Electronic Supplementary Material (ESI) for Dalton Transactions

Synthesis, Characterization, DNA binding and cleavage, BSA interaction and Anticancer Activity of dinuclear Zinc complexes

Chun-Yan Gao[a], Xin Qiao[b], Zhong-Ying Ma[b], Zhi-Gang Wang[a], Jing Lu[a], Jin-Lei Tian[a*], Jing-Yuan Xu[b], Guang-Jun Xu[c], Zhi-Ling Wang[c] and Shi-Ping Yan[a*]

[a] *Department of Chemistry, Nankai University, Tianjin 300071, P. R. China*

[b] *College of Pharmacy, Tianjin Medical University, Tianjin 300070, P. R. China*

[c] *Forth Mil Med Univ, Bethune Mil Med Coll, Shijiazhuang, 050081, P. R. China*

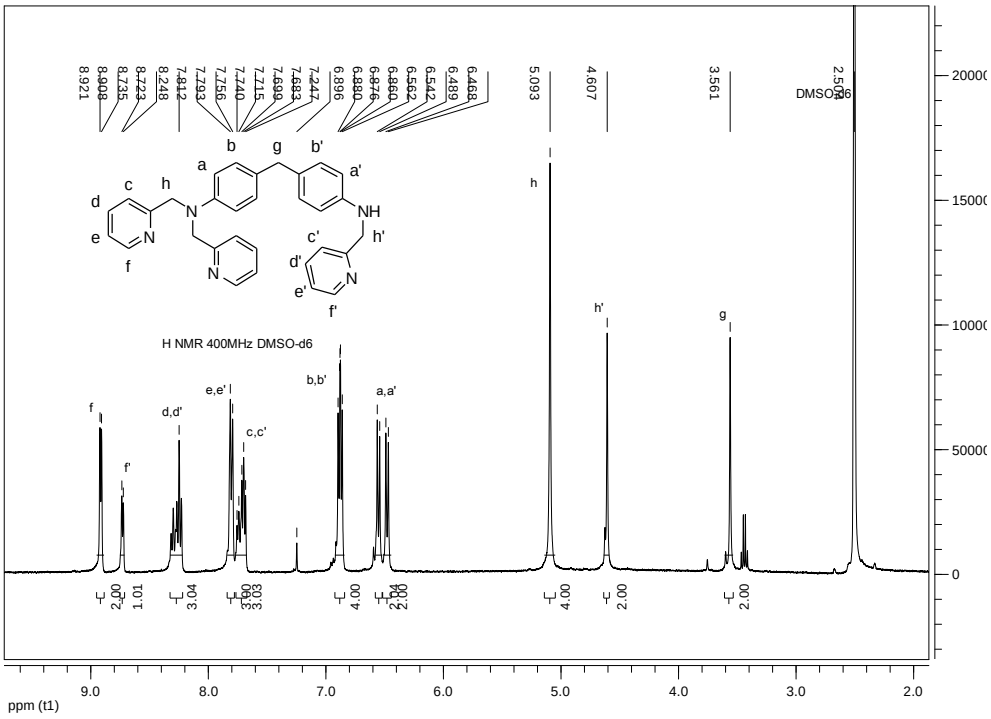

Fig. S1. ^{1}H NMR (400 MHz) spectra of the ligand **L^{1}** in DMSO-d6.

* Corresponding author: Tel.: +86-022-23505063; *Email address*: yansp@nankai.edu.cn

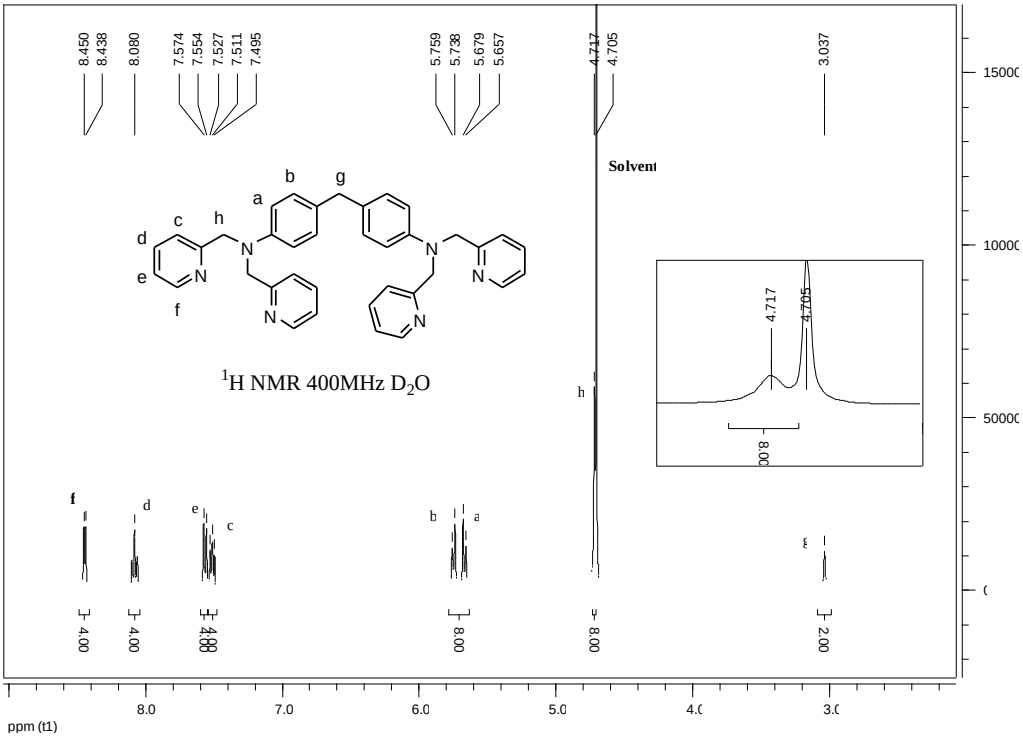

Fig. S2. ^{1}H NMR (400 MHz) spectra of the ligand $\mathbf{L}^2$ in D_2O.

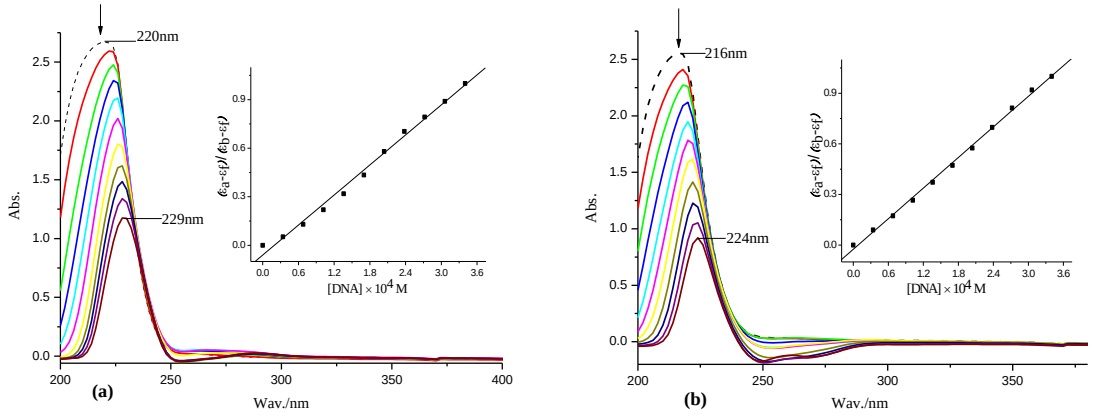

Fig. S3 (a-b) Absorption spectra of complexes **1** and **3** (1.96×10^{-6} M) in the absence (dashed line) and presence (solid line) of increasing amounts of CT-DNA (34, 68, 102, 136, 170, 204, 238, 272, 306, and 340 μM) in 5 mM Tris-HCl/50 mM NaCl buffer (pH = 7.2). The arrow shows the absorbance changes on increasing DNA concentration. Insert: Plot of $(\epsilon_a-\epsilon_f)/(\epsilon_b-\epsilon_f)$ versus [DNA] for the titration of DNA to complex.

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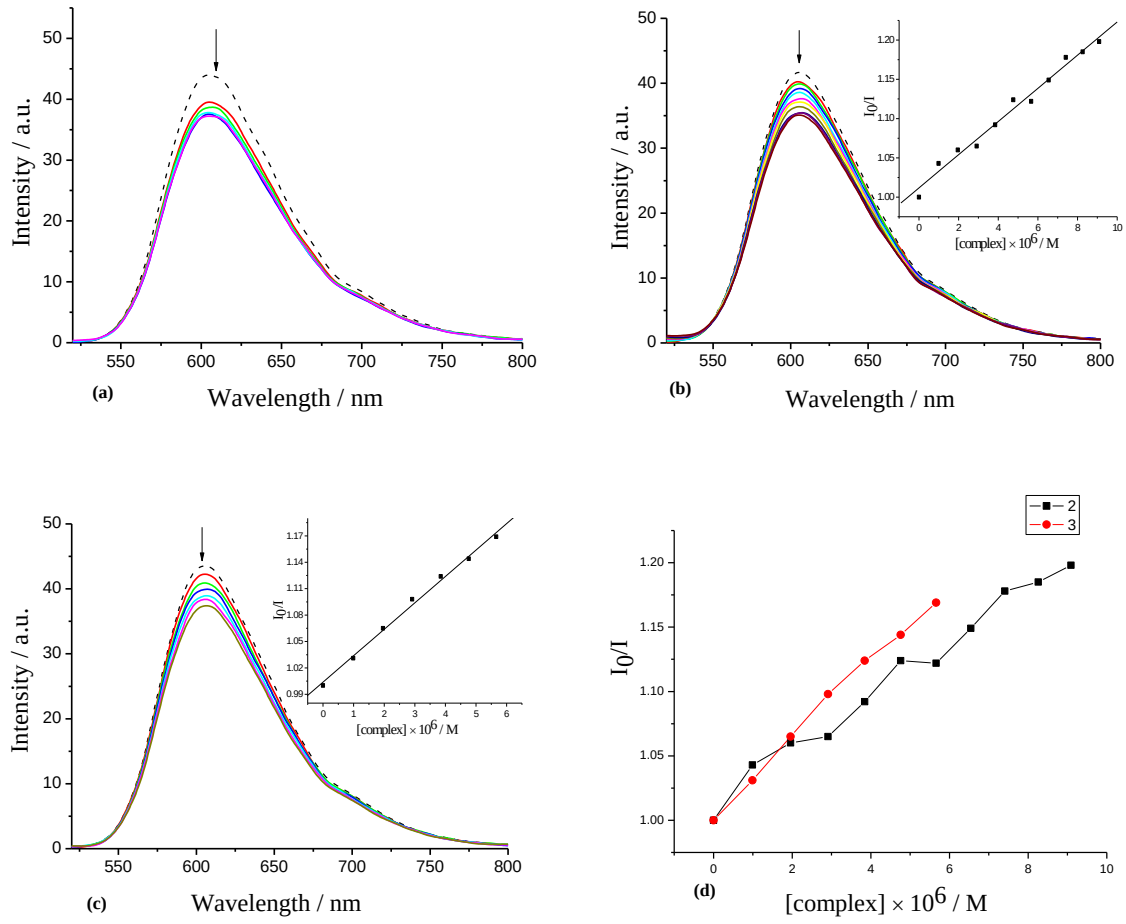
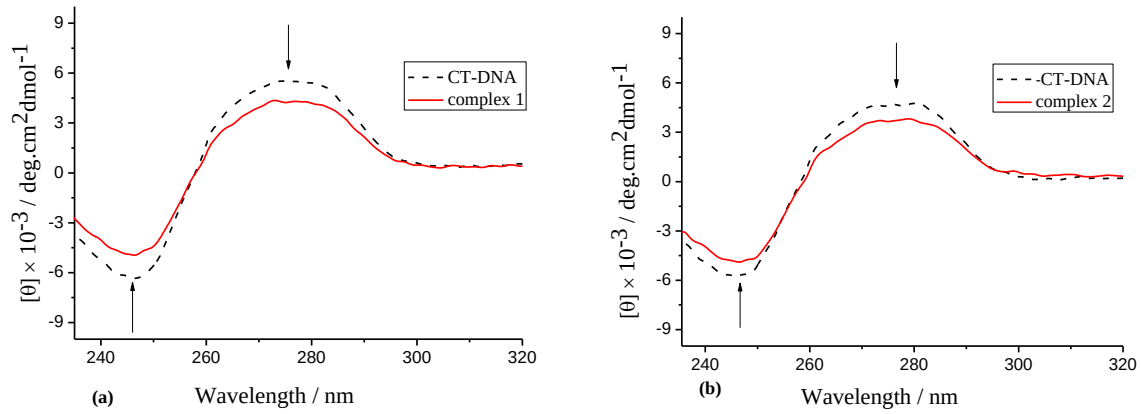


Fig. S4(a-c) Fluorescence emission spectra of the EB (2.4 μM) bound to CT-DNA (48 μM) system in the absence (dashed line) and presence (solid lines) of complexes **1**-**3** (0.99, 1.96, 2.91, 3.85, 4.76, 5.66, 6.54, 7.41, 8.26 and 9.09 μM). Inset: the plot of I_0/I versus the complex concentration. **(d)** The plot of I_0/I versus the concentration of complexes **2** and **3**.



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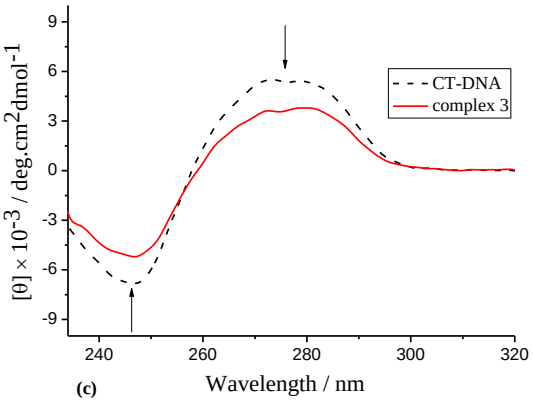


Fig. S5 (a-c) CD spectra of CT-DNA in the buffer solution (Tris-HCl) at 0.66 mM in the absence (dashed line) and presence (solid line)of 0.032 mM complex 1-3.

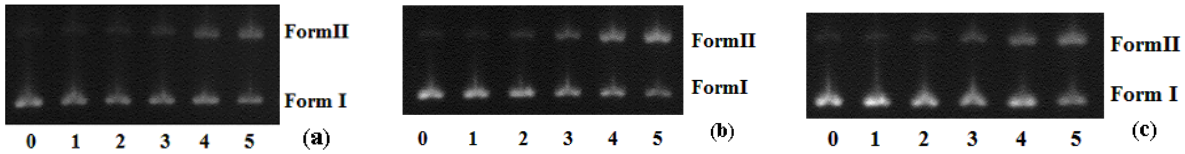


Fig. S6 (a-c) Gel electrophoresis diagram showing the cleavage of pBR322 DNA (0.1 μg/μL) for complexes **1-3** at different concentrations in Tris-HCl/NaCl buffer (pH = 7.2) and 37 ℃Lane 0: DNA control (4 h); Lane 1-5: DNA + **complex** (0.005, 0.025, 0.045, 0.065, 0.080 mM), respectively.

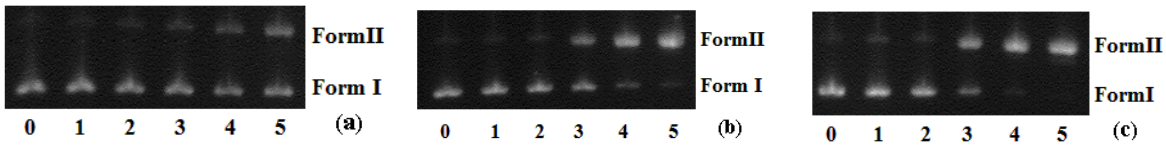


Fig. S7 (a-c) Gel electrophoresis diagrams showing the cleavage of pBR322 DNA (0.1 μg/μL) for **complexes 1-3** at different concentrations in Tris-HCl/NaCl buffer (pH = 7.2) and 37 ℃ Lane 0: DNA control (4 h); Lane 1: DNA + 0.25 mM H_2O_2; Lane 2-5: DNA + H_2O_2 + **complex** (0.005, 0.025, 0.045, 0.065 mM), respectively.

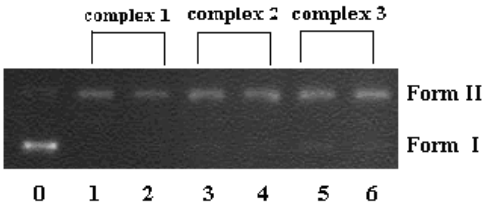
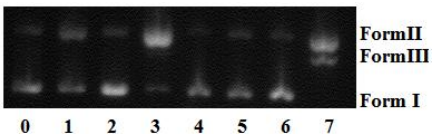


Fig. S8 Cleavage of plasmid pBR322 DNA (0.1 μg/μL) in presence of 0.065 mM complexes **1-3** and 20 U/mL Catalase inhibitors after 4 h incubation at 37 ℃. Lane 0: DNA control; Lane 1: DNA + 0.25 mM H_2O_2+ **complex** 1; Lane 2: DNA + 0.25 mM H_2O_2+ complex **1**+ Catalase; Lane 3-4 corresponds to complex **2**. Lane 5-6 corresponds to complex **3**



* Corresponding author: Tel.: +86-022-23505063; *Email address*: yansp@nankai.edu.cn

Fig. S9 Cleavage of pBR322 DNA (0.1 μg/μL) by complex **3** incubated for 4 h at pH 7.2 and 33 ℃ . Lane 0-3 (in N_2 atmosphere): DNA control; DNA + 0.075 mM complex; DNA +0.25 mM H_2O_2; DNA +0.25 mM H_2O_2+ 0.075 mM complex; (Lanes 4-7 aerobic conditions).

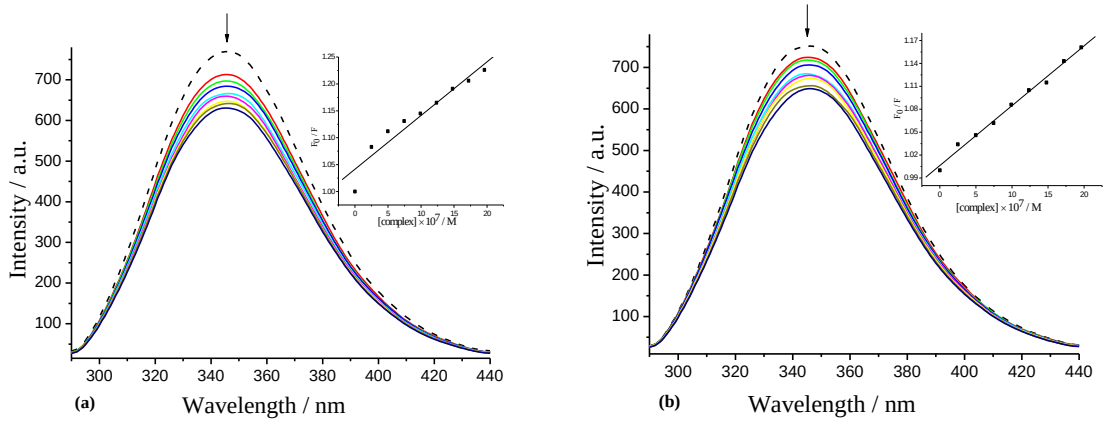


Fig. S10(a-b) Fluorescence emission spectra of the BSA (29.4 μM) system in the absence (dashed line) and presence (solid lines) of complexes **1** and **3** (0.25, 0.5, 0.74, 0.99, 1.23, 1.48, 1.72, and 1.96 μM, respectively). Inset: the plot of F_0/F versus the complex concentration.

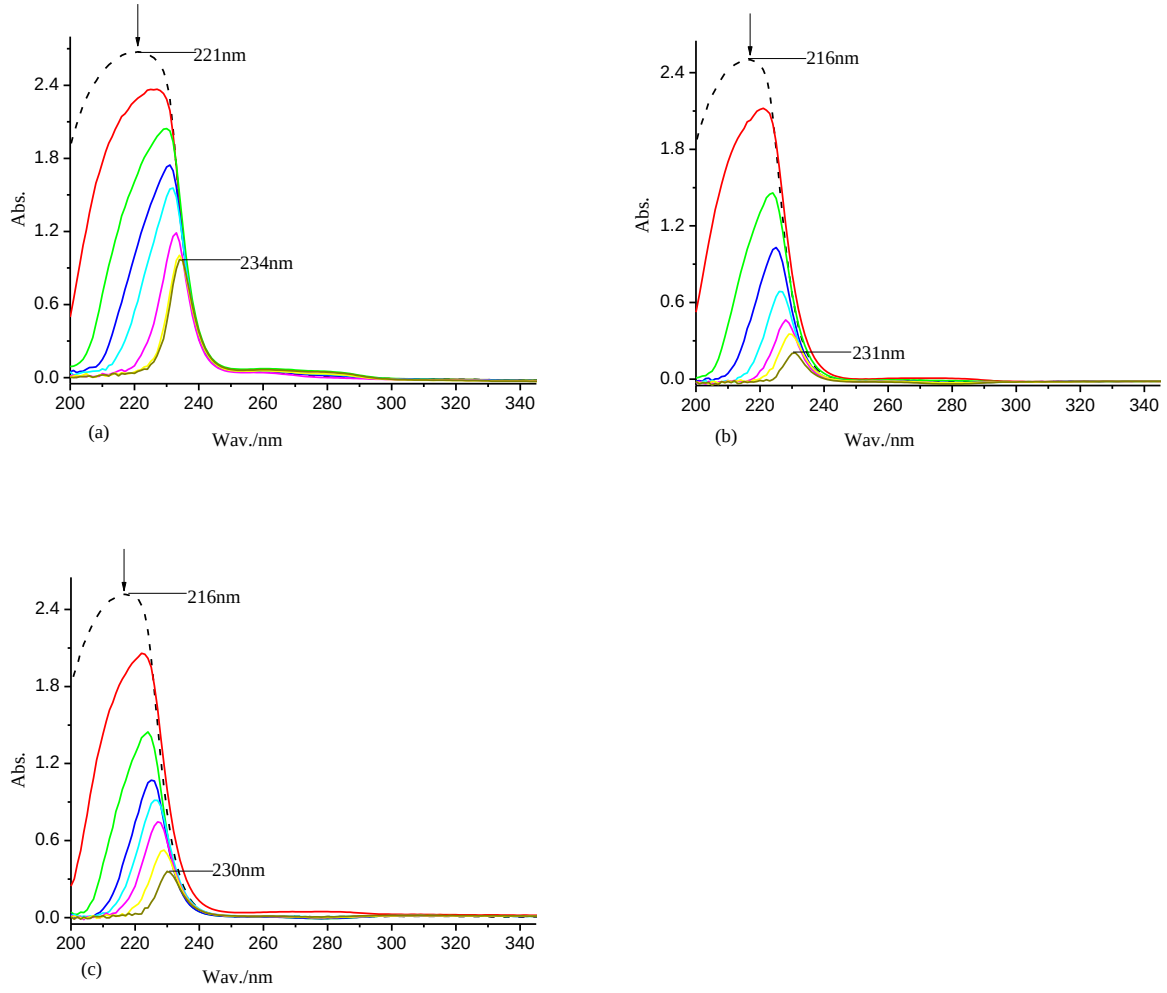


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Fig. S11 (a-c) Absorption spectra of complexes **1-3** (1.96 μM) in the absence (dashed line) and presence (solid line) of increasing amounts of BSA (0.59, 1.18, 1.76, 2.35, 2.94, 3.53 and 4.12 μM) in phosphate buffer (pH = 7.0).

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