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Supporting Information

Anti-proliferative activity and DNA/BSA interactions of five mono- or di-organotin(IV) compounds derived from 2-hydroxy-N'-[(2-hydroxy-3-methoxyphenyl)methylidene]-benzohydrazone

Min Hong,[†] Guoliang Chang,[†] Rui Li, Meiju Niu[*]

School of Chemistry and Chemical Engineering, Liaocheng University, Liaocheng 252059, China.

[*] Corresponding author. Tel.: +866358230633; Fax: +866358239121.
E-mail address: niumeiju@163.com (M.J. Niu).

Table S1 Selected bond lengths (Å) and angles (°) for complexes **1-5**.

Complex **1**			
Sn(1)-C(17)	2.094(5)	O(2)-C(7)	1.273(6)
Sn(1)-C(16)	2.100(5)	O(3)-C(14)	1.329(6)
Sn(1)-O(3)	2.198(3)	N(1)-C(7)	1.329(6)
Sn(1)-O(2)	2.199(3)	N(1)-N(2)	1.399(5)
Sn(1)-N(2)	2.258(4)	N(2)-C(8)	1.284(6)
C(17)-Sn(1)-C(16)	163.4(2)	C(17)-Sn(1)-O(3)	94.03(17)
O(3)-Sn(1)-O(2)	151.41(13)	C(16)-Sn(1)-O(3)	91.84(18)
C(17)-Sn(1)-N(2)	94.09(19)	C(17)-Sn(1)-O(2)	93.41(18)
C(16)-Sn(1)-N(2)	102.10(19)	C(16)-Sn(1)-O(2)	88.76(18)
O(3)-Sn(1)-N(2)	81.16(14)	O(2)-Sn(1)-N(2)	70.79(14)
Complex **2**			
Sn(1)-O(3)	2.050(3)	O(2)-C(7)	1.299(4)
Sn(1)-C(22)	2.122(4)	O(3)-C(14)	1.329(4)
Sn(1)-C(16)	2.122(4)	N(1)-C(7)	1.320(5)
Sn(1)-O(2)	2.125(2)	N(1)-N(2)	1.394(4)
Sn(1)-N(2)	2.169(3)	N(2)-C(8)	1.307(5)
C(22)-Sn(1)-C(16)	115.25(13)	O(2)-Sn(1)-N(2)	73.18(10)
O(3)-Sn(1)-O(2)	155.64(11)	O(3)-Sn(1)-C(22)	99.78(14)
O(3)-Sn(1)-N(2)	83.41(11)	O(3)-Sn(1)-C(16)	95.81(13)
C(22)-Sn(1)-N(2)	114.86(12)	C(22)-Sn(1)-O(2)	96.18(13)
C(16)-Sn(1)-N(2)	129.22(12)	C(16)-Sn(1)-O(2)	93.86(12)
Complex **3**			
Sn(1)-C(20)	2.109(4)	O(2)-C(7)	1.282(4)
Sn(1)-C(16)	2.117(3)	O(3)-C(14)	1.325(4)
Sn(1)-O(3)	2.165(2)	N(1)-C(7)	1.309(5)
Sn(1)-N(2)	2.211(3)	N(1)-N(2)	1.391(4)
Sn(1)-O(2)	2.213(3)	N(2)-C(8)	1.284(4)
C(20)-Sn(1)-C(16)	151.37(15)	C(20)-Sn(1)-O(3)	97.67(13)
C(20)-Sn(1)-N(2)	106.74(12)	C(16)-Sn(1)-O(3)	94.06(12)
C(16)-Sn(1)-N(2)	100.70(12)	C(20)-Sn(1)-O(2)	89.36(13)
O(3)-Sn(1)-N(2)	81.92(10)	C(16)-Sn(1)-O(2)	92.20(13)
O(3)-Sn(1)-O(2)	152.45(10)	N(2)-Sn(1)-O(2)	70.55(10)
Complex **4**			
Sn(1)-C(16)	2.120(5)	O(2)-C(7)	1.289(6)
Sn(1)-C(24)	2.111(5)	O(3)-C(14)	1.331(5)
Sn(1)-O(3)	2.175(3)	N(1)-C(7)	1.311(6)
Sn(1)-N(2)	2.214(4)	N(1)-N(2)	1.387(5)
Sn(1)-O(2)	2.212(3)	N(2)-C(8)	1.307(6)
C(16)-Sn(1)-C(24)	153.0(3)	C(16)-Sn(1)-O(2)	90.25(18)
C(16)-Sn(1)-O(3)	93.84(17)	C(24)-Sn(1)-O(2)	90.70(19)
C(24)-Sn(1)-O(3)	97.82(19)	O(3)-Sn(1)-O(2)	152.11(13)
C(16)-Sn(1)-N(2)	101.07(18)	N(2)-Sn(1)-O(2)	70.67(13)

C(24)-Sn(1)-N(2)	104.72(19)	O(3)-Sn(1)-N(2)	81.47(13)
Complex **5**			
Sn(1)-O(3)	2.040(3)	N(1)-C(7)	1.325(6)
Sn(1)-O(2)	2.088(3)	N(1)-N(2)	1.404(5)
Sn(1)-C(16)	2.126(4)	N(2)-C(8)	1.297(6)
Sn(1)-N(2)	2.171(4)	O(2)-C(7)	1.289(5)
Sn(1)-O(5)	2.302(3)	O(3)-C(10)	1.330(5)
Sn(1)-Cl(1)	2.4403(13)		
O(3)-Sn(1)-O(2)	157.23(15)	C(16)-Sn(1)-O(5)	90.15(16)
O(3)-Sn(1)-C(16)	98.84(15)	N(2)-Sn(1)-O(5)	81.96(13)
O(2)-Sn(1)-C(16)	100.38(15)	O(3)-Sn(1)-Cl(1)	95.43(10)
O(3)-Sn(1)-N(2)	85.36(13)	O(2)-Sn(1)-Cl(1)	93.35(11)
O(2)-Sn(1)-N(2)	73.93(13)	C(16)-Sn(1)-Cl(1)	99.46(14)
C(16)-Sn(1)-N(2)	170.68(16)	N(2)-Sn(1)-Cl(1)	88.35(10)
O(3)-Sn(1)-O(5)	84.15(13)	O(5)-Sn(1)-Cl(1)	170.31(9)
O(2)-Sn(1)-O(5)	83.70(14)		

Symmetry transformations used to generate equivalent atoms: Complex **1**: #1 = -x, -y, 2-z; Complex **3**: #1 = 2-x, 1-y, 1-z; Complex **4**: 1-x, 2-y, 1-z.

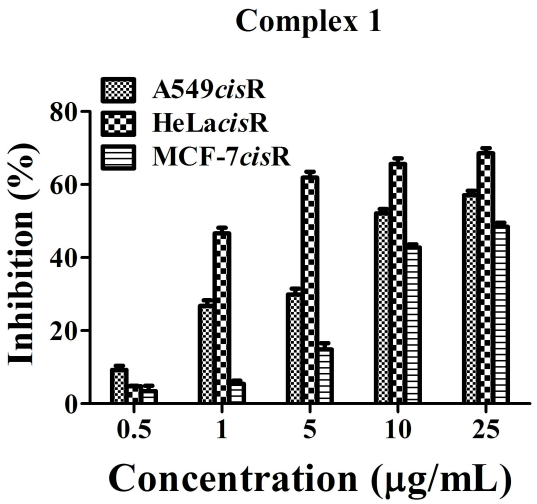

Fig. S1 The inhibition effects of complex **1** on the three cancer cell lines at different concentration.

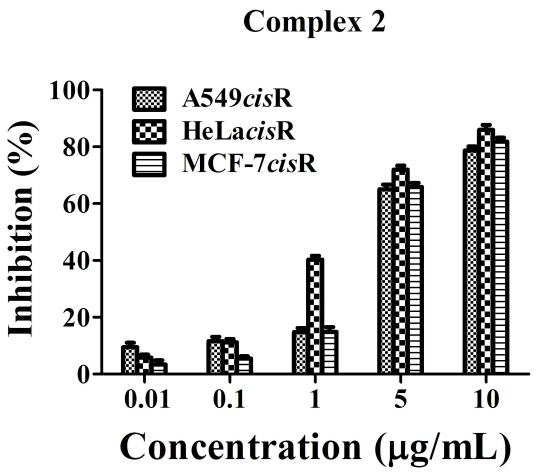

Fig. S2 The inhibition effects of complex **2** on the three cancer cell lines at different concentration.

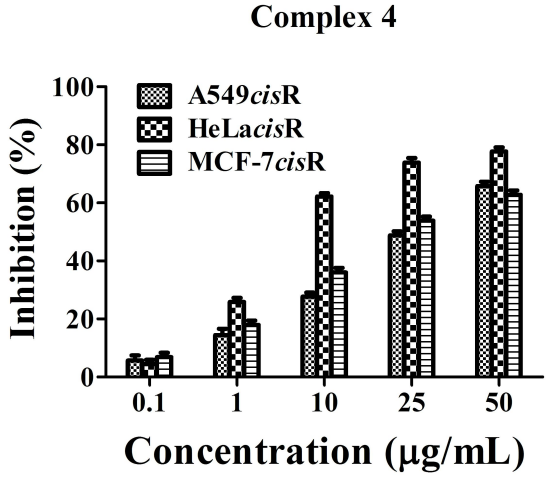

Fig. S3 The inhibition effects of complex **4** on the three cancer cell lines at different concentration.

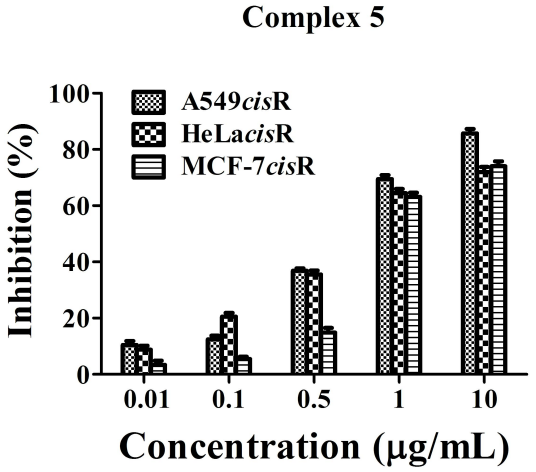

Fig. S4 The inhibition effects of complex **5** on the three cancer cell lines at different concentration.

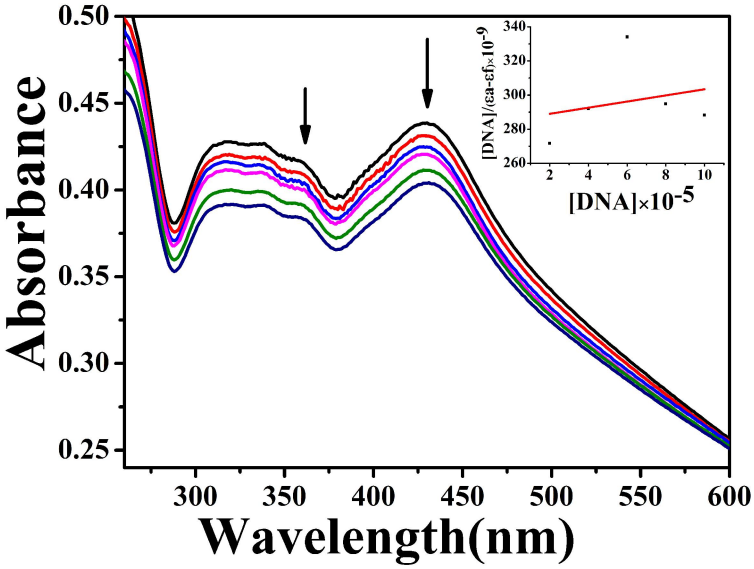

Fig. S5 UV–vis absorption spectrum of complex **1** (30 μM) in the absence and presence of CT-DNA, from 1 to 6, [DNA] = 0, 20, 40, 60, 80 and 100 μM, respectively. Arrows show the changes in absorbance with respect to an increase in the DNA concentration (Inset: plot between [DNA] and [DNA]/ [ε_a–ε_f]).

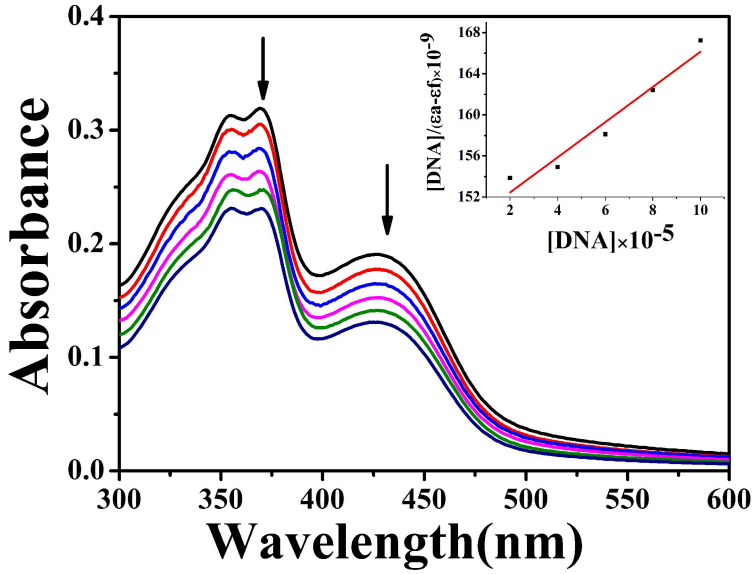

Fig. S6 UV–vis absorption spectrum of complex **2** (30 μM) in the absence and presence of CT-DNA, from 1 to 6, [DNA] = 0, 20, 40, 60, 80 and 100 μM, respectively. Arrows show the changes in absorbance with respect to an increase in the DNA concentration (Inset: plot between [DNA] and [DNA]/ [ε_a–ε_f]).

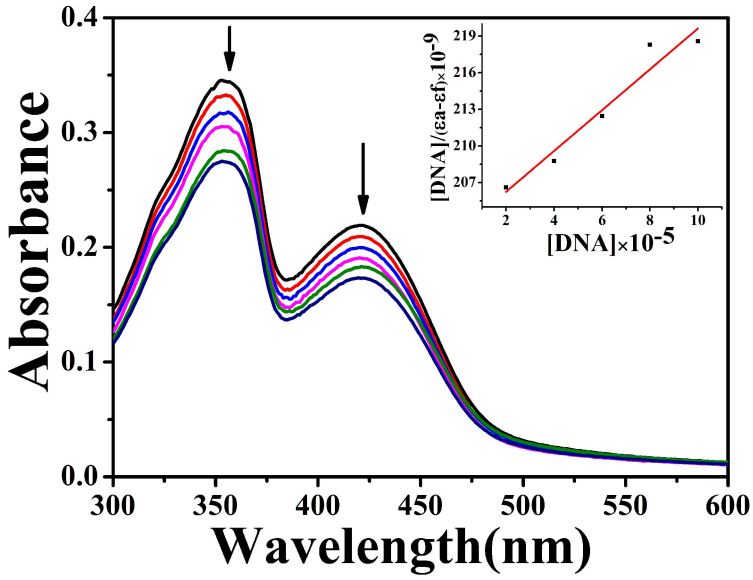

Fig. S7 UV–vis absorption spectrum of complex **4** (30 μM) in the absence and presence of CT-DNA, from 1 to 6, [DNA] = 0, 20, 40, 60, 80 and 100 μM, respectively. Arrows show the changes in absorbance with respect to an increase in the DNA concentration (Inset: plot between [DNA] and [DNA]/ [$\varepsilon_a-\varepsilon_f$]).

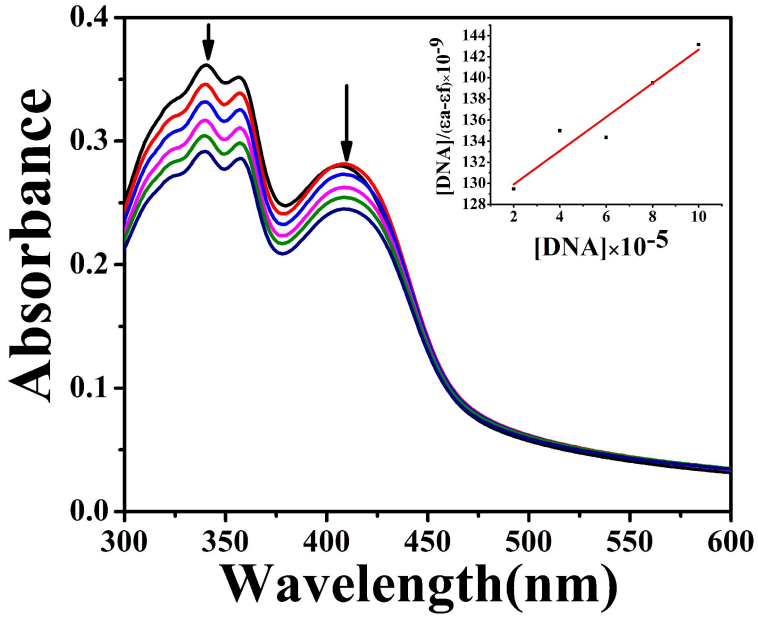

Fig. S8 UV–vis absorption spectrum of complex **5** (30 μM) in the absence and presence of CT-DNA, from 1 to 6, [DNA] = 0, 20, 40, 60, 80 and 100 μM, respectively. Arrows show the changes in absorbance with respect to an increase in the DNA concentration (Inset: plot between [DNA] and [DNA]/ [$\varepsilon_a-\varepsilon_f$]).

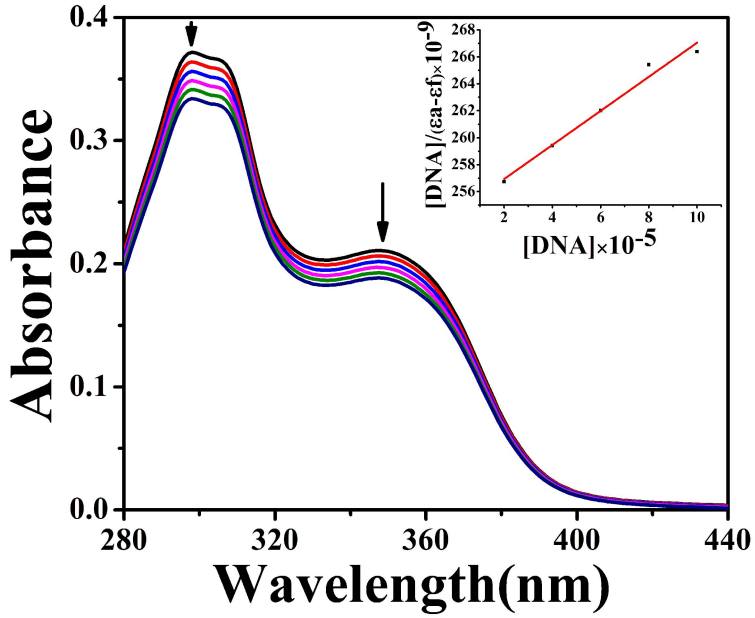

Fig. S9 UV–vis absorption spectrum of ligand HL (30 μM) in the absence and presence of CT-DNA, from 1 to 6, [DNA] ＝0, 20, 40, 60, 80 and 100 μM, respectively. Arrows show the changes in absorbance with respect to an increase in the DNA concentration (Inset: plot between [DNA] and [DNA]/ [ε_a−ε_f]).

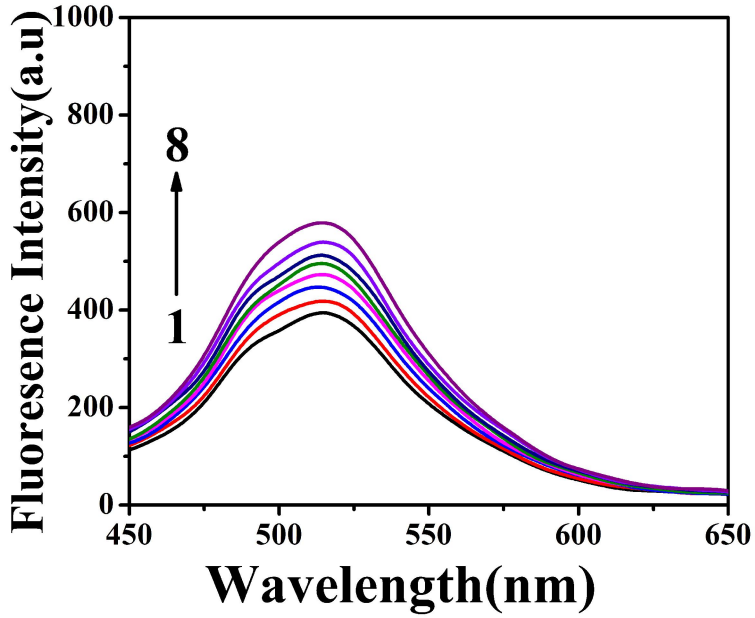

Fig. S10 Effects of the emission spectra (λ_{ex} = 346 nm) of 3 μM complex **1** with increasing concentrations of the DNA (0 - 250 μM).

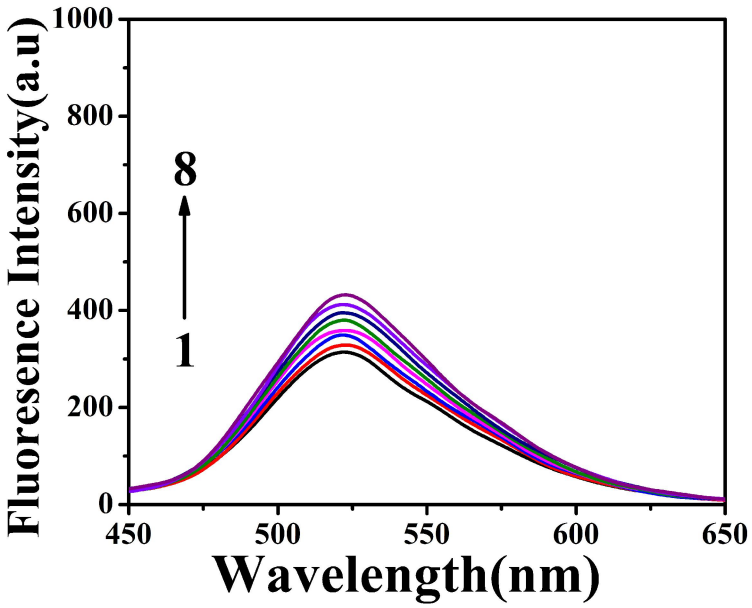

Fig. S11 Effects of the emission spectra (λ_{ex} = 346 nm) of 3 μM complex **2** with increasing concentrations of the DNA (0 - 250 μM).

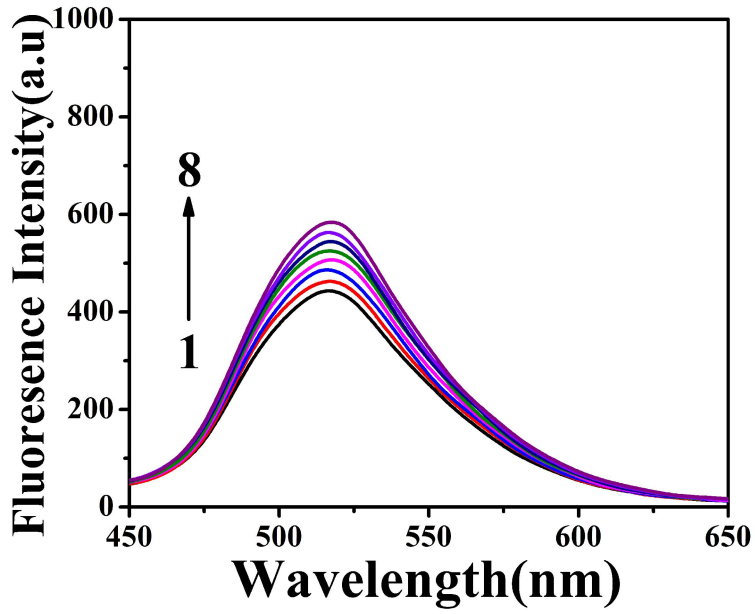

Fig. S12 Effects of the emission spectra (λ_{ex} = 346 nm) of 3 μM complex **4** with increasing concentrations of the DNA (0 - 250 μM).

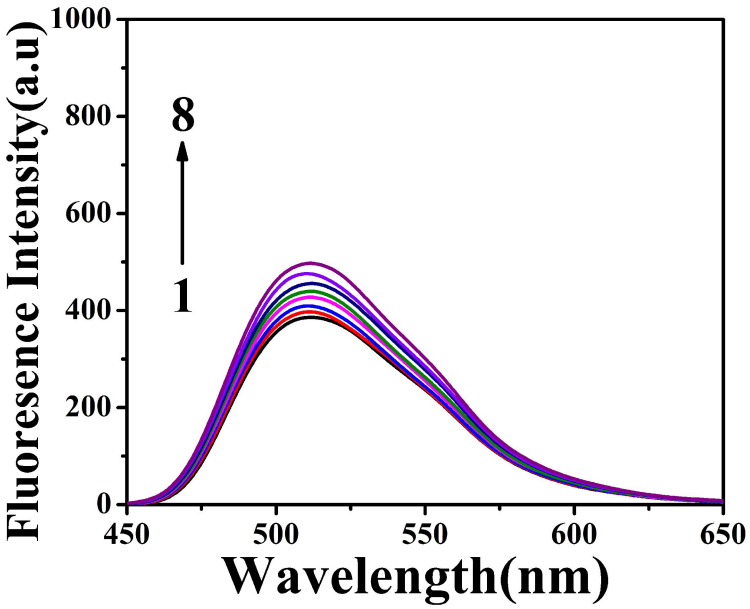

Fig. S13 Effects of the emission spectra (λ_{ex} = 346 nm) of 3 μM complex **5** with increasing concentrations of the DNA (0 - 250 μM).

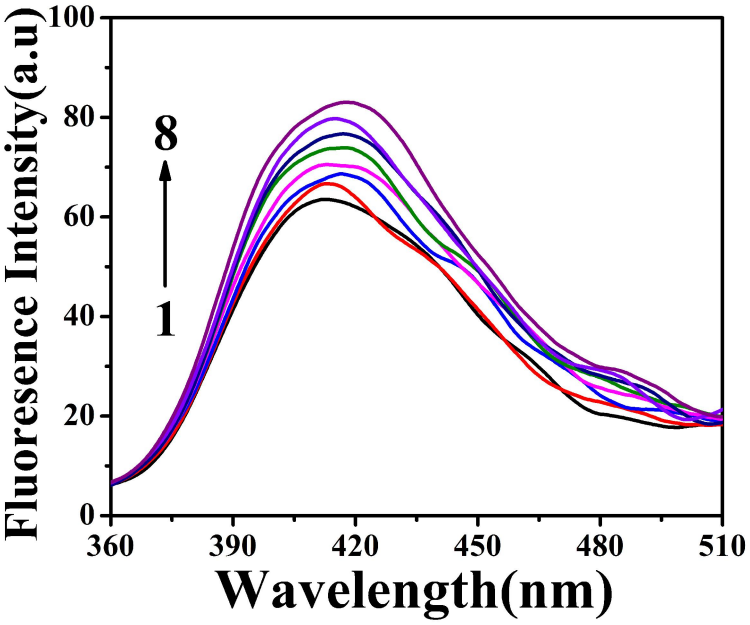

Fig. S14 Effects of the emission spectra (λ_{ex} = 346 nm) of 3 μM ligand HL with increasing concentrations of the DNA (0 - 250 μM).

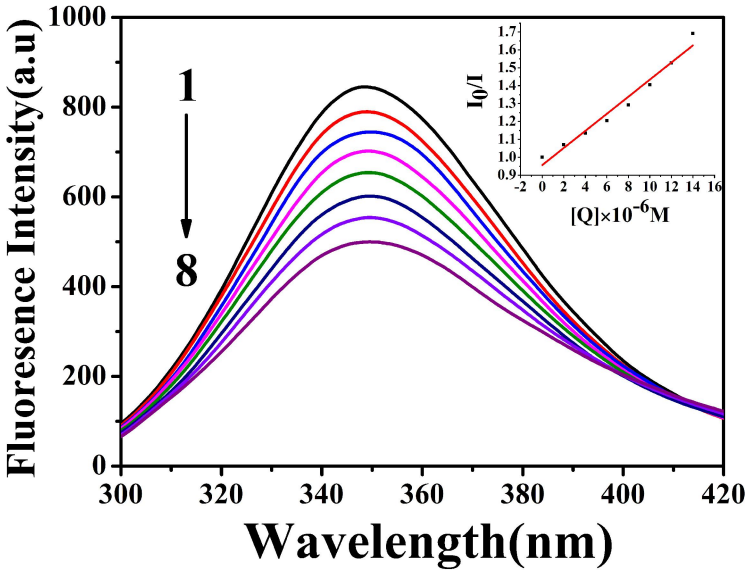

Fig. S15 Effects of complex **1** on the fluorescence spectra of BSA system. [BSA] = 1.0 × 10^{-6} M, [Complex] = 0, 2, 4, 6, 8, 10, 12 and 14 μM, respectively; λ_{ex} = 280 nm. (Inset: Plot of [Q] vs. I_0/I).

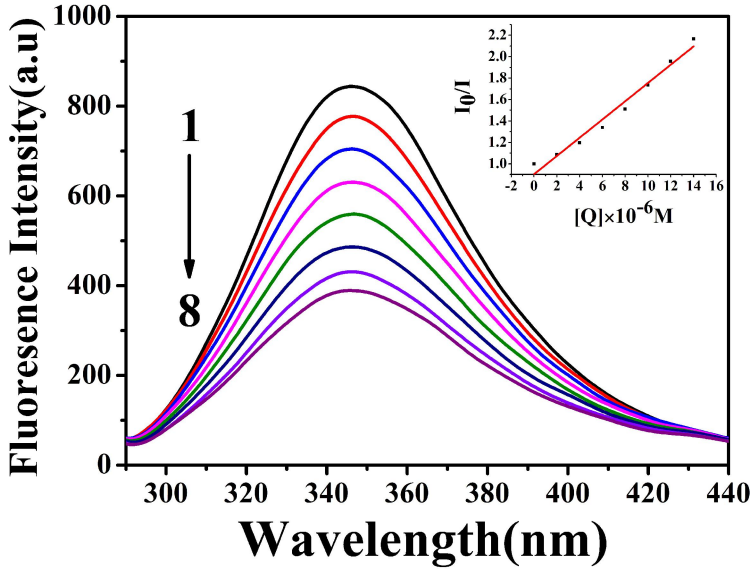

Fig. S16 Effects of complex **2** on the fluorescence spectra of BSA system. [BSA] = 1.0 × 10^{-6} M, [Complex] = 0, 2, 4, 6, 8, 10, 12 and 14 μM, respectively; λ_{ex} = 280 nm. (Inset: Plot of [Q] vs. I_0/I).

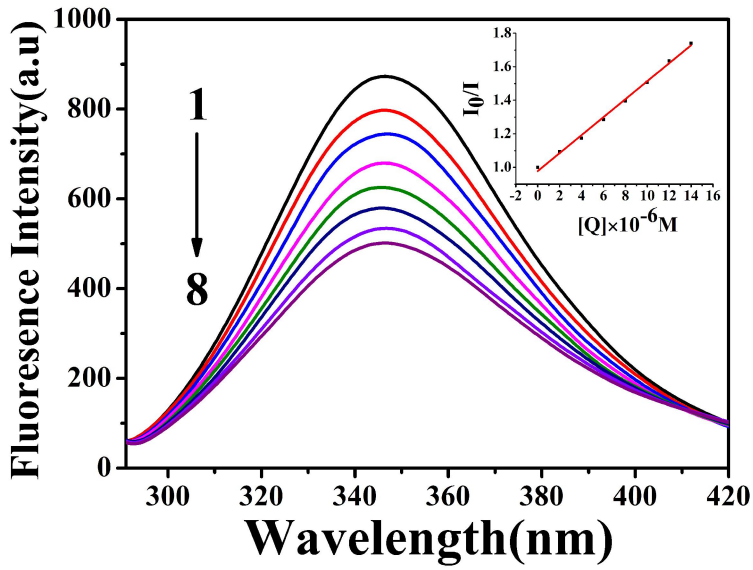

Fig. S17 Effects of complex **4** on the fluorescence spectra of BSA system. [BSA] = 1.0 × 10^{-6} M, [Complex] = 0, 2, 4, 6, 8, 10, 12 and 14 μM, respectively; λ_{ex} = 280 nm. (Inset: Plot of [Q] vs. I_0/I).

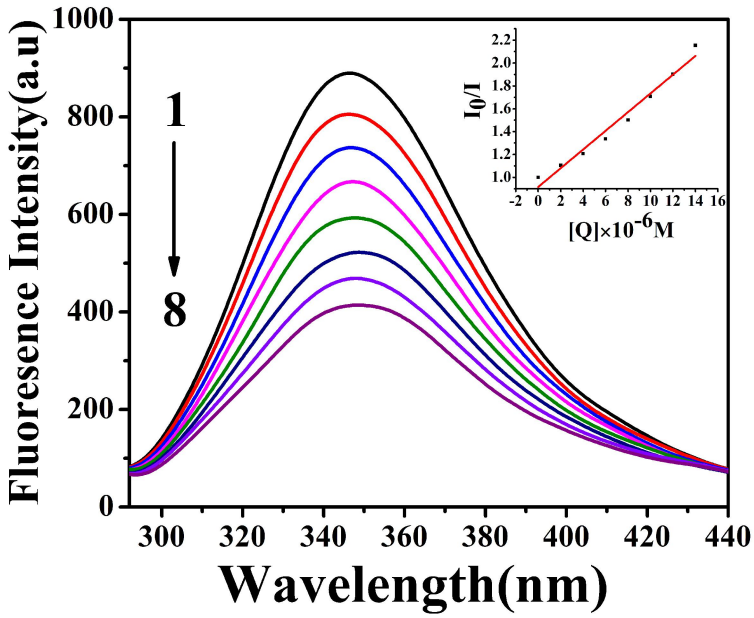

Fig. S18 Effects of complex **5** on the fluorescence spectra of BSA system. [BSA] = 1 μM, [Complex] = 0, 2, 4, 6, 8, 10, 12 and 14 μM, respectively; λ_{ex} = 280 nm. (Inset: Plot of [Q] vs. I_0/I).

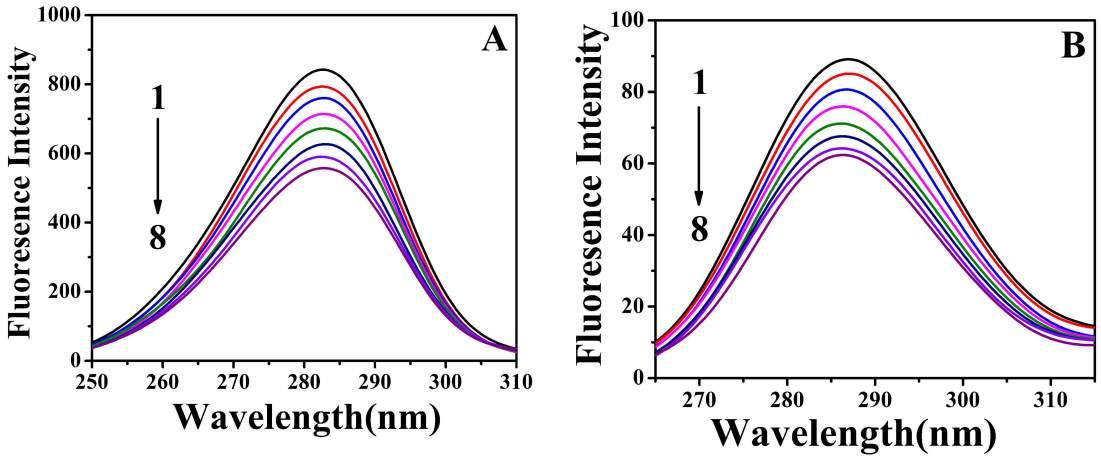

Fig. S19 Effects of complex **1** on the synchronous spectra of BSA system (A and B). [BSA] = 1.0 μM, from 1 to 8, [VOL] = 0, 1, 2, 3, 4, 5, 6 and 7μM, respectively. Δλ = 60 nm (A) and Δλ = 15 nm (B).

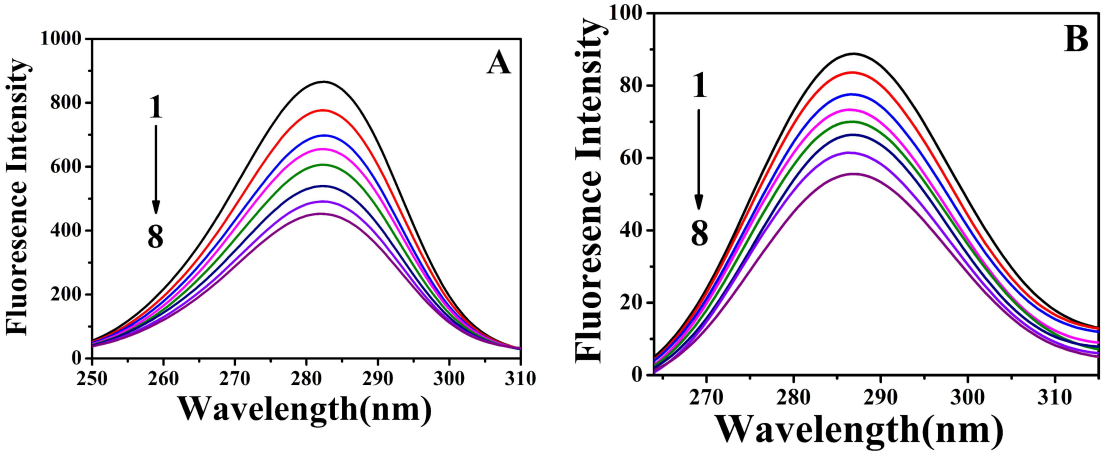

Fig. S20 Effects of complex **2** on the synchronous spectra of BSA system (A and B). [BSA] = 1.0 μM, from 1 to 8, [VOL] = 0, 1, 2, 3, 4, 5, 6 and 7 μM, respectively. Δλ = 60 nm (A) and Δλ = 15 nm (B).

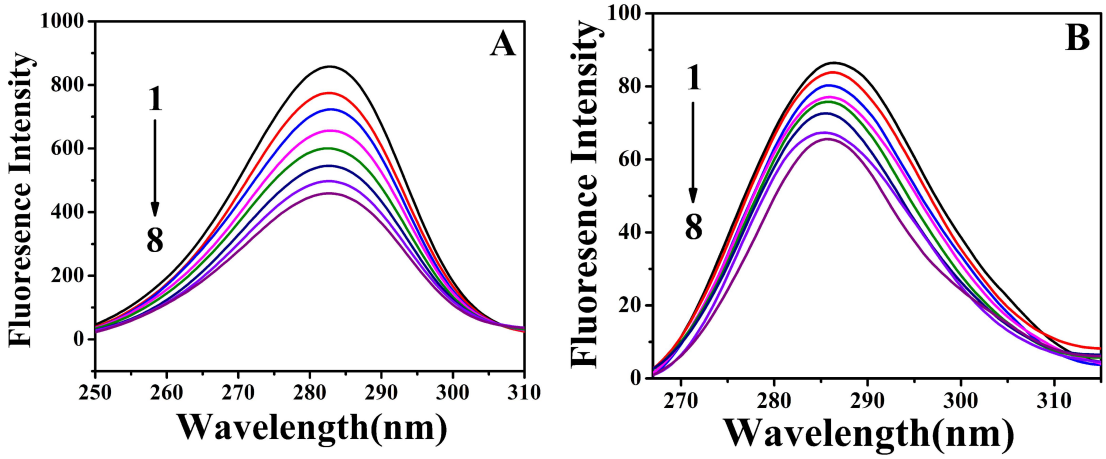

Fig. S21 Effects of complex **4** on the synchronous spectra of BSA system (A and B). [BSA] = 1.0 μM, from 1 to 8, [VOL] = 0, 1, 2, 3, 4, 5, 6 and 7 μM, respectively. Δλ = 60 nm (A) and Δλ = 15 nm (B).

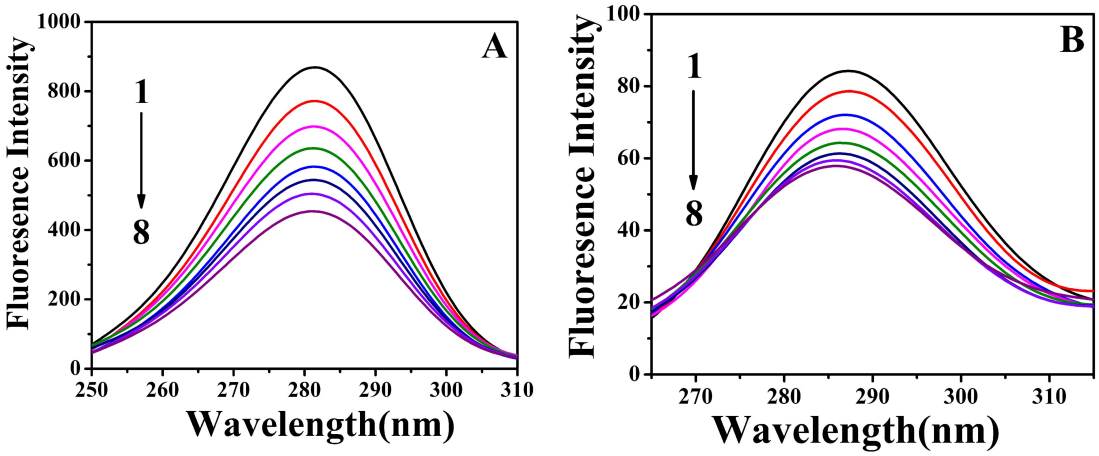

Fig. S22 Effects of complex **5** on the synchronous spectra of BSA system (A and B). [BSA] = 1.0 μM, from 1 to 8, [VOL] = 0, 1, 2, 3, 4, 5, 6 and 7 μM, respectively. Δλ = 60 nm (A) and Δλ = 15 nm (B).