

## **Supporting Information**

### **Evaluation on the role of terminal *N*-substitution in 6-methoxy-2-oxo-1,2-dihydroquinoline-3-carbaldehyde thiosemicarbazones on the biological properties of new water soluble nickel(II) complexes**

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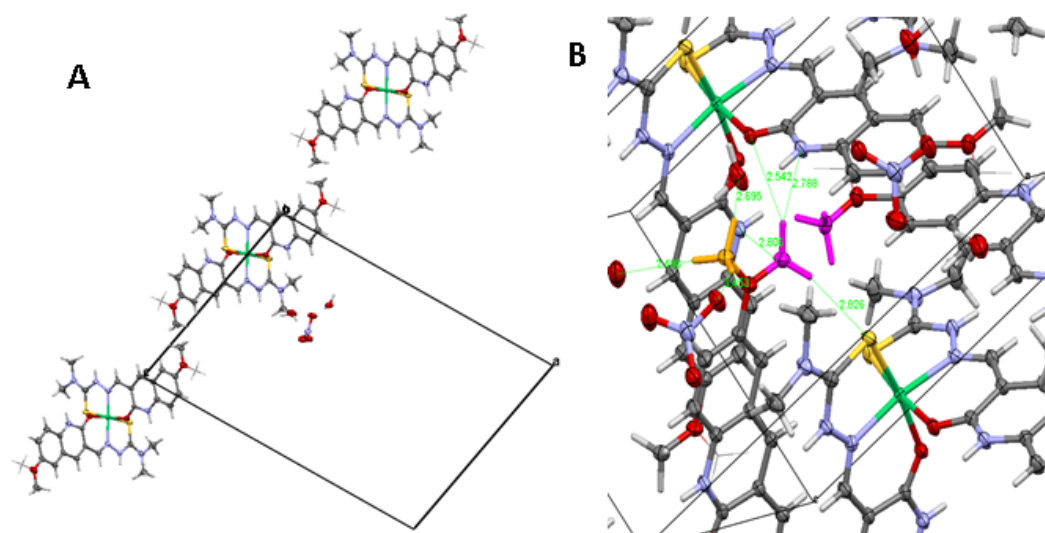


Figure S1: Depiction of the disorder present for the terminal methoxy groups. A: Three molecules arranged to show the steric interaction of methyl groups along the direction of the b-axis between neighbouring molecules. One of the methyl group positions (the one that avoids the steric interaction) is shown in wireframe view. B: close up view of steric interactions of both alternative methyl group positions (in pink and orange). C---H...O C---H...N and C---H...S interactions with neighboring groups are shown as dashed green lines with distances given in Ångstrom.

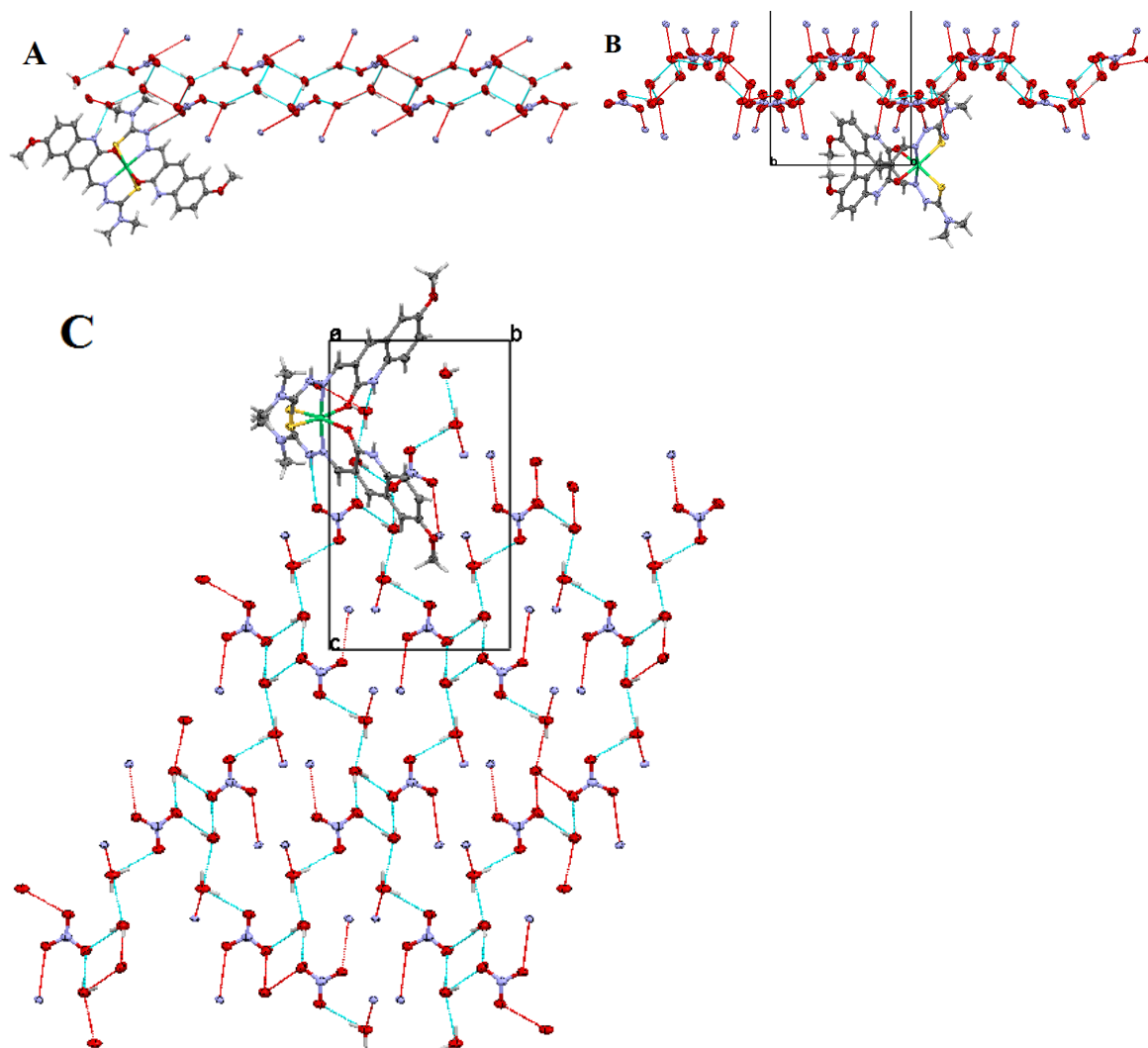


Figure S2: Hydrogen bonding interactions and formation of wave-like layers of water molecules and nitrate anions. (A) Down the b-axis, notice the regular ring pattern. Every disconnected nitrogen atom corresponds to a ligand molecule. (B) Down the c-axis, notice the alternating, wavy pattern. (C) Down the a-axis showing an entire aqueous layer connected by hydrogen bonds.

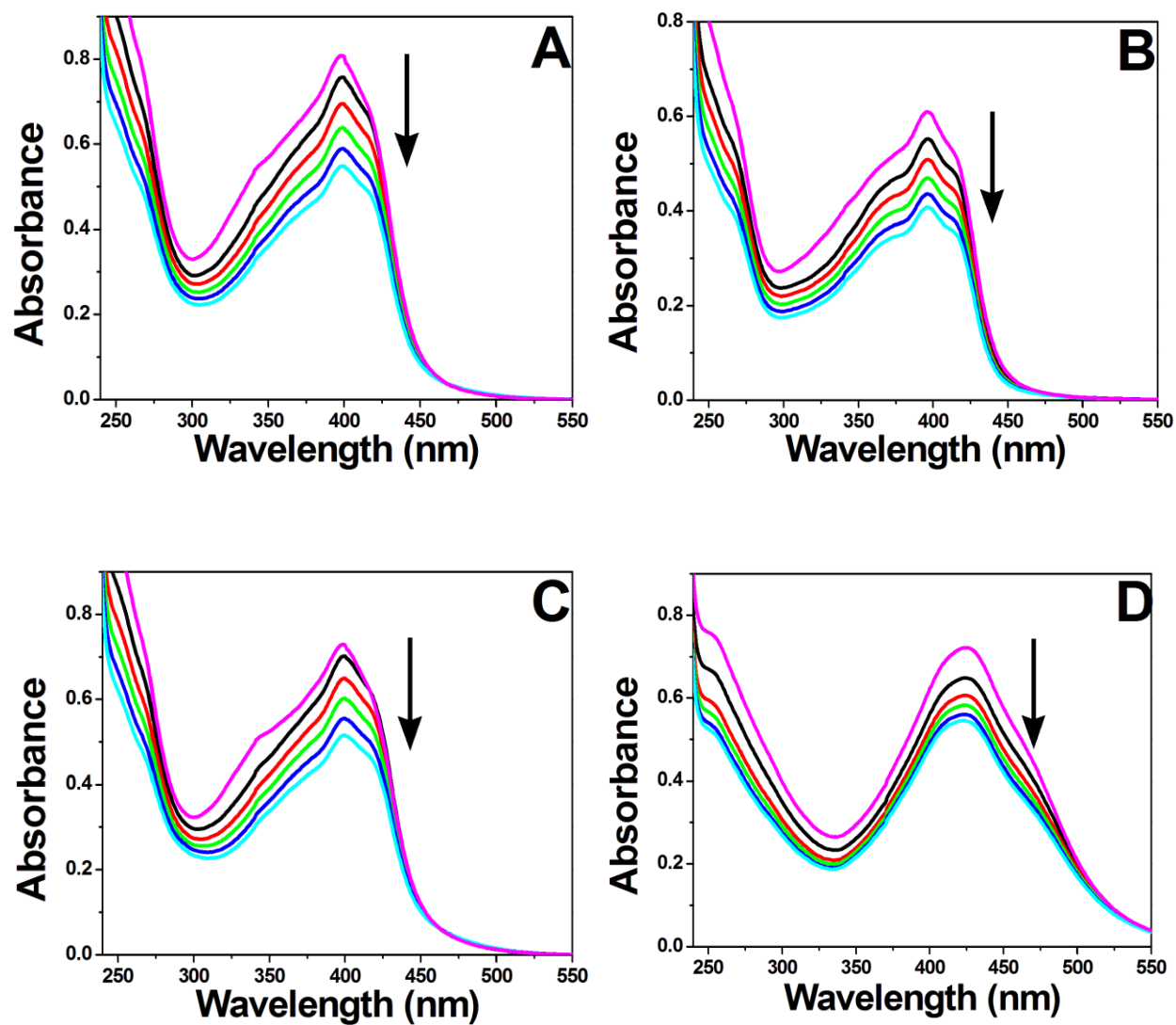


Figure S3: Electronic spectra of the complexes 1(A), 2(B), 3(C) and 5(D) in Tris-HCl buffer upon addition of CT-DNA. [Complex] = 25  $\mu$ M, [DNA] = 0-50  $\mu$ M. Arrow shows the absorption intensities decrease upon increasing DNA concentration.

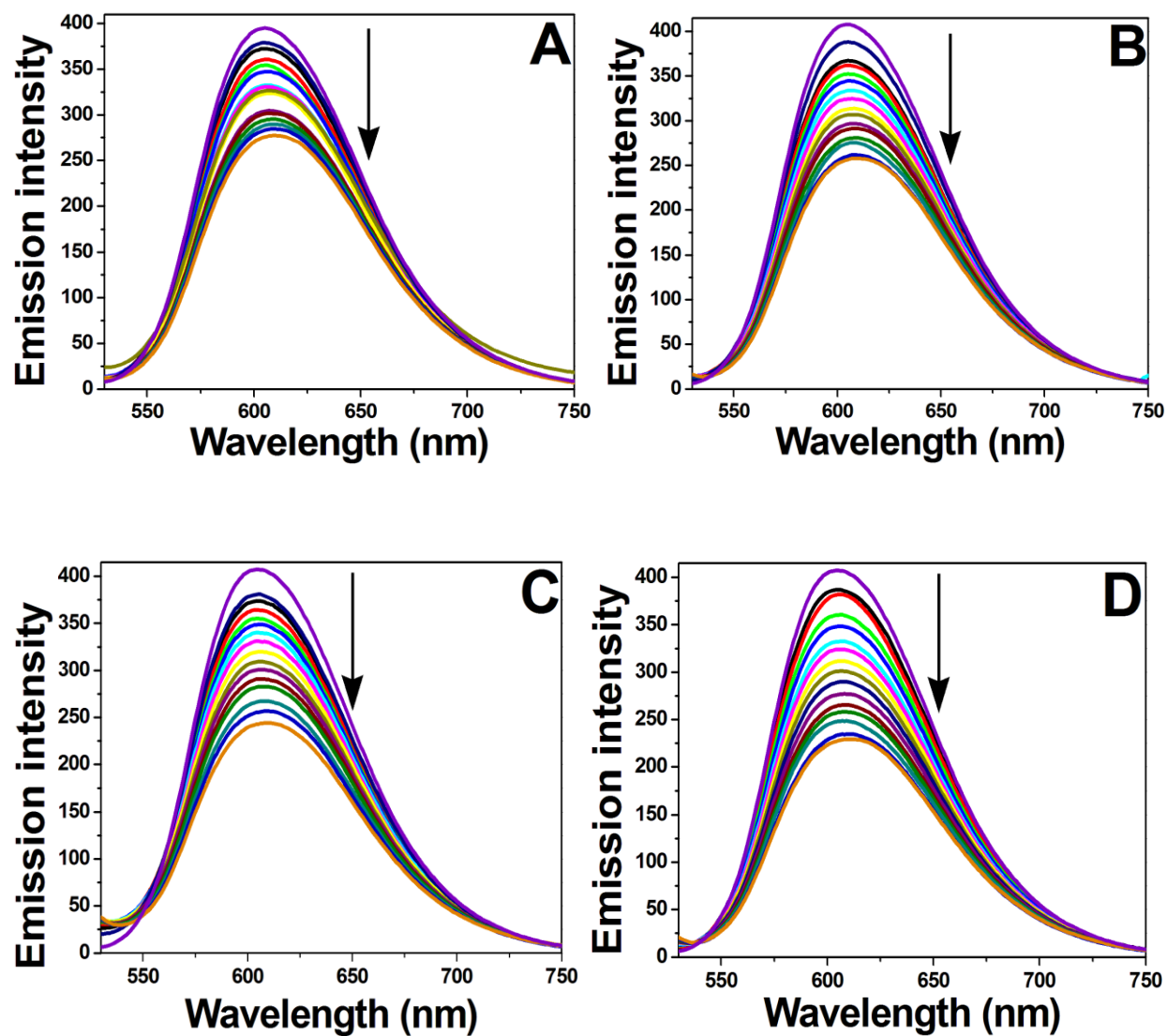


Figure S4: The emission spectra of DNA-EB system,  $\lambda_{\text{exi}} = 515$  nm,  $\lambda_{\text{emi}} = 530-750$  nm, in the presence of the complexes **1**(A), **2**(B), **3**(C) and **5**(D). [DNA] = 12 μM, [Complex] = 0-75 μM, [EB] = 12 μM. Arrow shows the emission intensity changes upon increasing complex concentration.

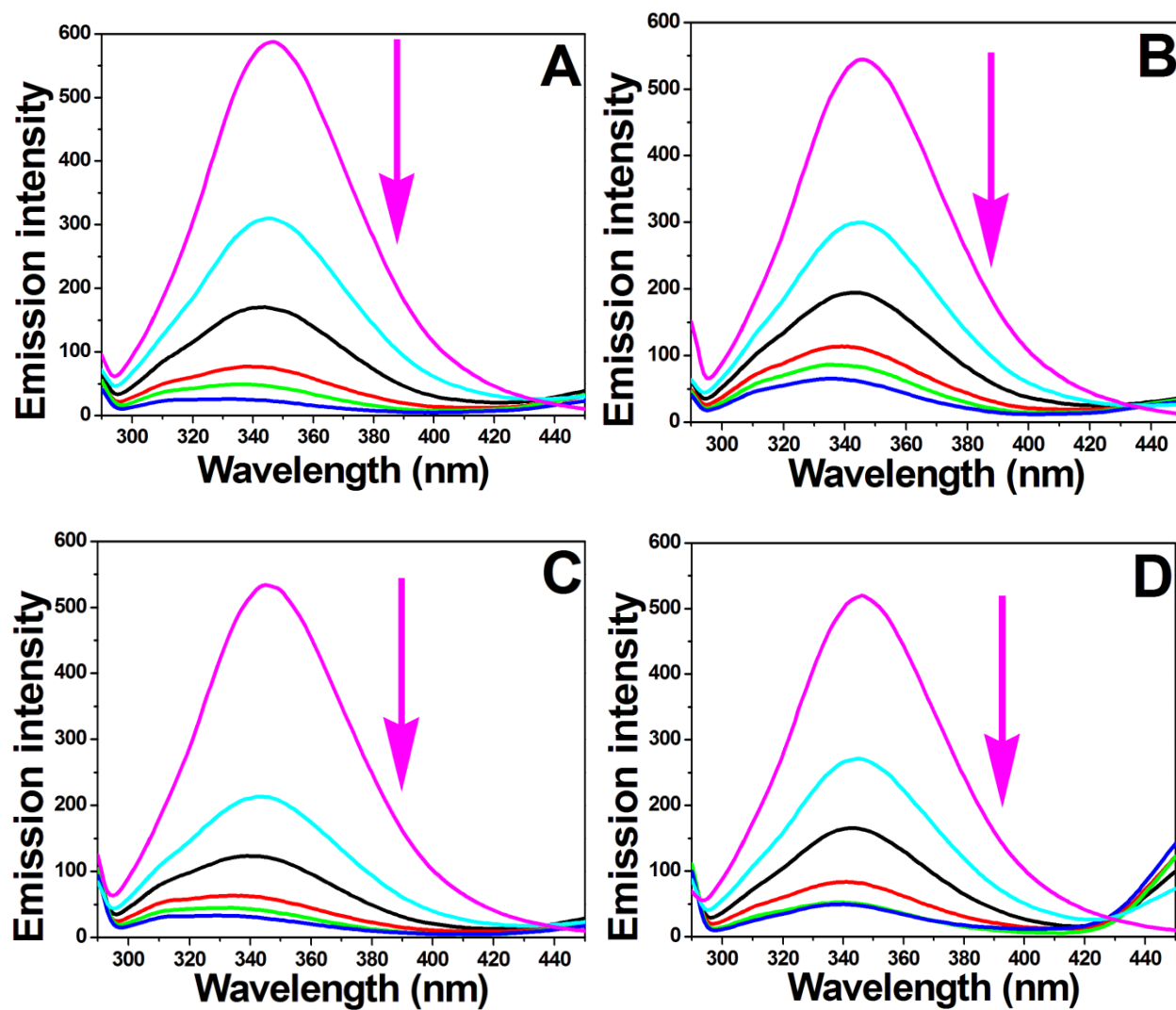


Figure S5: The emission spectrum of BSA (1  $\mu\text{M}$ ;  $\lambda_{\text{exi}} = 280 \text{ nm}$ ;  $\lambda_{\text{emi}} = 346 \text{ nm}$ ) in the presence of increasing amounts of the complexes 1(A), 2(B), 3(C) and 5(D) (0-25  $\mu\text{M}$ ). Arrow shows the emission intensity changes upon increasing complex concentration.

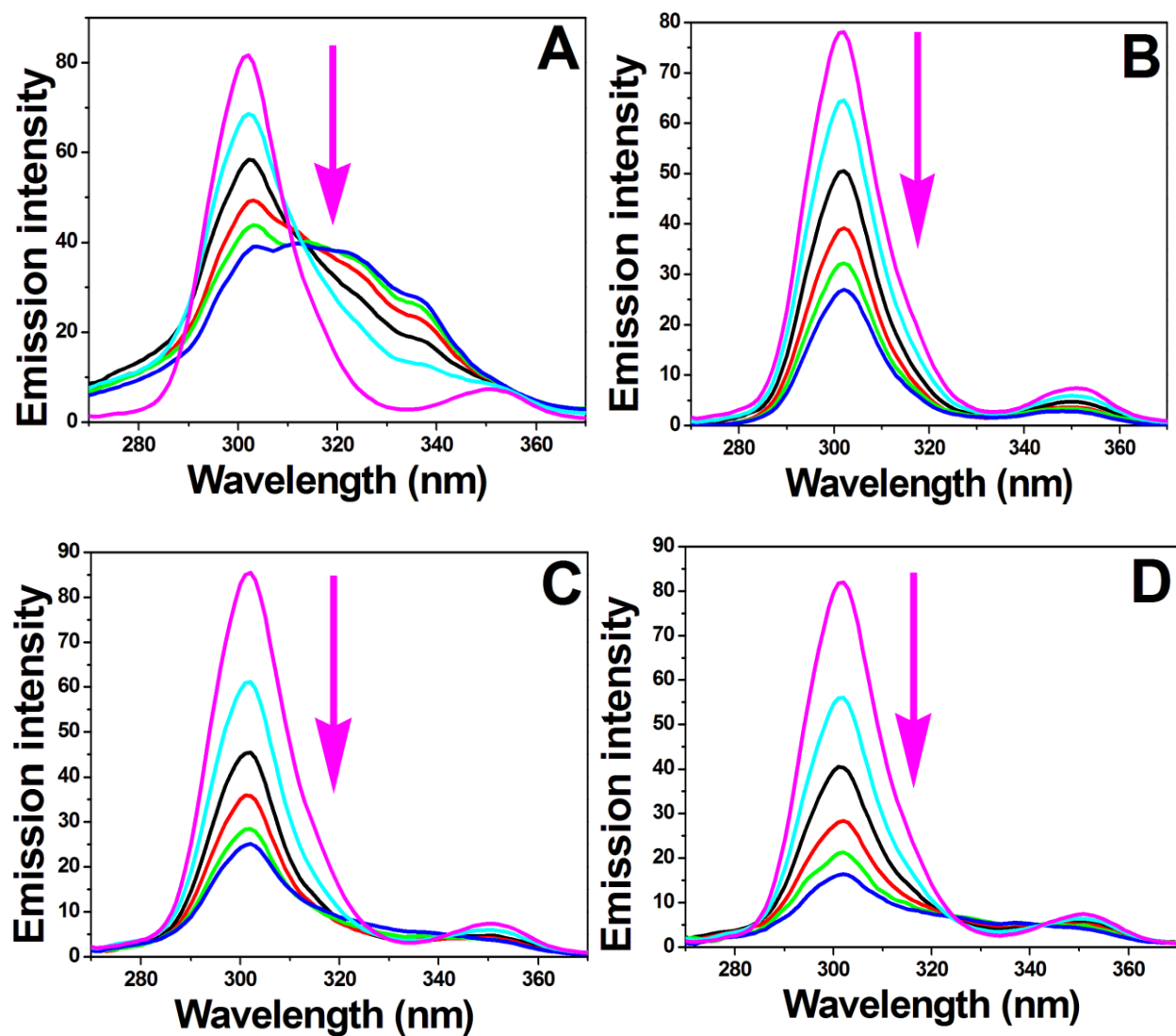


Figure S6: Synchronous spectra of BSA (1  $\mu\text{M}$ ) in the presence of increasing amounts of the complexes 1(A), 2(B), 3(C) and 5(D) (0-25  $\mu\text{M}$ ) in the wavelength difference of  $\Delta\lambda = 15$  nm. Arrow shows the emission intensity changes upon the increasing concentration of complex.

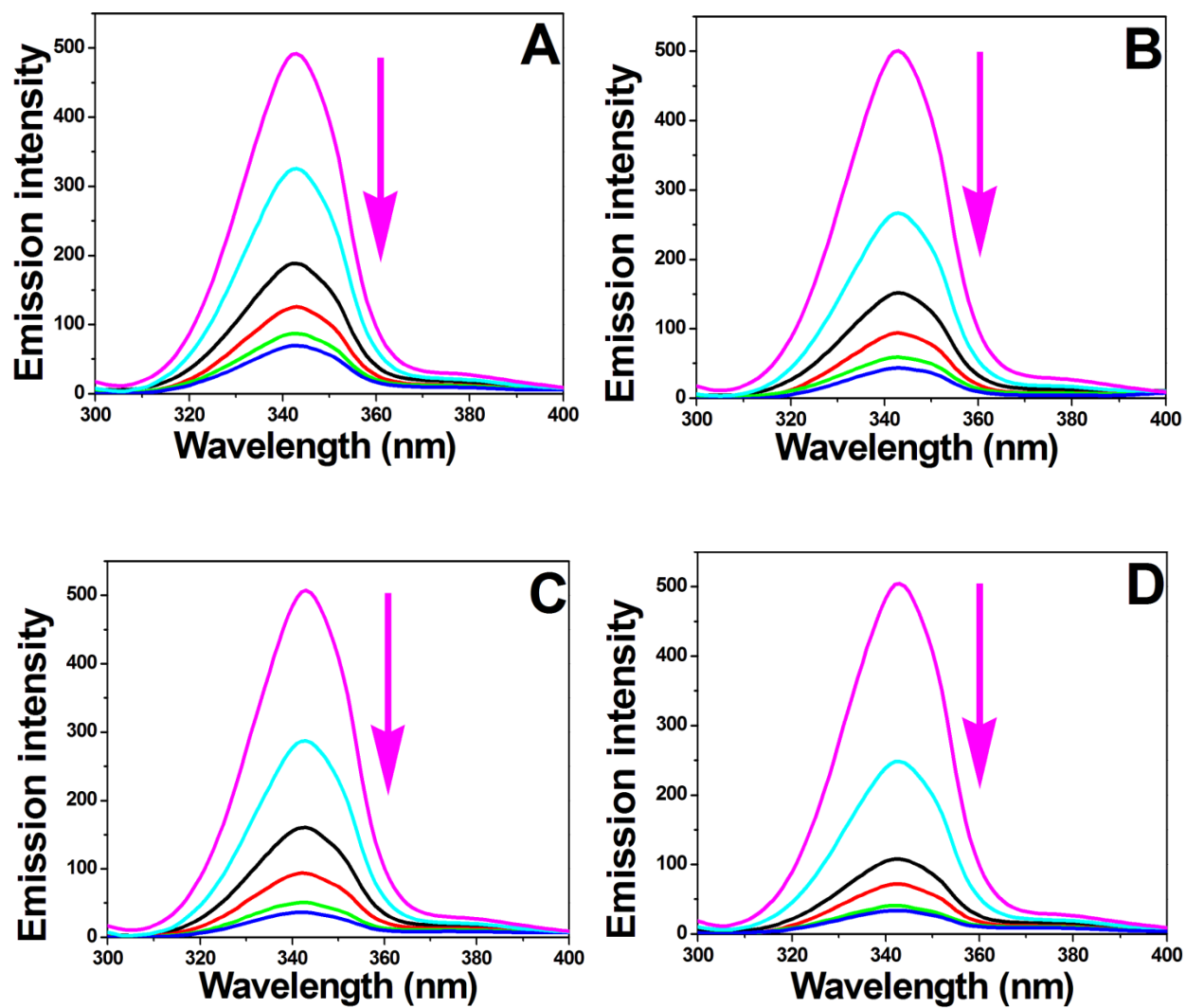


Figure S7: Synchronous spectra of BSA (1 μM) in the presence of increasing amounts of the complexes 1(A), 2(B), 3(C) and 5(D) (0-25 μM) in the wavelength difference of  $\Delta\lambda = 60$  nm. Arrow shows the emission intensity changes upon the increasing concentration of complex.