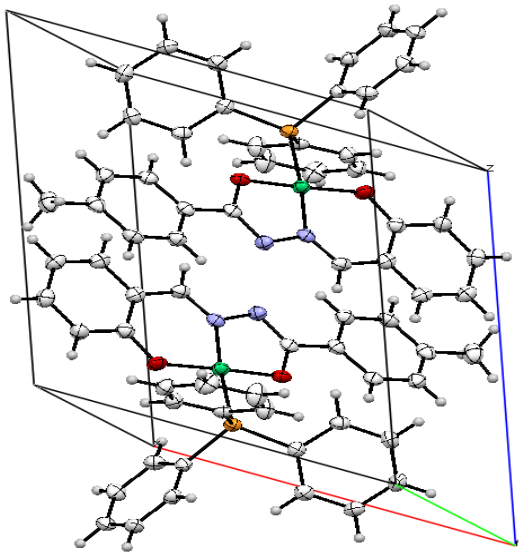

Figure S1. Packing diagram for the unit cell of complex **5**.

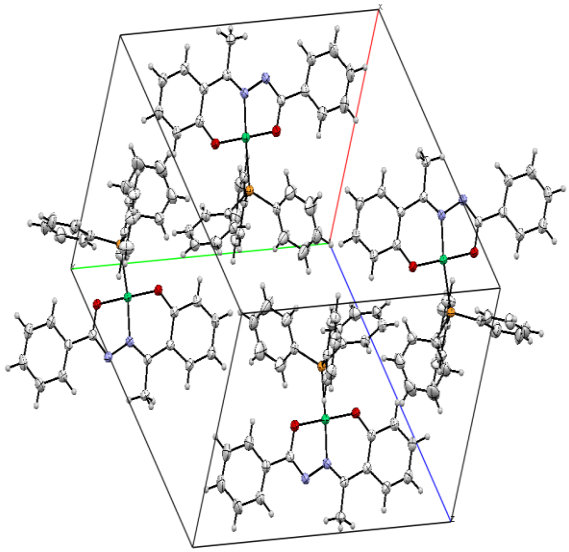

Figure S2. Packing diagram for the unit cell of complex **7**.

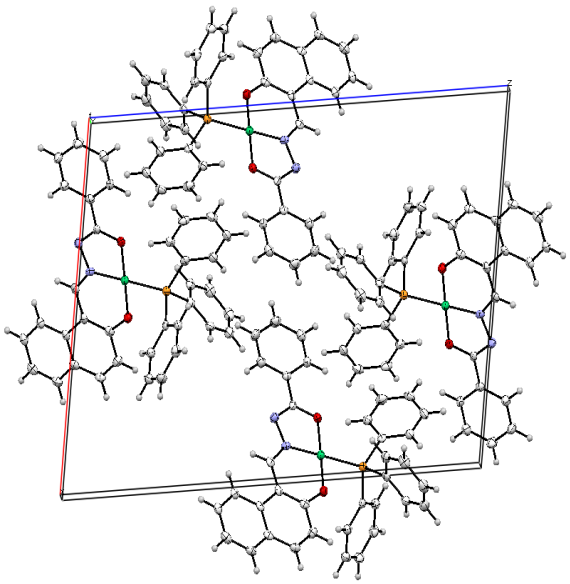

Figure S3. Packing diagram for the unit cell of complex **8**.

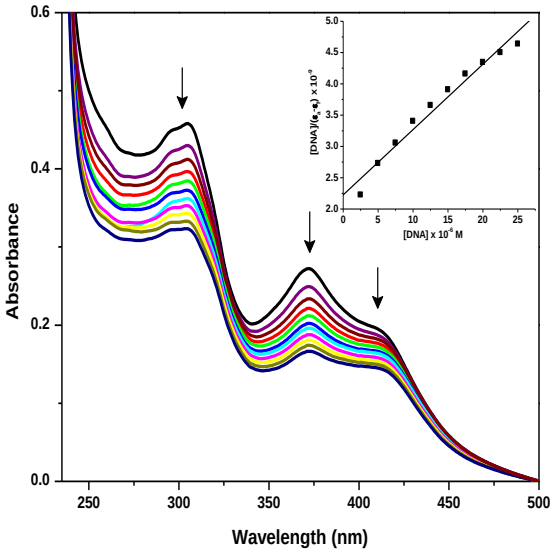

Figure S4. Electronic absorption spectra of complex **5** (25 μM) in the absence and presence of increasing amounts of CT DNA (2.5, 5.0, 7.5, 10.0, 12.5, 15.0, 17.5 and 20.0, 22.5 and 25 μM). Arrows show the changes in absorbance with respect to an increase in the DNA concentration (Inset: Plot of [DNA] vs [DNA]/(ε_a- ε_f)).

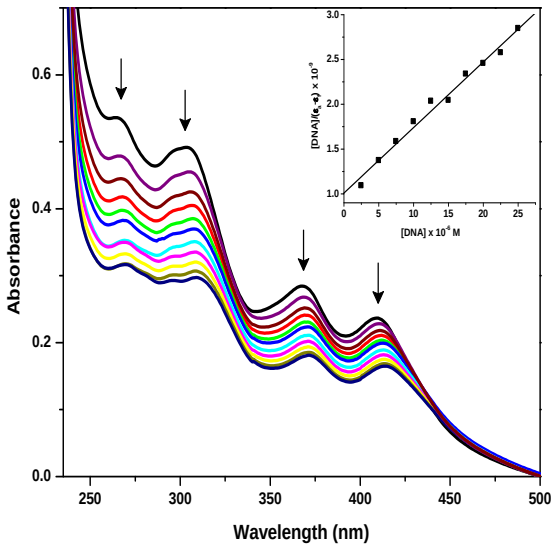

Figure S5. Electronic absorption spectra of complex **6** (25 μM) in the absence and presence of increasing amounts of CT DNA (2.5, 5.0, 7.5, 10.0, 12.5, 15.0, 17.5 and 20.0, 22.5 and 25 μM). Arrows show the changes in absorbance with respect to an increase in the DNA concentration (Inset: Plot of [DNA] vs [DNA]/(ε_a- ε_f)).

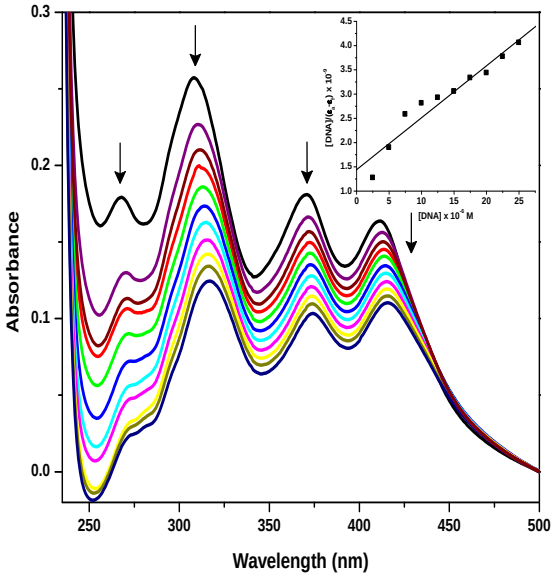

Figure S6. Electronic absorption spectra of complex **7** (25 μM) in the absence and presence of increasing amounts of CT DNA (2.5, 5.0, 7.5, 10.0, 12.5, 15.0, 17.5 and 20.0, 22.5 and 25 μM). Arrows show the changes in absorbance with respect to an increase in the DNA concentration (Inset: Plot of [DNA] vs [DNA]/(ε_a- ε_f)).

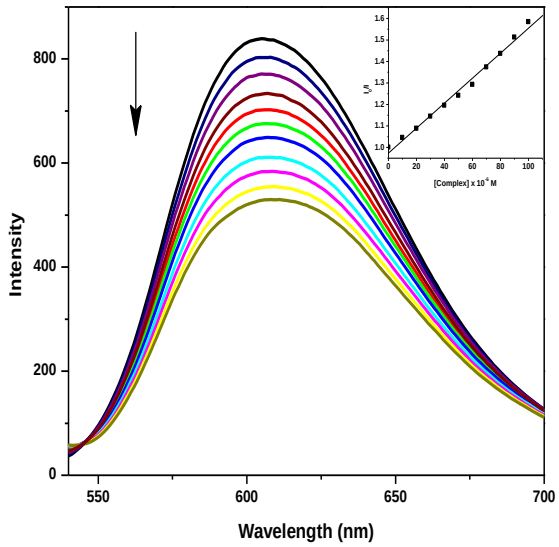

Figure S7. Emission spectra of DNA-EB (10 µM), in the presence of 0, 10, 20, 30, 40, 50, 60, 70, 80, 90 and 100 µM of complex **5**. Arrow indicates the changes in the emission intensity as a function of complex concentration. Inset: Stern-Volmer plot of the fluorescence titration data corresponding to the complex **5**.

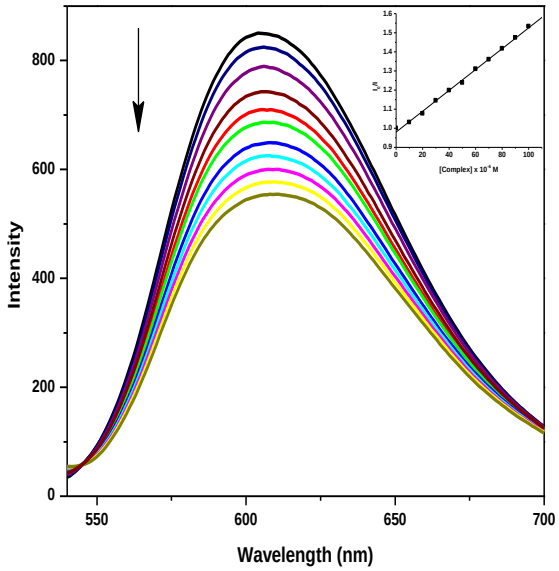

Figure S8. Emission spectra of DNA-EB (10 µM), in the presence of 0, 10, 20, 30, 40, 50, 60, 70, 80, 90 and 100 µM of complex **6**. Arrow indicates the changes in the emission intensity as a function of complex concentration. Inset: Stern-Volmer plot of the fluorescence titration data corresponding to the complex **6**.

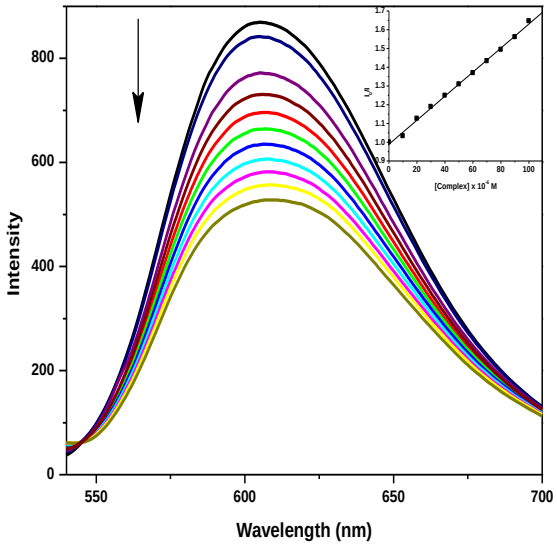

Figure S9. Emission spectra of DNA-EB (10 µM), in the presence of 0, 10, 20, 30, 40, 50, 60, 70, 80, 90 and 100 µM of complex **7**. Arrow indicates the changes in the emission intensity as a function of complex concentration. Inset: Stern-Volmer plot of the fluorescence titration data corresponding to the complex **7**.

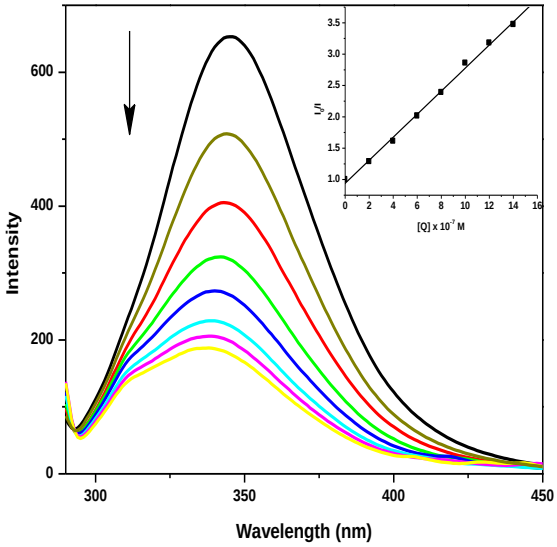

Figure S10. Emission spectrum of BSA (1 x 10^{-6} M; λ_{exi} = 280 nm; λ_{emi} = 345 nm) as a function of concentration of the complex **5** (0, 2, 4, 6, 8, 10, 12 and 14 x 10^{-7} M). Arrow indicates the effect of metal complex **5** on the fluorescence emission of BSA.

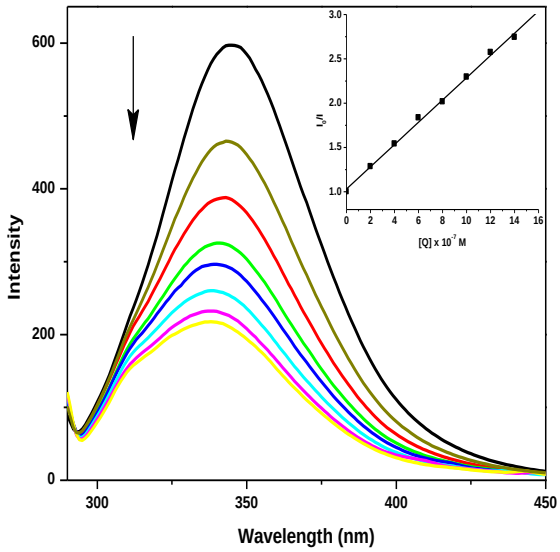

Figure S11. Emission spectrum of BSA (1 x 10^{-6} M; λ_{exi} = 280 nm; λ_{emi} = 345 nm) as a function of concentration of the complex **6** (0, 2, 4, 6, 8, 10, 12 and 14 x 10^{-7} M). Arrow indicates the effect of metal complex **6** on the fluorescence emission of BSA**.**

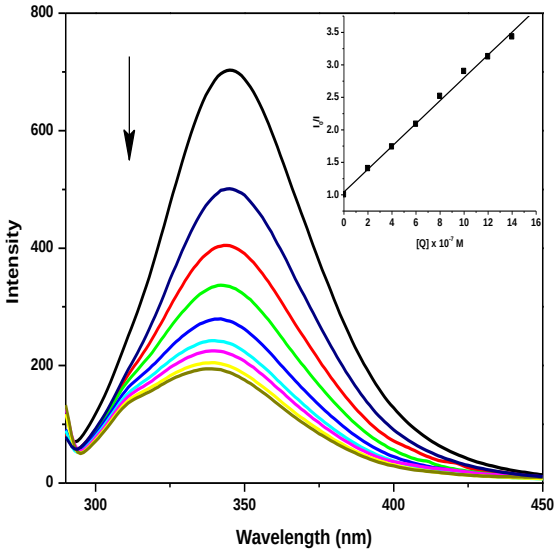

Figure S12. Emission spectrum of BSA (1 x 10^{-6} M; λ_{exi} = 280 nm; λ_{emi} = 345 nm) as a function of concentration of the complex **7** (0, 2, 4, 6, 8, 10, 12 and 14 x 10^{-7} M). Arrow indicates the effect of metal complex **7** on the fluorescence emission of BSA**.**

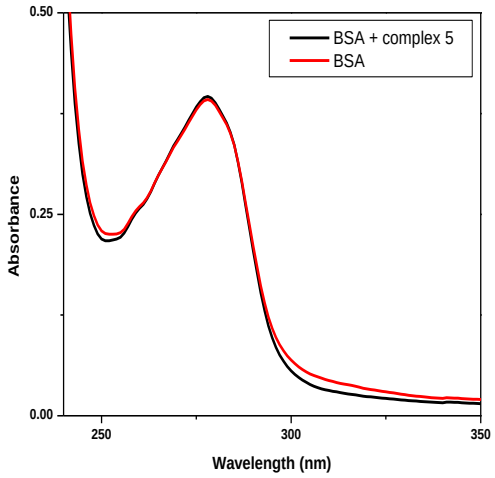

Figure S13. The absorption spectra of BSA (1 x 10^{-5} M) and BSA-Complex **5** (BSA= 1 x 10^{-5} M and Complex **5** = 1 x 10^{-6} M).

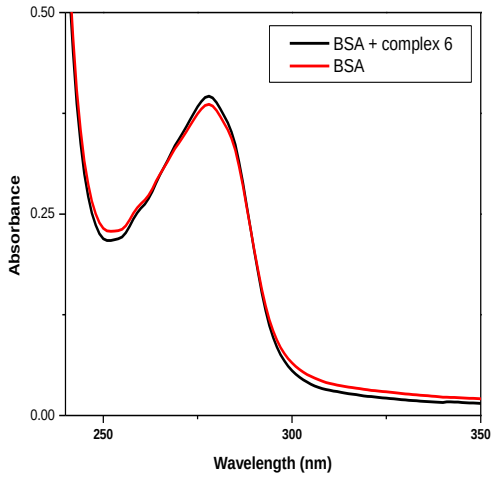

Figure S14. The absorption spectra of BSA (1 x 10^{-5} M) and BSA-Complex **6** (BSA= 1 x 10^{-5} M and Complex **6** = 1 x 10^{-6} M).

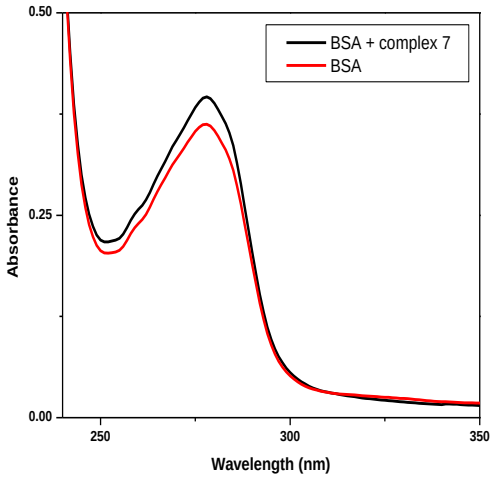

Figure S15. The absorption spectra of BSA (1 x 10^{-5} M) and BSA-Complex **7** (BSA= 1 x 10^{-5} M and Complex **7** = 1 x 10^{-6} M).

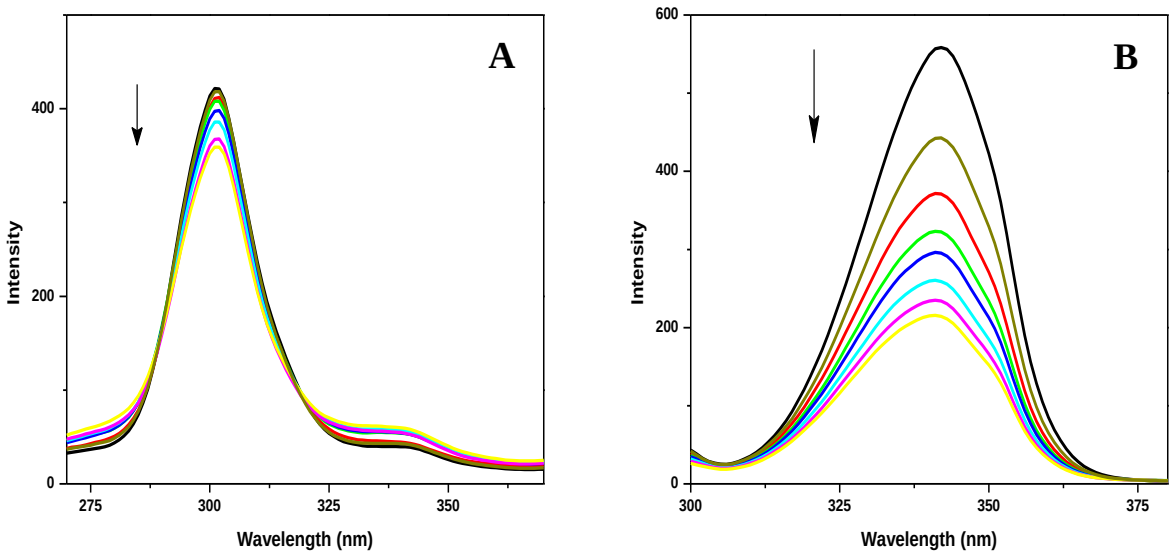

Figure S16. Synchronous spectra of BSA (1 x 10^{-6} M) as a function of concentration concentration of the complex **5** (0, 2, 4, 6, 8, 10, 12 and 14 x 10^{-7} M) with wavelength difference of $\Delta\lambda$ = 15 nm (A) and $\Delta\lambda$ = 60 nm (B). Arrow indicates the decrease in emission intensity accompanied by hypsochromic shift (B) w.r.t various concentration of complex **5**.

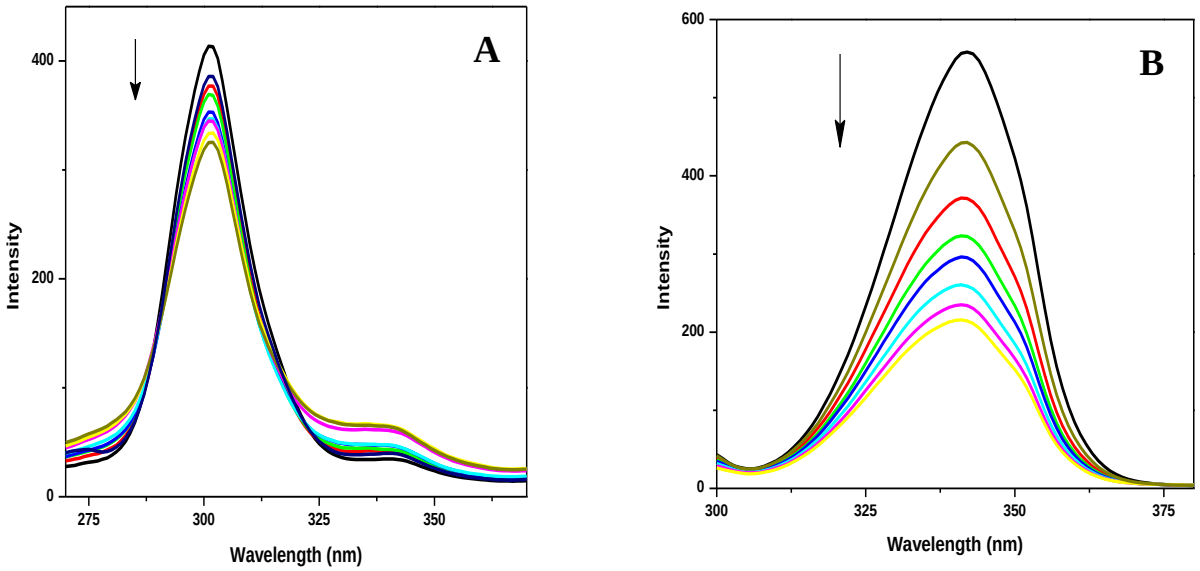

Figure S17. Synchronous spectra of BSA (1 x 10^{-6} M) as a function of concentration concentration of the complex **6** (0, 2, 4, 6, 8, 10, 12 and 14 x 10^{-7} M) with wavelength difference of $\Delta\lambda$ = 15 nm (A) and $\Delta\lambda$ = 60 nm (B). Arrow indicates the decrease in emission intensity accompanied by hypsochromic shift (B) w.r.t various concentration of complex **6**.

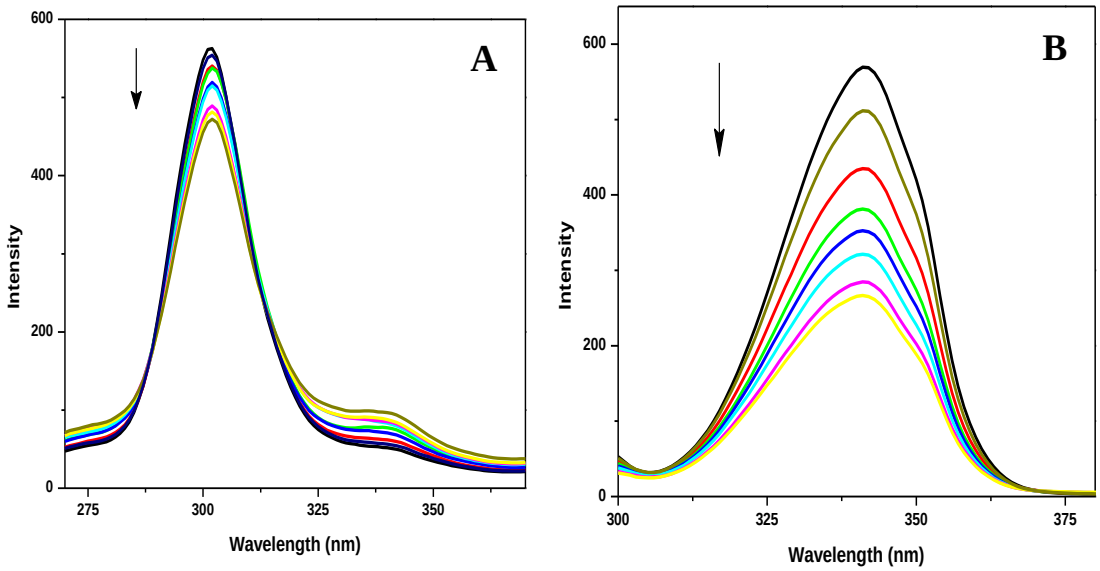

Figure S18. Synchronous spectra of BSA (1 x 10^{-6} M) as a function of concentration concentration of the complex **7** (0, 2, 4, 6, 8, 10, 12 and 14 x 10^{-7} M) with wavelength difference of $\Delta\lambda$ = 15 nm (A) and $\Delta\lambda$ = 60 nm (B). Arrow indicates the decrease in emission intensity accompanied by hypsochromic shift (B) w.r.t various concentration of complex **7**.