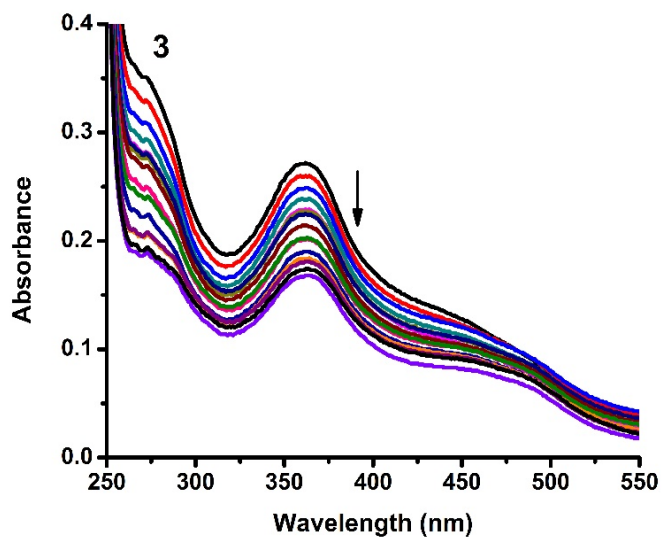
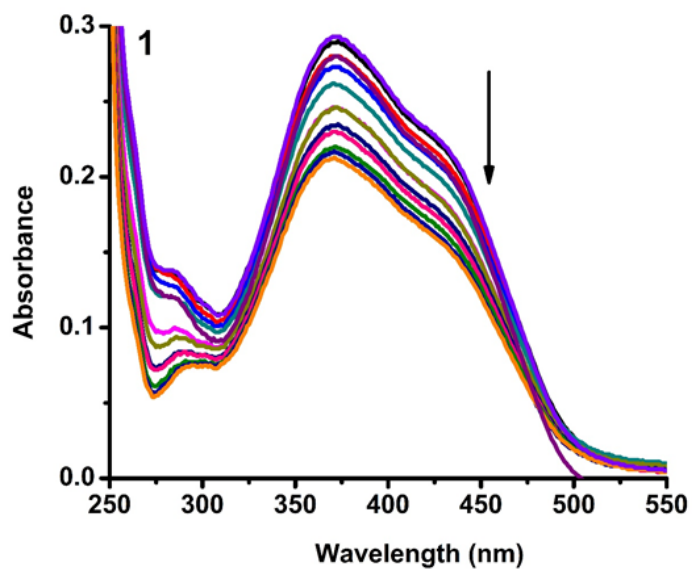


Synthesis, DNA/protein binding, molecular docking, DNA cleavage and *in vitro* anticancer activity of nickel(II) bis(thiosemicarbazone) complexes

Jebiti Haribabu, Kumaramangalam Jeyalakshmi, Yuvaraj Arun, Nattamai S. P. Bhuvanesh,
Paramasivan Thirumalai Perumal, and Ramasamy Karvembu

Supplementary Information



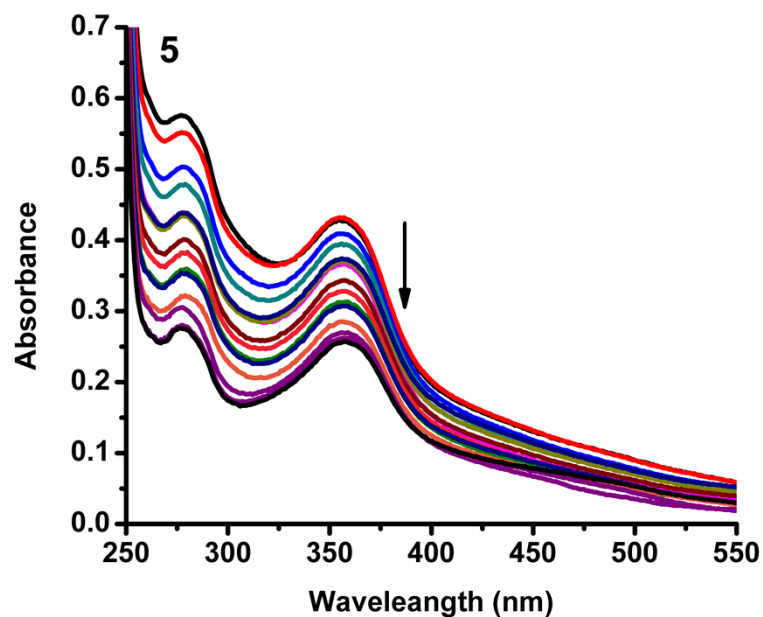
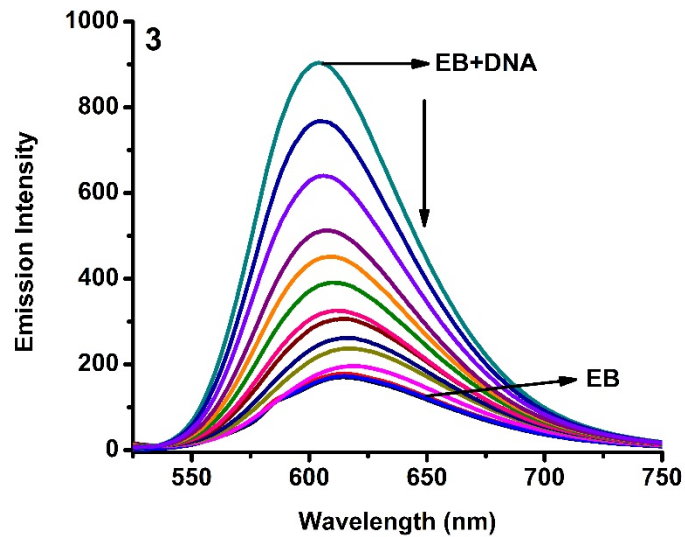
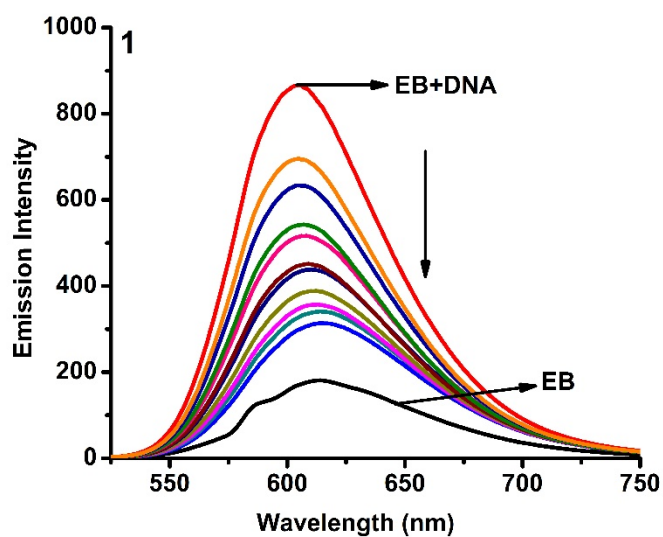


Fig. S1 Absorption spectra of complexes **1**, **3** and **5** in Tris-HCl buffer upon addition of CT DNA. [Complex] = 1.5×10^{-5} M, [DNA] = 0-50 μ M. Arrow shows that the absorption intensities decrease upon increasing DNA concentration.



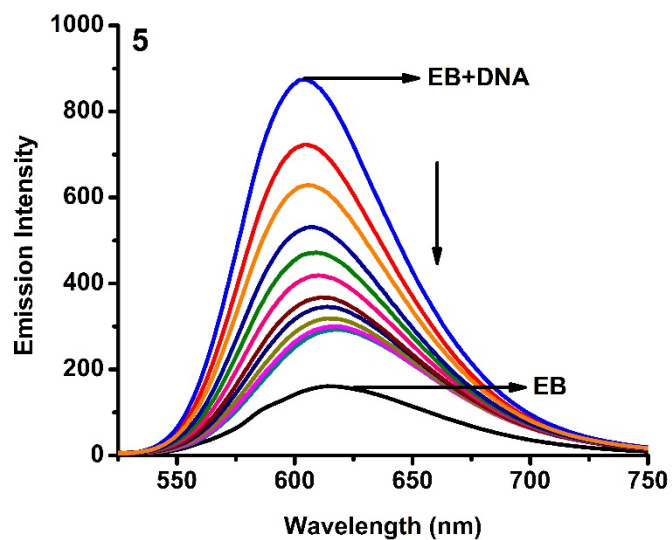


Fig. S2 Fluorescence quenching curves of EB bound to DNA in the presence of **1**, **3** and **5**. [DNA] = 5 μ M, [EB] = 5 μ M and [complex] = 0-50 μ M.

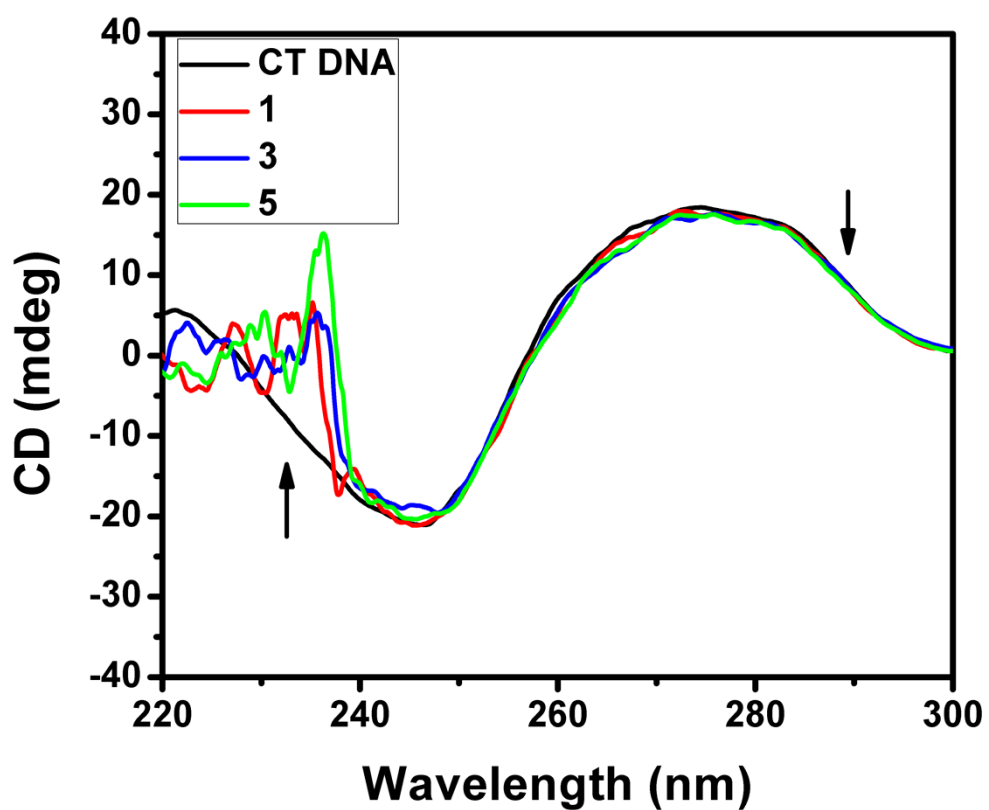


Fig. 3 CD spectra of CT DNA (200 μ M) in the absence and presence of 40 μ M of complexes **1**, **3** and **5**.

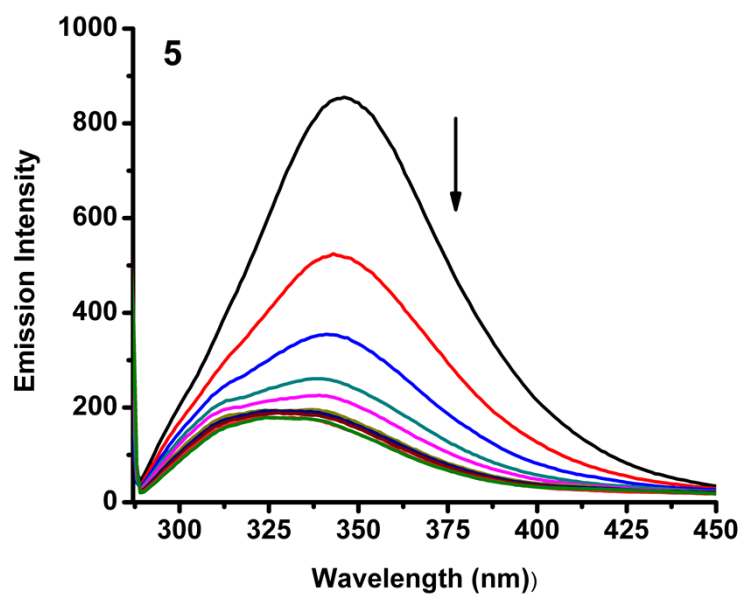
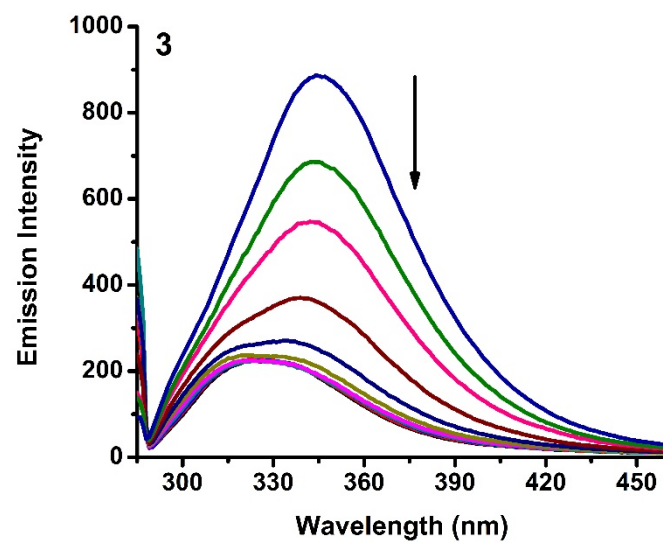
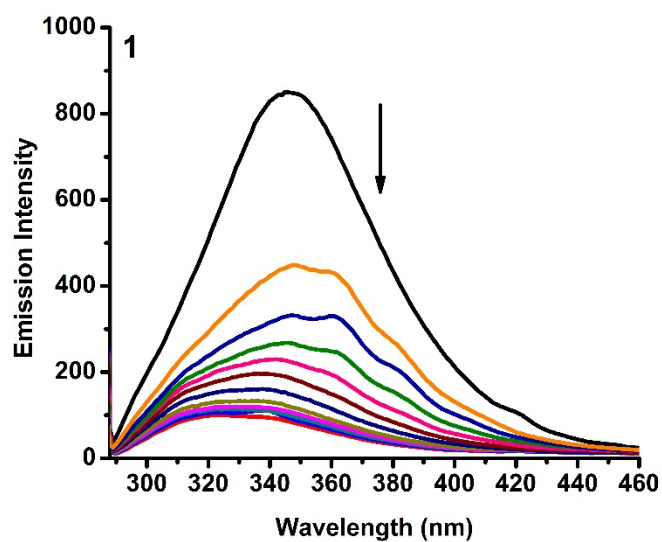


Fig. S4 Fluorescence quenching curves of BSA in the absence and presence of **1**, **3** and **5**. [BSA] = 1 μ M and [complex] = 0-50 μ M.

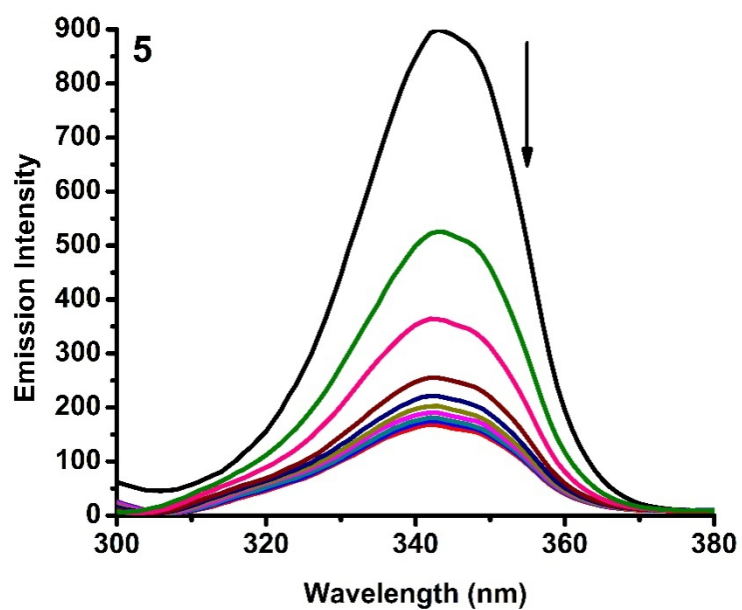
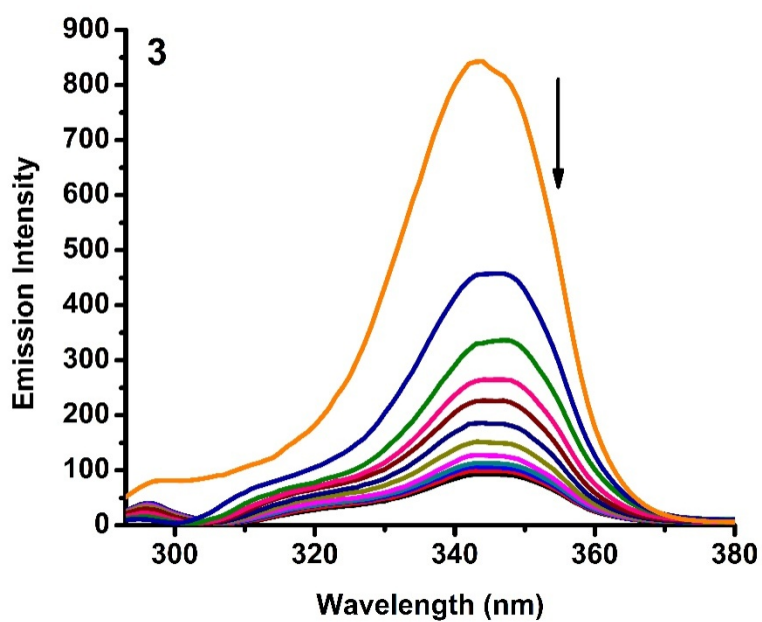
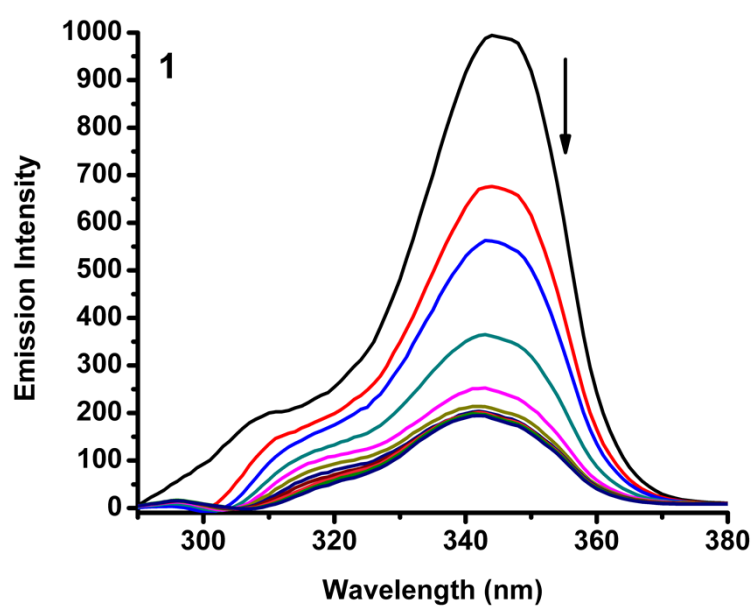


Fig. S5 Synchronous spectra of BSA (1 μM) as a function of concentration of **1**, **3** and **5** (0-50 μM) with $\Delta\lambda = 60$ nm.

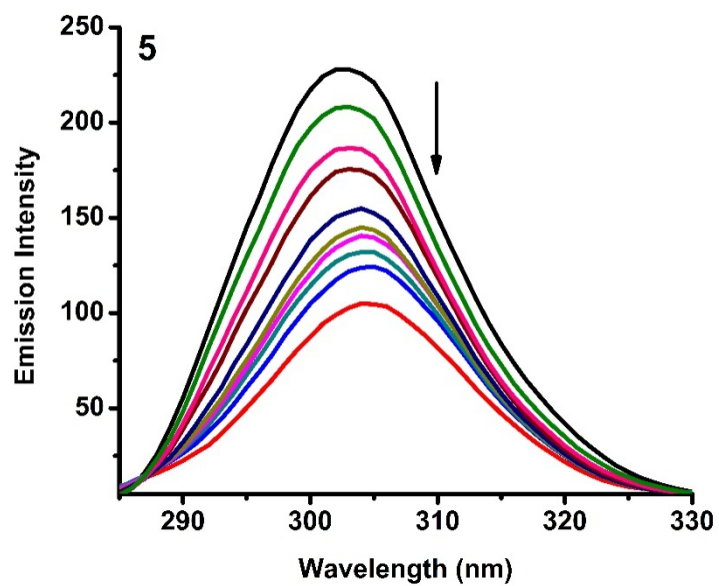
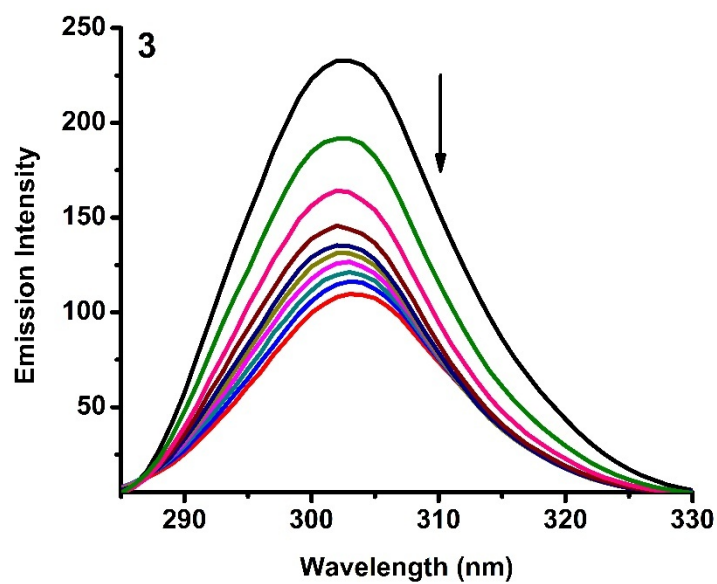
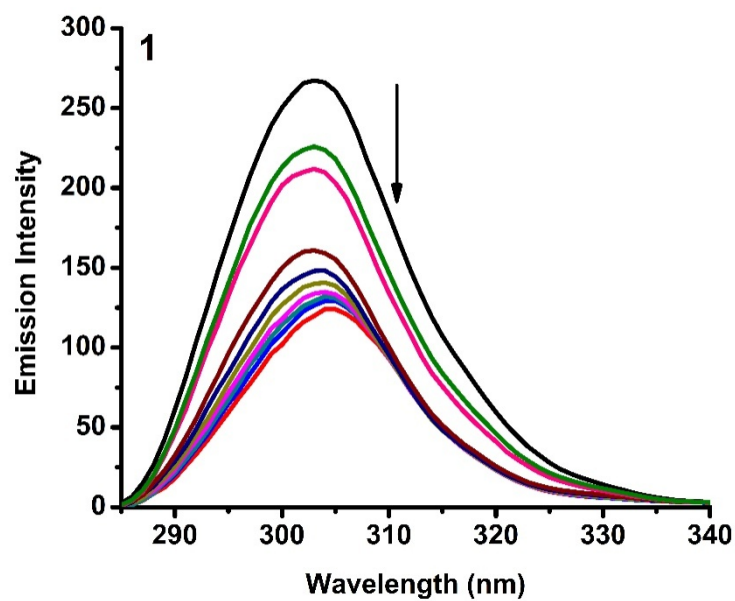
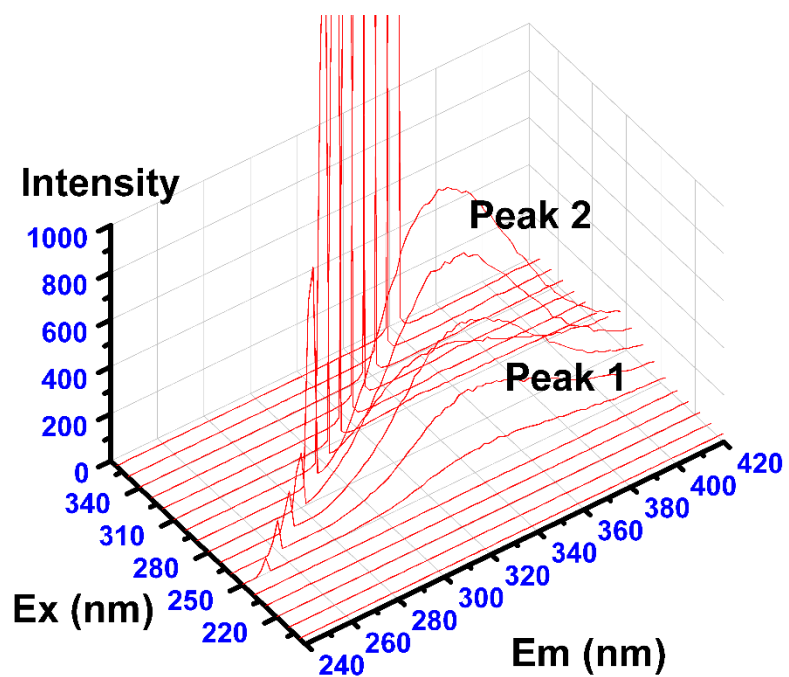
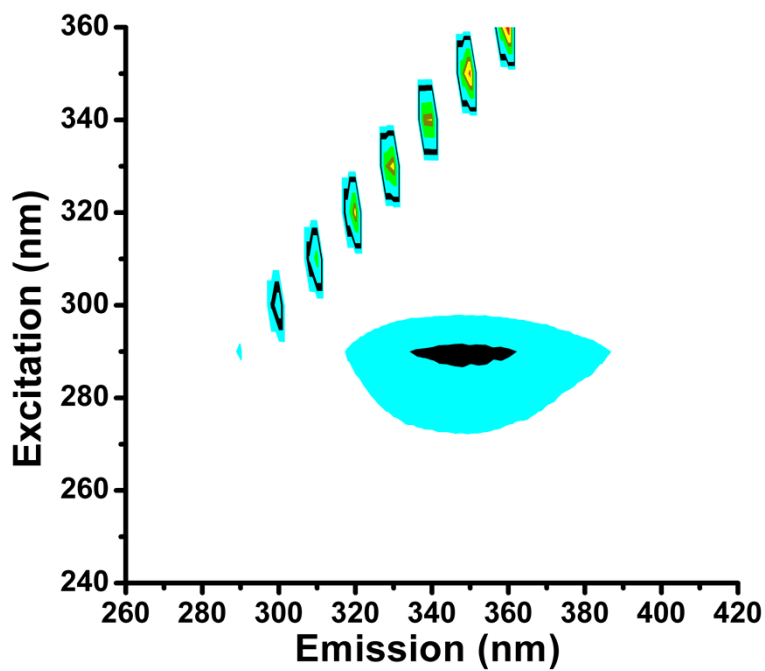
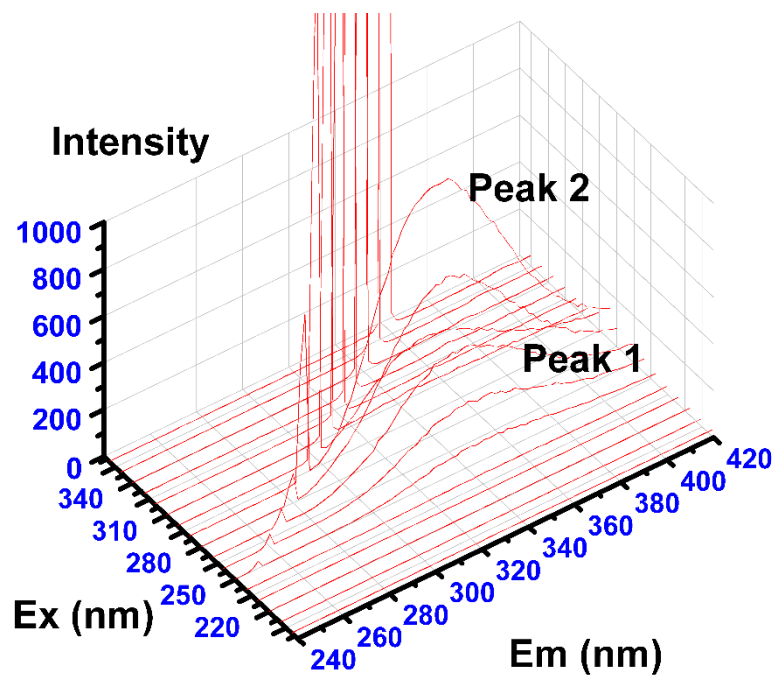
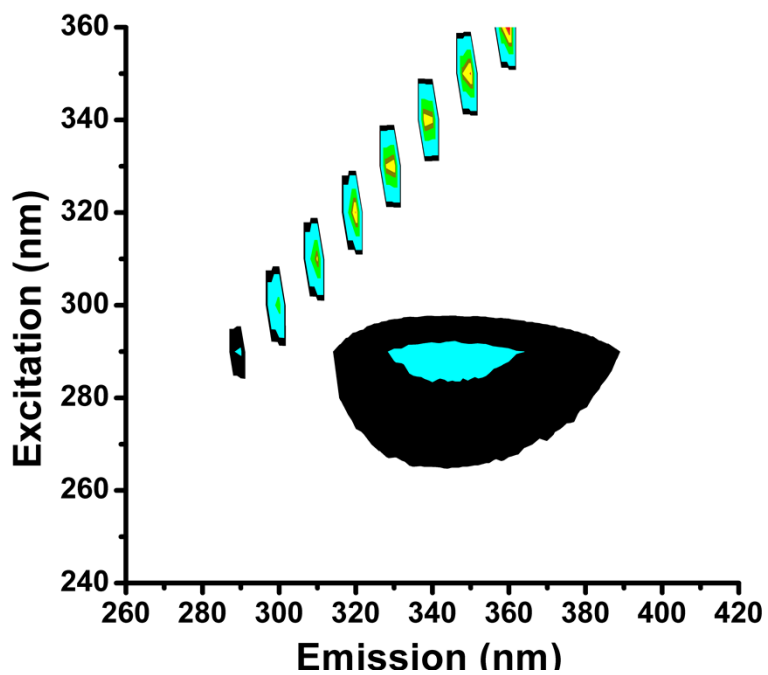


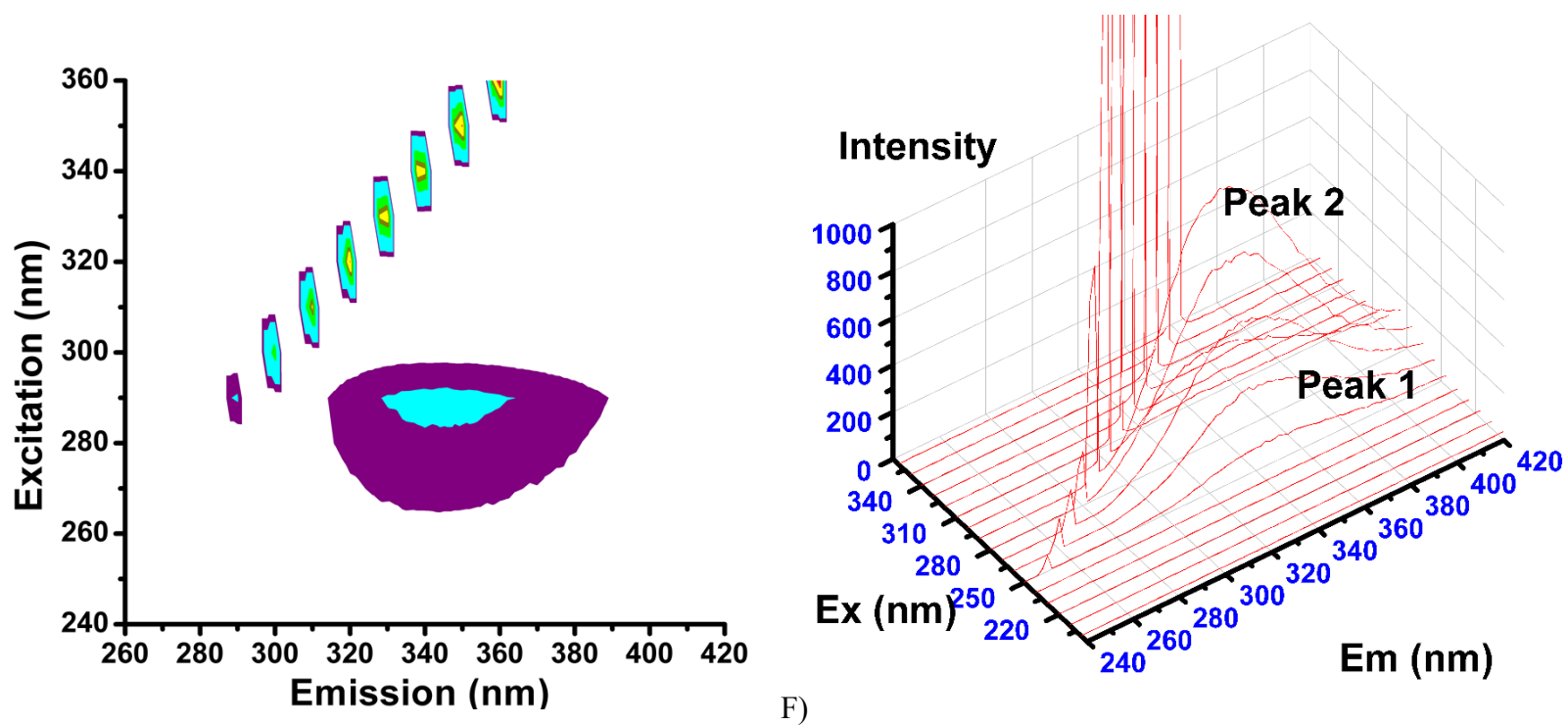
Fig. S6 Synchronous spectra of BSA (1 μM) as a function of concentration of **1**, **3** and **5** (0-50 μM) with $\Delta\lambda = 15$ nm.



D)

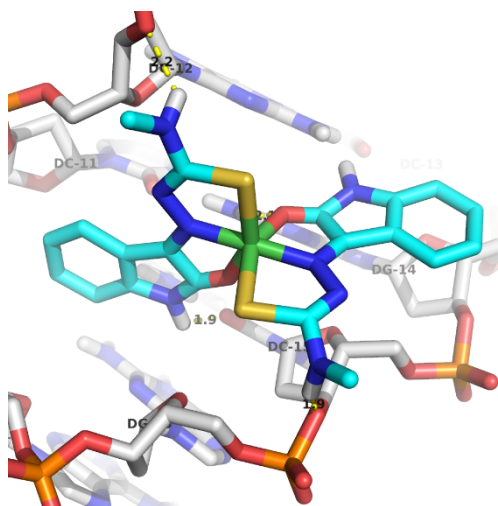
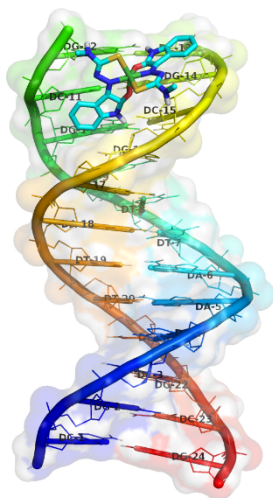


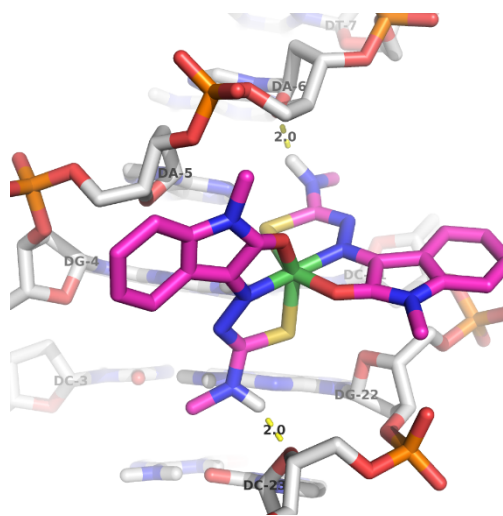
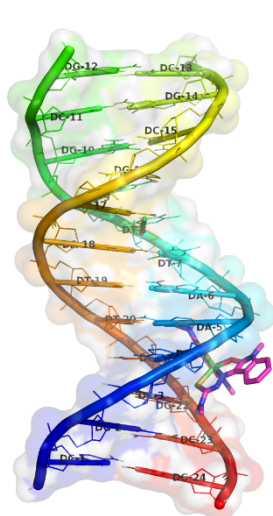
E)



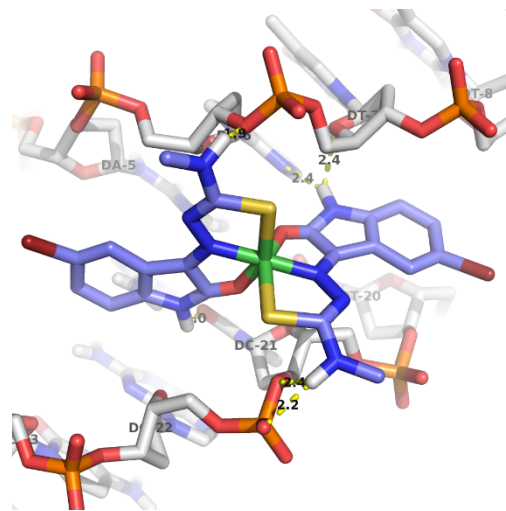
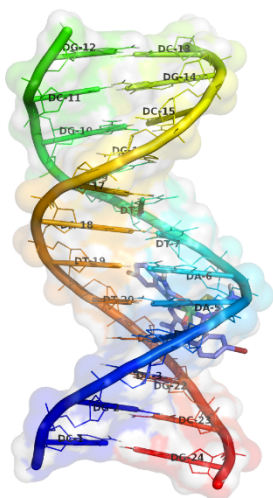
F)

Fig. S7 Three dimensional fluorescence spectra of D) BSA-1, E) BSA-3 and F) BSA-5



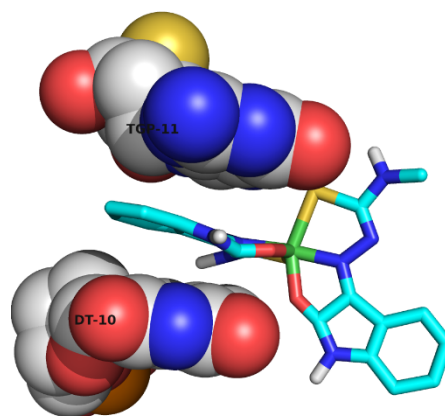
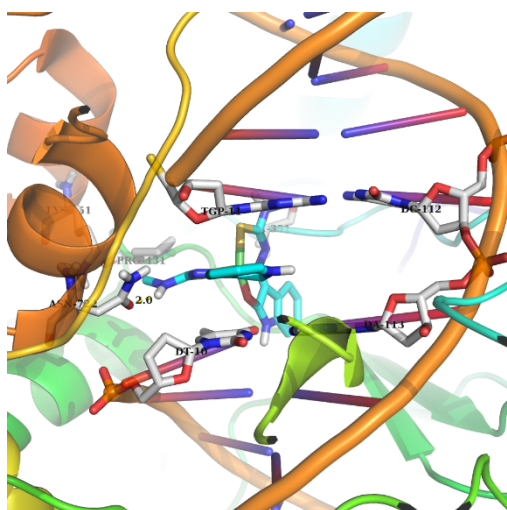


3

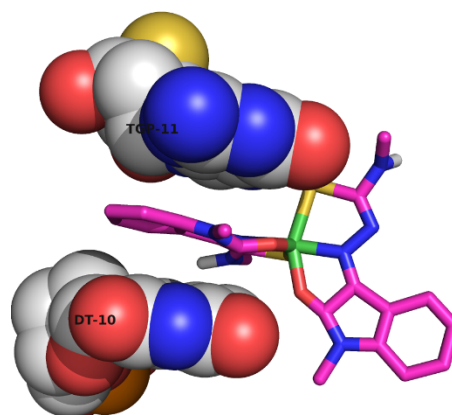
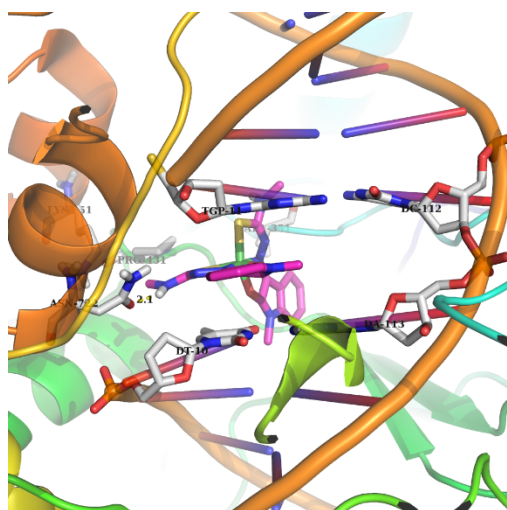


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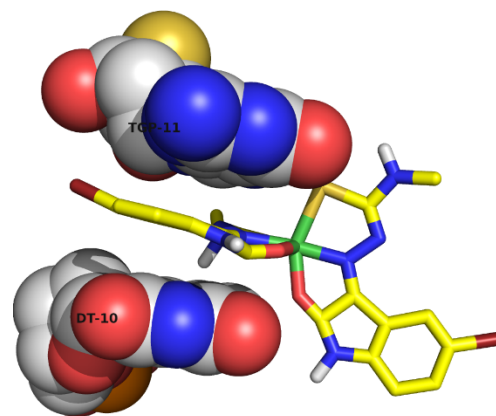
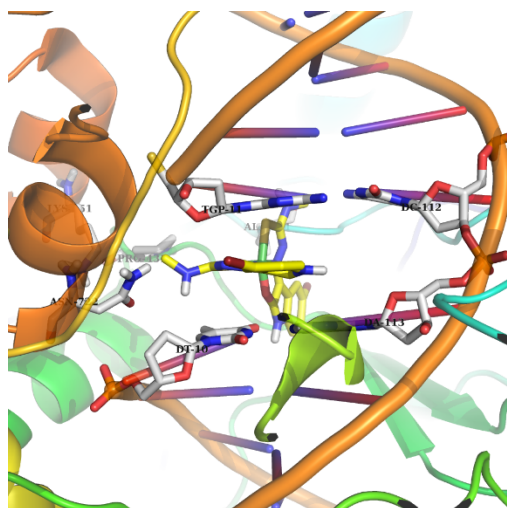
Fig. S8 Docking pose of nickel complexes **1**, **3** and **5** with B-DNA (1BNA).



1

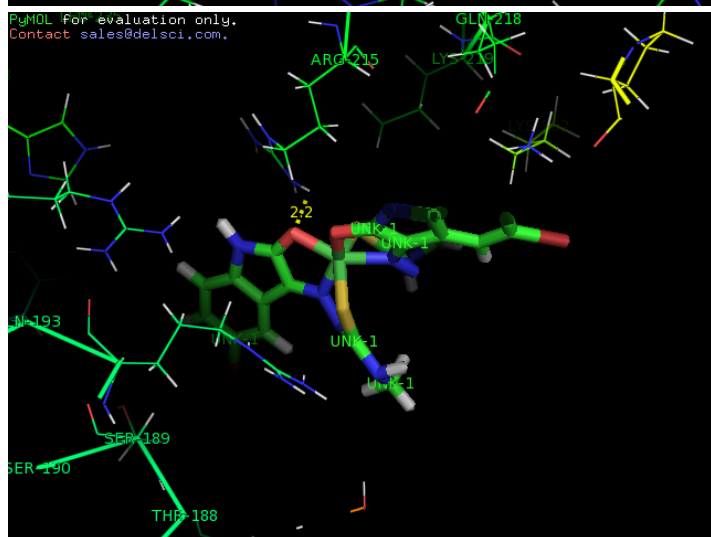
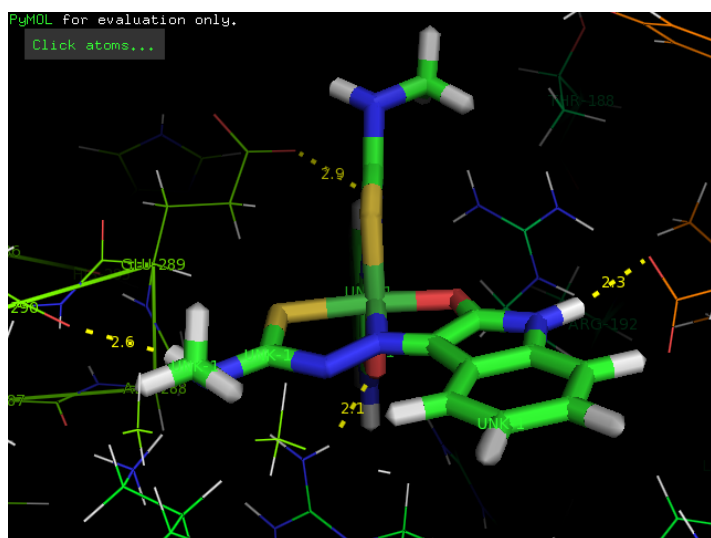


3



5

Fig. S9 Docking pose of nickel complexes **1**, **3** and **5** with DNA-Topoisomerase I (1SC7).



5

Fig. S10 Docking pose of nickel complexes **1**, **3** and **5** with protein (3V03).