

Supporting Information

Cadmium(II) complexes with a 4-acyl pyrazolone derivative and co-ligands: crystal structure and antitumor activity

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Table S1 Selected bond lengths (Å) and angles (°) for ligand and complexes **1-3**.

H₂L			
C7-O1	1.2619(19)	C11-N3	1.3320(19)
C18-O2	1.2398(18)	C18-N4	1.3463(19)
N3-N4	1.3853(17)		
Complex 1			
Cd1-O3	2.313(3)	Cd1-O2	2.315(3)
Cd1-N3	2.340(4)		
O3-Cd1-O3A	82.28(16)	O2A-Cd1-N3	123.46(12)
O3-Cd1-O2A	83.11(12)	O2-Cd1-N3	70.48(12)
O3-Cd1-N3A	97.87(12)	O3-Cd1-O2	83.16(12)
O3A-Cd1-O2	83.11(12)	O2A-Cd1-O2	161.73(17)
O2-Cd1-N3A	123.46(12)	O3-Cd1-N3	153.36(12)
N3-Cd1-N3A	93.64(19)	O3A-Cd1-N3	97.87(12)
Complex 2			
Cd1-O4	2.299(5)	Cd1-N3	2.338(5)
Cd1-N10	2.319(6)	Cd1-N7	2.357(6)
Cd1-O2	2.337(5)	Cd1-N9	2.370(6)
O4-Cd1-N10	158.19(18)	O2-Cd1-N7	86.19(18)
O4-Cd1-O2	87.24(17)	N3-Cd1-N7	155.56(19)
N10-Cd1-O2	114.39(18)	O4-Cd1-N9	87.68(18)
O4-Cd1-N3	101.15(17)	N10-Cd1-N9	70.51(19)
N10-Cd1-N3	89.49(19)	O2-Cd1-N9	170.20(17)
O2-Cd1-N3	70.16(17)	N3-Cd1-N9	119.11(19)
O4-Cd1-N7	70.70(18)	N7-Cd1-N9	84.22(19)
N10-Cd1-N7	106.4(2)		
Complex 3			
Cd1-O4	2.301(4)	Cd1-N10	2.348(5)
Cd1-N3	2.307(5)	Cd1-N9	2.354(5)

Cd1-O2	2.339(4)	Cd1-N7	2.370(5)
O4-Cd1-N3	95.21(15)	O2-Cd1-N9	94.72(16)
O4-Cd1-O2	96.36(14)	N10-Cd1-N9	71.37(18)
N3-Cd1-O2	70.58(15)	O4-Cd1-N7	70.67(14)
O4-Cd1-N10	98.72(16)	N3-Cd1-N7	158.92(16)
N3-Cd1-N10	119.50(16)	O2-Cd1-N7	94.87(14)
O2-Cd1-N10	160.79(16)	N10-Cd1-N7	79.09(16)
O4-Cd1-N9	168.19(17)	N9-Cd1-N7	112.43(17)
N3-Cd1-N9	84.64(17)		

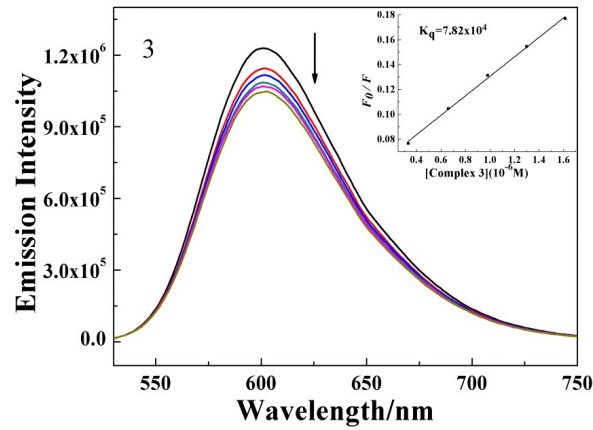
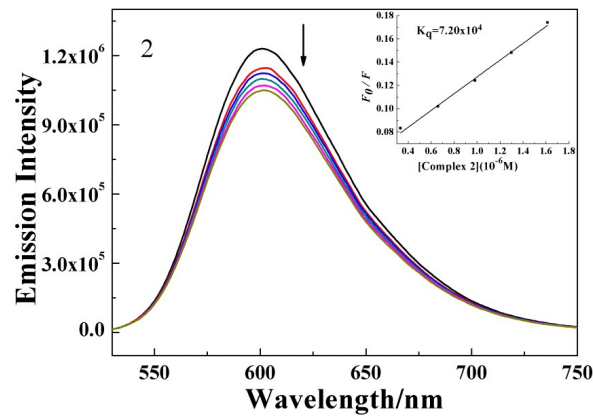
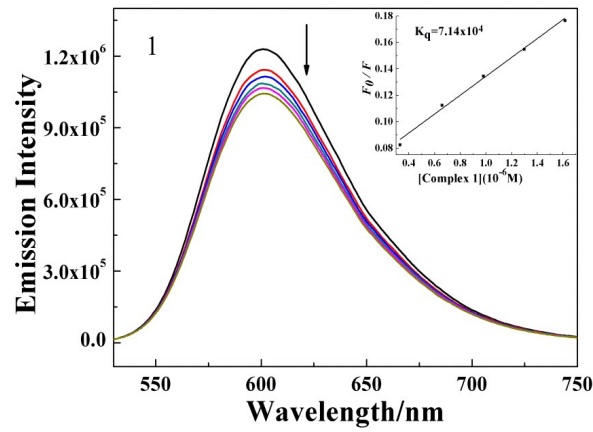
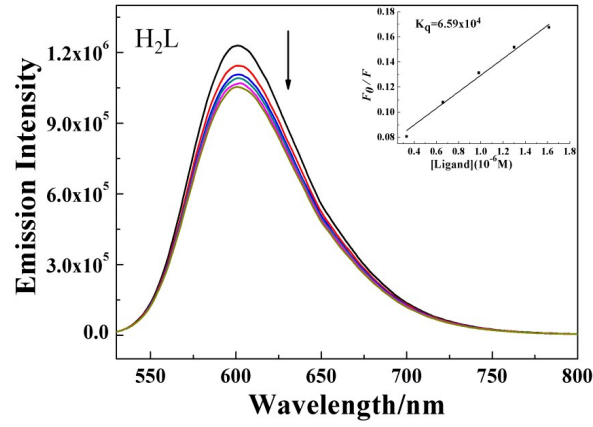


Fig. S1 The emission spectra of EB-DNA system in the absence and presence of increasing amount of the ligand and complexes **1-3**. $\lambda_{\text{ex}} = 530.0 \text{ nm}$, $\lambda_{\text{em}} = 590 \text{ nm}$, $[\text{DNA}] = 271 \text{ } \mu\text{M}$, $[\text{EB}] = 9.0 \text{ } \mu\text{M}$, $[\text{complex}] = 0-1.6 \text{ } \mu\text{M}$ from up to down respectively. Arrow shows the changes on addition of the ligand and complexes.

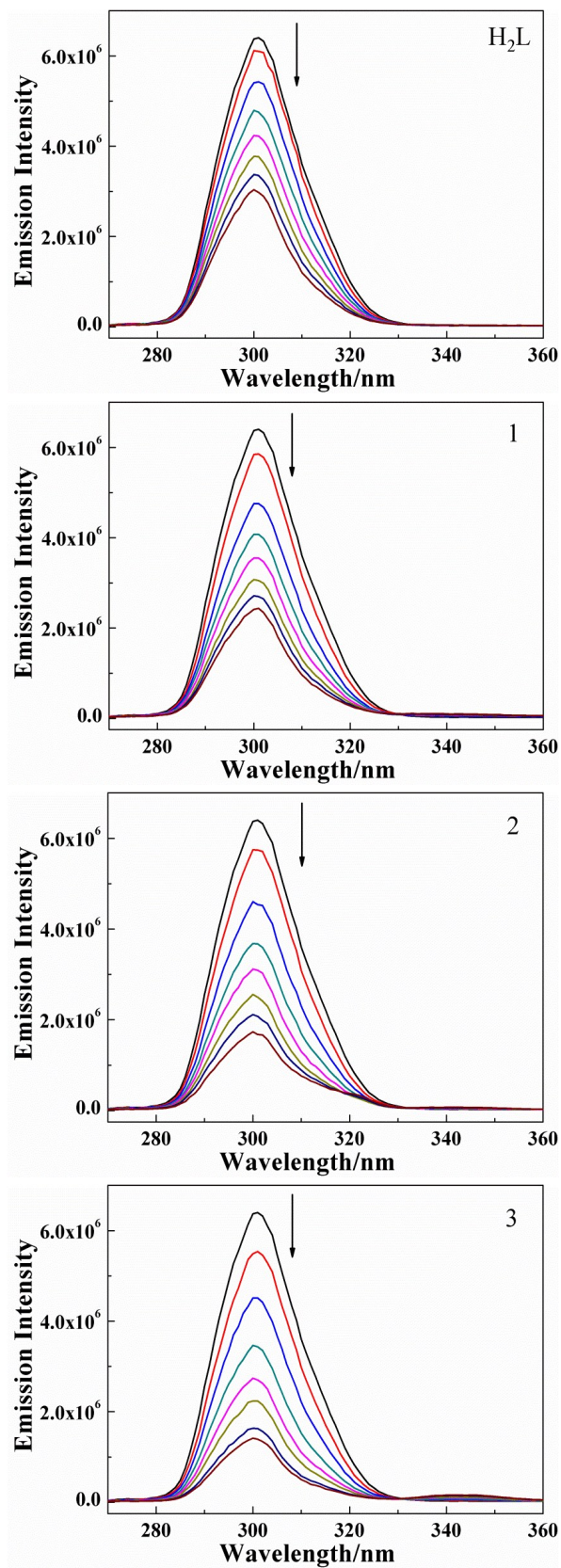


Fig. S2 Synchronous spectra of BSA (5.1 μ M) in the presence of increasing amounts of ligand and complexes **1-3** at a wavelength difference of $\Delta\lambda = 15$ nm.

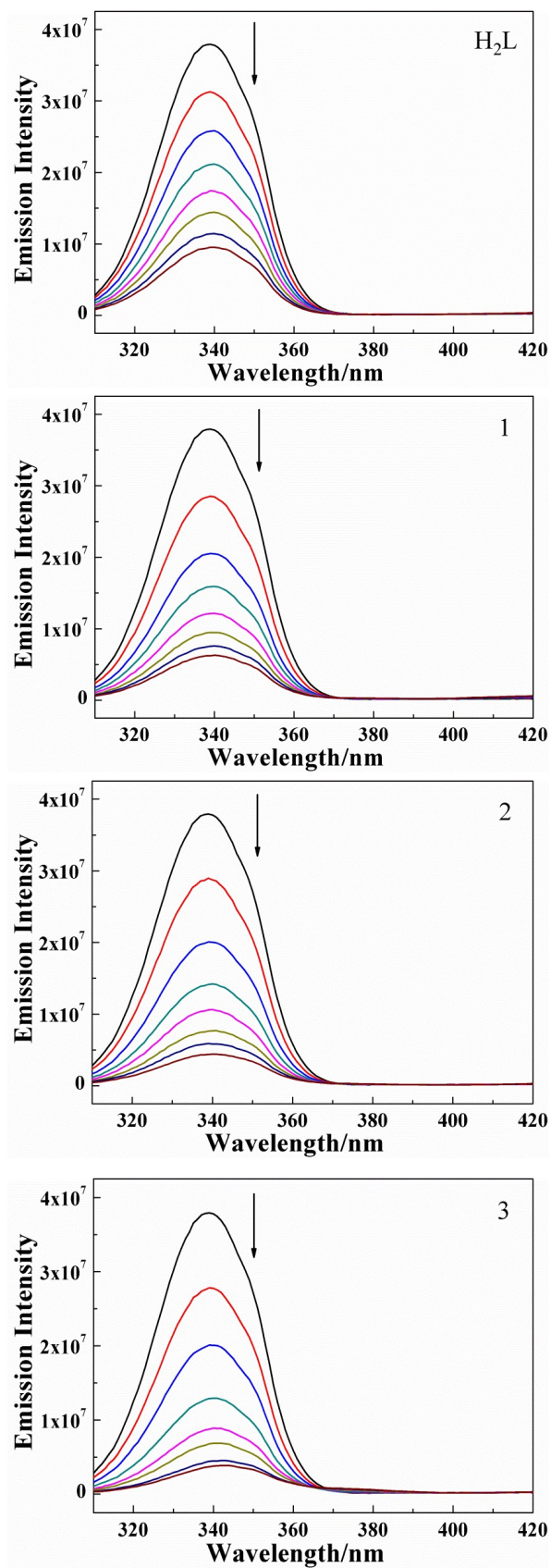


Fig. S3 Synchronous spectra of BSA (5.1 μM) in the presence of increasing amounts of ligand and complexes **1-3** at a wavelength difference of $\Delta\lambda = 60$ nm.

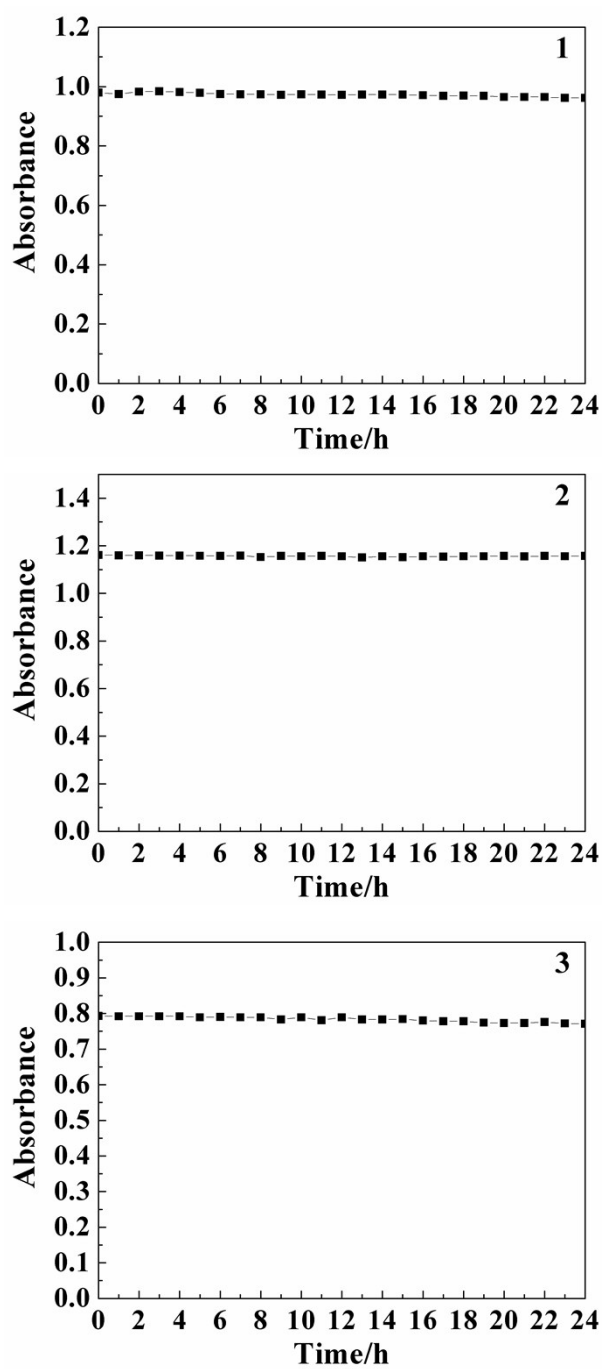


Fig. S4 The time-dependent UV absorbance of the complexes **1-3** at 250, 252 and 262 nm, respectively. The complexes were dissolved in the solution used for the biological tests and keep the solution at 37 °C.