## Supplementary material for

## Variation in the biomolecular interactions of nickel(II) hydrazone complexes upon tuning the hydrazide fragment

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Figures



Figure S1. Unit cell packing diagram of the complex 4.



Figure S2. Unit cell packing diagram of the complex 5.



**Figure S3.** Electronic absorption spectra of ligands **1-3** (25  $\mu$ M) 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  $\mu$ M). Arrows show the changes in absorbance as a function of increasing DNA concentration (Inset: Plot of [DNA] vs [DNA]/( $\epsilon_a$ - $\epsilon_f$ )).



**Figure S4.** Electronic absorption spectra of complexes **4** and **5** (25  $\mu$ M) 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  $\mu$ M). Arrows show the changes in absorbance as a function of increasing DNA concentration (Inset: Plot of [DNA] vs [DNA]/( $\epsilon_a$ - $\epsilon_f$ )).



**Figure S5.** Emission spectra of DNA-EB, in the presence of 0, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 110, 120, 130,140 and 150  $\mu$ M of ligands 1-3. Arrow indicates the change in the emission intensity as a function of ligand concentration (Inset: Stern-Volmer plot of the fluorescence titration data corresponding to the ligands).



**Figure S6.** Emission spectra of DNA-EB, in the presence of 0, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 110, 120, 130,140 and 150  $\mu$ M of complexes 4 and 5. Arrow indicates the change in the emission intensity as a function of complex concentration (Inset: Stern-Volmer plot of the fluorescence titration data corresponding to the complex).



**Figure S7**. Emission spectra of BSA ( $1 \times 10^{-6}$  M;  $\lambda_{exi} = 280$  nm;  $\lambda_{emi} = 345$  nm) as a function of concentration of the ligands **1-3** (0, 2, 4, 6, 8, 10, 12 and  $14 \times 10^{-7}$  M). Arrow indicates the effect of the ligands on the fluorescence emission of BSA (Inset: Plot between [Q] and I<sub>0</sub>/I).



**Figure S8**. Emission spectra of BSA ( $1 \times 10^{-6}$  M;  $\lambda_{exi} = 280$  nm;  $\lambda_{emi} = 345$  nm) as a function of concentration of the complexes **4** and **5** (0, 2, 4, 6, 8, 10, 12 and  $14 \times 10^{-7}$  M). Arrow indicates the effect of metal complexes **4** and **5** on the fluorescence emission of BSA (Inset: Plot between [Q] and I<sub>0</sub>/I).



**Figure S9.** Synchronous spectra of BSA  $(1 \times 10^{-6} \text{ M})$  as a function of concentration of the ligands **1-3** (0, 2, 4, 6, 8, 10, 12 and  $14 \times 10^{-7} \text{ M}$ ) with wavelength difference of  $\Delta \lambda = 15$  nm (a) and  $\Delta \lambda = 60$  nm (b). Arrow indicates the change in emission intensity w.r.t various concentration of the ligands.



**Figure S10.** Synchronous spectra of BSA  $(1 \times 10^{-6} \text{ M})$  as a function of concentration of the complexes **4** and **5** (0, 2, 4, 6, 8, 10, 12 and  $14 \times 10^{-7} \text{ M}$ ) with wavelength difference of  $\Delta \lambda = 15 \text{ nm}$  (a) and  $\Delta \lambda = 60 \text{ nm}$  (b). Arrow indicates the change in emission intensity w.r.t various concentration of the complexes.



**Figure S11**. % Cell inhibition of NIH 3T3, HeLa, HepG-2 and A431 cell lines as a function of concentration of nickel hydrazones **4**, **5** and **6**.