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 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 as a function of increasing DNA concentration (Inset: Plot of [DNA] vs [DNA]/(ε<sub>a</sub>-ε<sub>f</sub>)).
Figure S4. Electronic absorption spectra of complexes 4 and 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 as a function of increasing DNA concentration (Inset: Plot of [DNA] vs [DNA]/(ε_a-ε_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 µM 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 µM 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 (1×10⁻⁶ M; λ<sub>exi</sub> = 280 nm; λ<sub>emi</sub> = 345 nm) as a function of concentration of the ligands 1-3 (0, 2, 4, 6, 8, 10, 12 and 14×10⁻⁷ M). Arrow indicates the effect of the ligands on the fluorescence emission of BSA (Inset: Plot between [Q] and I₀/I).
Figure S8. Emission spectra of BSA (1×10^{-6} M; \(\lambda_{\text{exi}} = 280\) nm; \(\lambda_{\text{emi}} = 345\) nm) as a function of concentration of the complexes 4 and 5 (0, 2, 4, 6, 8, 10, 12 and 14×10^{-7} M). Arrow indicates the effect of metal complexes 4 and 5 on the fluorescence emission of BSA (Inset: Plot between [Q] and \(I_0/I\)).
Figure S9. Synchronous spectra of BSA (1×10⁻⁶ M) as a function of concentration of the ligands 1-3 (0, 2, 4, 6, 8, 10, 12 and 14×10⁻⁷ M) with wavelength difference of Δλ = 15 nm (a) and Δλ = 60 nm (b). Arrow indicates the change in emission intensity w.r.t various concentration of the ligands.
**Figure S10.** Synchronous spectra of BSA (1×10⁻⁶ M) as a function of concentration of the complexes 4 and 5 (0, 2, 4, 6, 8, 10, 12 and 14×10⁻⁷ M) with wavelength difference of Δλ = 15 nm (a) and Δλ = 60 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.