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Supplementary Material

Lanthanide based Polymers with Charged Ligand Backbones:

Triple-stranded Chain Structures and their DNA Cleavage Studies

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Figure Legends:

**Fig. S1** Agarose GE patterns for the cleavage of pBR322 DNA by complex **3** and complex **4** in the presence of  $H_2O_2$  (25  $\mu$ M). Lane 1: 0.5 kb DNA Ladder; Lane 2: pBR322 DNA alone; Lanes 3-7: DNA with complex **3** at the concentrations of 0.01, 0.03, 0.05, 0.07 and 0.1 mM; Lane 8: pBR322 DNA alone; Lanes 9-13: DNA with complex **4** at the concentrations of 0.01, 0.03, 0.05, 0.07 and 0.1 mM, respectively. **Fig. S2**. Agarose GE patterns for the cleavage of pBR322 DNA by complex **1** in the

presence of  $H_2O_2$  (25 µM). Lane 1: 0.5 kb DNA Ladder; Lane 2: pBR322 DNA alone; Lanes 3-7: pBR322 DNA with complex **1** at the concentrations of 0.1, 0.3, 0.5, 0.7 and 1 mM with reaction time 5 h; Lanes 8-12: the time of reactions were 0, 3, 5, 7 and 9 h with concentration of 0.1 mM.

**Fig. S3.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.01 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction

products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 2.0, 3.0, 4.0 and 5.0 h, respectively.

**Fig. S4.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.02 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 2.0, 3.0, 4.0 and 5.0 h, respectively.

**Fig. S5.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.04 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 1.5, 2.0, 2.5 and 3.0 h, respectively.

**Fig. S6.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.05 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 20, 40, 60, 80, 100 and 120 min, respectively.

**Fig. S7.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.06 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively. **Fig. S8.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.07 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively. **Fig. S9.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.08 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively. **Fig. S10.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.09 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively. **Fig. S10.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.09 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively.

**Fig. S11.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.1 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 5, 10, 15, 20, 25 and 30 min, respectively.

**Fig. S12.** Time course of pBR322 DNA cleavage promoted by complex **2** (0.01 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 2.0, 3.0, 4.0 and 5.0 h, respectively.

**Fig. S13.** Time course of pBR322 DNA cleavage promoted by complex **2** (0.02 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 2.0, 3.0, 4.0 and 5.0 h, respectively.

**Fig. S14.** Time course of pBR322 DNA cleavage promoted by complex **2** (0.04 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 1.5, 2.0, 2.5 and 3.0 h, respectively.

**Fig. S15.** Time course of pBR322 DNA cleavage promoted by complex **2** (0.06 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 20, 40, 60, 80, 100 and 120 min, respectively.

**Fig. S16.** Time course of pBR322 DNA cleavage promoted by complex **2** (0.07 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 20, 40, 60, 80, 100 and 120 min, respectively.

**Fig. S17.** Time course of pBR322 DNA cleavage promoted by complex **2** (0.08 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 5, 10, 15, 20, 25 and 30 min, respectively.

**Fig. S18.** Time course of pBR322 DNA cleavage promoted by complex **2** (0.1 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 5, 10, 15, 20, 25 and 30 min, respectively. **Fig. S19.** Time course of pBR322 DNA cleavage promoted by complex **3** (0.2 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction

products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 2.0, 3.0, 4.0 and 5.0 h, respectively.

**Fig. S20.** Time course of pBR322 DNA cleavage promoted by complex **3** (0.3 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 1.5, 2.0, 2.5 and 3.0 h, respectively.

**Fig. S21.** Time course of pBR322 DNA cleavage promoted by complex **3** (0.4 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 1.5, 2.0 and 2.5 h, respectively.

**Fig. S22.** Time course of pBR322 DNA cleavage promoted by complex **3** (0.6 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 20, 40, 60, 80, 100 and 120 min, respectively.

**Fig. S23.** Time course of pBR322 DNA cleavage promoted by complex **3** (0.7 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively. **Fig. S24.** Time course of pBR322 DNA cleavage promoted by complex **3** (0.8 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively. **Fig. S25.** Time course of pBR322 DNA cleavage promoted by complex **3** (1.0 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively. **Fig. S26.** Time course of pBR322 DNA cleavage promoted by complex **4** (0.2 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively. **Fig. S26.** Time course of pBR322 DNA cleavage promoted by complex **4** (0.2 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 1.5, 2.0, 3.0 and 4.0 h, respectively.

**Fig. S27.** Time course of pBR322 DNA cleavage promoted by complex **4** (0.3 mM) at 37 °C and pH 7.00 with H<sub>2</sub>O<sub>2</sub>. Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 1.5, 2.0, 2.5 and 3.0 h, respectively.

**Fig. S28.** Time course of pBR322 DNA cleavage promoted by complex **4** (0.4 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 20, 40, 60, 80, 100 and 120 min, respectively.

**Fig. S29.** Time course of pBR322 DNA cleavage promoted by complex **4** (0.6 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 20, 40, 60, 80, 100 and 120 min, respectively.

**Fig. S30.** Time course of pBR322 DNA cleavage promoted by complex **4** (0.7 mM) at 37 °C and pH 7.00 with H<sub>2</sub>O<sub>2</sub>. Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively. **Fig. S31.** Time course of pBR322 DNA cleavage promoted by complex **4** (0.8 mM) at 37 °C and pH 7.00 with H<sub>2</sub>O<sub>2</sub>. Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively. **Fig. S32.** Time course of pBR322 DNA cleavage promoted by complex **4** (1.0 mM) at 37 °C and pH 7.00 with H<sub>2</sub>O<sub>2</sub>. Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively. **Fig. S32.** Time course of pBR322 DNA cleavage promoted by complex **4** (1.0 mM) at 37 °C and pH 7.00 with H<sub>2</sub>O<sub>2</sub>. Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively. **Fig. S33.** (a) Time course of pBR322 DNA cleavage promoted by complex **1** (0.04 mM) at pH 7.0 and 37 °C. Inset: agarose GE patterns of the time-variable reaction products. Lanes1-7, reaction time were 0, 0.5, 1.0, 1.5, 2.0, 2.5 and 3.0 h, respectively. (b) Saturation kinetics plot of  $k_{obs}$  versus the concentrations of complex **1**.

**Fig. S34.** (a) Time course of pBR322 DNA cleavage promoted by complex **2** (0.1 mM) at pH 7.0 and 37 °C. Inset: agarose GE patterns of the time-variable reaction products. Lanes 1–7, reaction time were 0, 5, 10, 15, 20, 25 and 30 min, respectively. (b) Saturation kinetics plot of  $k_{obs}$  versus the concentrations of complex **2**.

**Fig. S35.** (a) Time course of pBR322 DNA cleavage promoted by complex **3** (0.4 mM) at pH 7.0 and 37 °C. Inset: agarose GE patterns of the time-variable reaction products. Lanes 1–7, reaction time were 0, 0.5, 1.0, 1.5, 2.0, 2.5 and 3.0 h, respectively. (b) Saturation kinetics plot of  $k_{obs}$  versus the concentrations of complex **3**.

Fig. S36. (a) Time course of pBR322 DNA cleavage promoted by complex 4 (0.04

mM) at pH 7.0 and 37 °C. Inset: agarose GE patterns of the time-variable reaction products. Lanes 1–7, reaction time were 0, 0.5, 1.0, 1.5, 2.0, 2.5 and 3.0 h, respectively. (b) Saturation kinetics plot of  $k_{obs}$  versus the concentrations of complex **4**.

**Fig. S37.** Agarose GE patterns for the cleavage of pBR322 DNA by complex **2** (0.01 mM) at pH 7.0 and 37°C for 5 h with  $H_2O_2$  (25  $\mu$ M), in the presence of DMSO (1 M, Lane 3), MeOH (1 M, Lane 4), KI (0.1 M, Lane 5), NaN<sub>3</sub> (0.1 M, Lane 6), EDTA (0.1 M, Lane 7). Lane 1, DNA alone and Lane 2: DNA + complex **2**.

**Fig. S38.** Agarose GE patterns for the cleavage of pBR322 DNA by complex **3** (0.8 mM) at pH 7.0 and 37°C for 5 h with  $H_2O_2$  (25  $\mu$ M), in the presence of DMSO (1 M, Lane 3), MeOH (1 M, Lane 4), KI (0.1 M, Lane 5), NaN<sub>3</sub> (0.1 M, Lane 6), EDTA (0.1 M, Lane 7). Lane 1, DNA alone and Lane 2: DNA + complex **3**.

**Fig. S39.** Agarose GE patterns for the cleavage of pBR322 DNA by complex **4** (0.8 mM) at pH 7.0 and 37°C for 5 h with  $H_2O_2$  (25  $\mu$ M), in the presence of DMSO (1 M, Lane 3), MeOH (1 M, Lane 4), KI (0.1 M, Lane 5), NaN<sub>3</sub> (0.1 M, Lane 6), EDTA (0.1 M, Lane 7). Lane 1, DNA alone and Lane 2: DNA + complex **4**.

**Fig. S40.** Fluorescence decrease of EB (3.03  $\mu$ M) induced by the competitive binding of complex **1** to CT DNA (2.4  $\mu$ M) in 5 mM Tris-HCl buffer (5 mM NaCl, pH 7.0) at room temperature, excitation 510 nm, emission 590 nm. Arrow shows the intensity changes upon the increase in the concentrations of complex **1**. The total concentrations of complex **1** were 0, 1.33, 3.32, 6.62, 11.86, 18.32, 37.86, 40.31, 58.38, 87.04, 129.43, 177.18, 239.74, 309.71  $\mu$ M.

**Fig. S41.** Plots of the relative fluorescence intensity (FI,  $I/I_0$ ) of EB against the concentrations of complex **1** in 5 mM Tris-HCl buffer (5 mM NaCl, pH 7.0) at room temperature, excitation 510 nm, emission 590 nm.

**Fig. S42.** Fluorescence decrease of EB (3.03  $\mu$ M) induced by the competitive binding of complex **2** to CT DNA (2.4  $\mu$ M) in 5 mM Tris-HCl buffer (5 mM NaCl, pH 7.0) at room temperature, excitation 510 nm, emission 590 nm. Arrow shows the intensity changes upon the increase in the concentrations of complex **2**. The total concentrations of complex **2** were 0, 1.33, 3.32, 6.62, 11.86, 18.32, 26.61, 35.99,

48.22, 66.00, 110.32, 160.13, 225.21, 297.75, 357.88 μM.

**Fig. S43.** Plots of the relative fluorescence intensity (FI,  $I/I_0$ ) of EB against the concentrations of complex **2** in 5 mM Tris-HCl buffer (5 mM NaCl, pH 7.0) at room temperature, excitation 510 nm, emission 590 nm.

**Fig. S44.** Fluorescence decrease of EB (3.03  $\mu$ M) induced by the competitive binding of complex **3** to CT DNA (2.4  $\mu$ M) in 5 mM Tris-HCl buffer (5 mM NaCl, pH 7.0) at room temperature, excitation 510 nm, emission 590 nm. Arrow shows the intensity changes upon the increase in the concentrations of complex **3**. The total concentrations of complex **3** were 0, 1.33, 3.32, 6.62, 11.86, 18.32, 27.88, 40.31, 58.38, 81.45, 114.00, 153.98, 199.15, 258.53, 325.24, 380.93, 428.14, 468.65  $\mu$ M.

**Fig. S45.** Plots of the relative fluorescence intensity (FI,  $I/I_0$ ) of EB against the concentrations of complex **3** in 5 mM Tris-HCl buffer (5 mM NaCl, pH 7.0) at room temperature, excitation 510 nm, emission 590 nm.

**Fig. S46.** Fluorescence decrease of EB (3.03  $\mu$ M) induced by the competitive binding of complex **4** to CT DNA (2.4  $\mu$ M) in 5 mM Tris-HCl buffer (5 mM NaCl, pH 7.0) at room temperature, excitation 510 nm, emission 590 nm. Arrow shows the intensity changes upon the increase in the concentration of complex **4**. The total concentrations of complex **4** were 0, 1.33, 4.64, 9.90, 16.39, 25.97, 38.46, 56.60, 85.37, 127.91, 175.82, 238.58, 308.76, 367.09, 416.34, 458.48  $\mu$ M.

**Fig. S47.** Plots of the relative fluorescence intensity (FI,  $I/I_0$ ) of EB against the concentrations of complex **4** in 5 mM Tris-HCl buffer (5 mM NaCl, pH 7.0) at room temperature, excitation 510 nm, emission 590 nm.



**Fig. S1** Agarose GE patterns for the cleavage of pBR322 DNA by complex **3** and complex **4** in the presence of  $H_2O_2$  (25  $\mu$ M). Lane 1: 0.5 kb DNA Ladder; Lane 2: pBR322 DNA alone; Lanes 3-7: DNA with complex **3** at the concentrations of 0.01, 0.03, 0.05, 0.07 and 0.1 mM; Lane 8: pBR322 DNA alone; Lanes 9-13: DNA with complex **4** at the concentrations of 0.01, 0.03, 0.05, 0.07 and 0.1 mM, respectively.



**Fig. S2**. Agarose GE patterns for the cleavage of pBR322 DNA by complex **1** in the presence of  $H_2O_2$  (25  $\mu$ M). Lane 1: 0.5 kb DNA Ladder; Lane 2: pBR322 DNA alone; Lanes 3-7: pBR322 DNA with complex **1** at the concentrations of 0.1, 0.3, 0.5, 0.7 and 1 mM with reaction time 5 h; Lanes 8-12: the time of reactions were 0, 3, 5, 7 and 9 h with concentration of 0.1 mM.



**Fig. S3.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.01 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 2.0, 3.0, 4.0 and 5.0 h, respectively.



**Fig. S4.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.02 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 2.0, 3.0, 4.0 and 5.0 h, respectively.



**Fig. S5.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.04 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 1.5, 2.0, 2.5 and 3.0 h, respectively.



**Fig. S6.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.05 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 20, 40, 60, 80, 100 and 120 min, respectively.



**Fig. S7.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.06 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively.



**Fig. S8.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.07 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively.



**Fig. S9.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.08 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively.



**Fig. S10.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.09 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively.



**Fig. S11.** Time course of pBR322 DNA cleavage promoted by complex **1** (0.1 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 5, 10, 15, 20, 25 and 30 min, respectively.



**Fig. S12.** Time course of pBR322 DNA cleavage promoted by complex **2** (0.01 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 2.0, 3.0, 4.0 and 5.0 h, respectively.



**Fig. S13.** Time course of pBR322 DNA cleavage promoted by complex **2** (0.02 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 2.0, 3.0, 4.0 and 5.0 h, respectively.



**Fig. S14.** Time course of pBR322 DNA cleavage promoted by complex **2** (0.04 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 1.5, 2.0, 2.5 and 3.0 h, respectively.



**Fig. S15.** Time course of pBR322 DNA cleavage promoted by complex **2** (0.06 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 20, 40, 60, 80, 100 and 120 min, respectively.



**Fig. S16.** Time course of pBR322 DNA cleavage promoted by complex **2** (0.07 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 20, 40, 60, 80, 100 and 120 min, respectively.



**Fig. S17.** Time course of pBR322 DNA cleavage promoted by complex **2** (0.08 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 5, 10, 15, 20, 25 and 30 min, respectively.



**Fig. S18.** Time course of pBR322 DNA cleavage promoted by complex **2** (0.1 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 5, 10, 15, 20, 25 and 30 min, respectively.



**Fig. S19.** Time course of pBR322 DNA cleavage promoted by complex **3** (0.2 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 2.0, 3.0, 4.0 and 5.0 h, respectively.



**Fig. S20.** Time course of pBR322 DNA cleavage promoted by complex **3** (0.3 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 1.5, 2.0, 2.5 and 3.0 h, respectively.



**Fig. S21.** Time course of pBR322 DNA cleavage promoted by complex **3** (0.4 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 1.5, 2.0 and 2.5 h, respectively.



**Fig. S22.** Time course of pBR322 DNA cleavage promoted by complex **3** (0.6 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 20, 40, 60, 80, 100 and 120 min, respectively.



**Fig. S23.** Time course of pBR322 DNA cleavage promoted by complex **3** (0.7 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively.



**Fig. S24.** Time course of pBR322 DNA cleavage promoted by complex **3** (0.8 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively.



**Fig. S25.** Time course of pBR322 DNA cleavage promoted by complex **3** (1.0 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively.



**Fig. S26.** Time course of pBR322 DNA cleavage promoted by complex **4** (0.2 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 1.5, 2.0, 3.0 and 4.0 h, respectively.



**Fig. S27.** Time course of pBR322 DNA cleavage promoted by complex **4** (0.3 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 0.5, 1.0, 1.5, 2.0, 2.5 and 3.0 h, respectively.



**Fig. S28.** Time course of pBR322 DNA cleavage promoted by complex **4** (0.4 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 20, 40, 60, 80, 100 and 120 min, respectively.



**Fig. S29.** Time course of pBR322 DNA cleavage promoted by complex **4** (0.6 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 20, 40, 60, 80, 100 and 120 min, respectively.



**Fig. S30.** Time course of pBR322 DNA cleavage promoted by complex **4** (0.7 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively.



**Fig. S31.** Time course of pBR322 DNA cleavage promoted by complex **4** (0.8 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively.



**Fig. S32.** Time course of pBR322 DNA cleavage promoted by complex **4** (1.0 mM) at 37 °C and pH 7.00 with  $H_2O_2$ . Inset: agarose GE patterns of the time-variable reaction products. Lanes 1-7, reaction time were 0, 10, 20, 30, 40, 50 and 60 min, respectively.



**Fig. S33.** (a) Time course of pBR322 DNA cleavage promoted by complex **1** (0.04 mM) at pH 7.0 and 37 °C. Inset: agarose GE patterns of the time-variable reaction products. Lanes 1–7, reaction time were 0, 0.5, 1.0, 1.5, 2.0, 2.5 and 3.0 h, respectively. (b) Saturation kinetics plot of  $k_{obs}$  versus the concentrations of complex **1**.



**Fig. S34.** (a) Time course of pBR322 DNA cleavage promoted by complex **2** (0.1 mM) at pH 7.0 and 37 °C. Inset: agarose GE patterns of the time-variable reaction products. Lanes 1–7, reaction time were 0, 5, 10, 15, 20, 25 and 30 min, respectively. (b) Saturation kinetics plot of  $k_{obs}$  versus the concentrations of complex **2**.



**Fig. S35.** (a) Time course of pBR322 DNA cleavage promoted by complex **3** (0. 4 mM) at pH 7.0 and 37 °C. Inset: agarose GE patterns of the time-variable reaction products. Lanes 1–7, reaction time were 0, 0.5, 1.0, 1.5, 2.0, 2.5 and 3.0 h, respectively. (b) Saturation kinetics plot of  $k_{obs}$  versus the concentrations of complex **3**.



**Fig. S36.** (a) Time course of pBR322 DNA cleavage promoted by complex **4** (0.04 mM) at pH 7.0 and 37 °C. Inset: agarose GE patterns of the time-variable reaction products. Lanes 1–7, reaction time were 0, 0.5, 1.0, 1.5, 2.0, 2.5 and 3.0 h, respectively. (b) Saturation kinetics plot of  $k_{obs}$  versus the concentrations of complex **4**.



**Fig. S37.** Agarose GE patterns for the cleavage of pBR322 DNA by complex **2** (0.01 mM) at pH 7.0 and 37°C for 5 h with  $H_2O_2$  (25  $\mu$ M), in the presence of DMSO (1 M, Lane 3), MeOH (1 M, Lane 4), KI (0.1 M, Lane 5), NaN<sub>3</sub> (0.1 M, Lane 6), EDTA (0.1 M, Lane 7). Lane 1, DNA alone and Lane 2: DNA + complex **2**.



**Fig. S38.** Agarose GE patterns for the cleavage of pBR322 DNA by complex **3** (0.8 mM) at pH 7.0 and 37°C for 5 h with  $H_2O_2$  (25  $\mu$ M), in the presence of DMSO (1 M, Lane 3), MeOH (1 M, Lane 4), KI (0.1 M, Lane 5), NaN<sub>3</sub> (0.1 M, Lane 6), EDTA (0.1 M, Lane 7). Lane 1, DNA alone and Lane 2: DNA + complex **3**.



**Fig. S39.** Agarose GE patterns for the cleavage of pBR322 DNA by Complex **4** (0.8 mM) at pH 7.0 and 37°C for 5 h with  $H_2O_2$  (25  $\mu$ M), in the presence of DMSO (1 M, Lane 3), MeOH (1 M, Lane 4), KI (0.1 M, Lane 5), NaN<sub>3</sub> (0.1 M, Lane 6), EDTA (0.1 M, Lane 7). Lane 1, DNA alone and Lane 2: DNA + complex **4**.



**Fig. S40.** Fluorescence decrease of EB (3.03  $\mu$ M) induced by the competitive binding of complex **1** to CT DNA (2.4  $\mu$ M) in 5 mM Tris-HCl buffer (5 mM NaCl, pH 7.0) at room temperature, excitation 510 nm, emission 590 nm. Arrow shows the intensity changes upon the increase in the concentrations of complex **1**. The total concentrations of complex **1** were 0, 1.33, 3.32, 6.62, 11.86, 18.32, 37.86, 40.31, 58.38, 87.04, 129.43, 177.18, 239.74, 309.71  $\mu$ M.



**Fig. S41.** Plots of the relative fluorescence intensity (FI,  $I/I_0$ ) of EB against the concentrations of complex **1** in 5 mM Tris-HCl buffer (5 mM NaCl, pH 7.0) at room temperature, excitation 510 nm, emission 590 nm.



**Fig. S42.** Fluorescence decrease of EB (3.03  $\mu$ M) induced by the competitive binding of complex **2** to CT DNA (2.4  $\mu$ M) in 5 mM Tris-HCl buffer (5 mM NaCl, pH 7.0) at room temperature, excitation 510 nm, emission 590 nm. Arrow shows the intensity changes upon the increase in the concentrations of complex **2**. The total concentrations of complex **2** were 0, 1.33, 3.32, 6.62, 11.86, 18.32, 26.61, 35.99, 48.22, 66.00, 110.32, 160.13, 225.21, 297.75, 357.88  $\mu$ M.



**Fig. S43.** Plots of the relative fluorescence intensity (FI,  $I/I_0$ ) of EB against the concentrations of complex **2** in 5 mM Tris-HCl buffer (5 mM NaCl, pH 7.0) at room temperature, excitation 510 nm, emission 590 nm.



**Fig. S44.** Fluorescence decrease of EB (3.03  $\mu$ M) induced by the competitive binding of complex **3** to CT DNA (2.4  $\mu$ M) in 5 mM Tris-HCl buffer (5 mM NaCl, pH 7.0) at room temperature, excitation 510 nm, emission 590 nm. Arrow shows the intensity changes upon the increase in the concentrations of complex **3**. The total concentrations of complex **3** were 0, 1.33, 3.32, 6.62, 11.86, 18.32, 27.88, 40.31, 58.38, 81.45, 114.00, 153.98, 199.15, 258.53, 325.24, 380.93, 428.14, 468.65  $\mu$ M.



**Fig. S45.** Plots of the relative fluorescence intensity (FI,  $I/I_0$ ) of EB against the concentrations of complex **3** in 5 mM Tris-HCl buffer (5 mM NaCl, pH 7.0) at room temperature, excitation 510 nm, emission 590 nm.



**Fig. S46.** Fluorescence decrease of EB (3.03  $\mu$ M) induced by the competitive binding of complex **4** to CT DNA (2.4  $\mu$ M) in 5 mM Tris-HCl buffer (5 mM NaCl, pH 7.0) at room temperature, excitation 510 nm, emission 590 nm. Arrow shows the intensity changes upon the increase in the concentration of complex **4**. The total concentrations of complex **4** were 0, 1.33, 4.64, 9.90, 16.39, 25.97, 38.46, 56.60, 85.37, 127.91, 175.82, 238.58, 308.76, 367.09, 416.34, 458.48  $\mu$ M.



**Fig. S47.** Plots of the relative fluorescence intensity (FI,  $I/I_0$ ) of EB against the concentrations of complex **4** in 5 mM Tris-HCl buffer (5 mM NaCl, pH 7.0) at room temperature, excitation 510 nm, emission 590 nm.