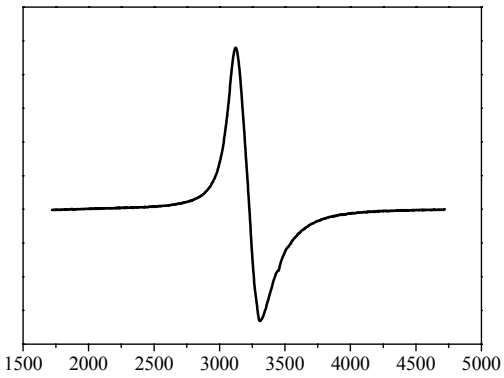
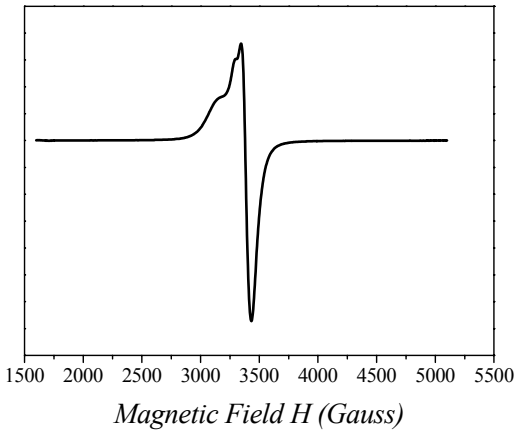
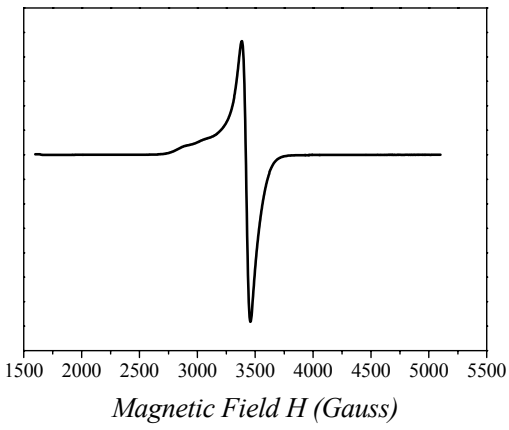


(1)

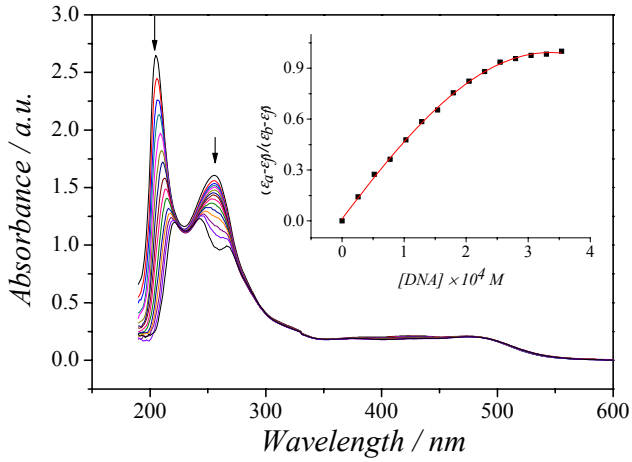


(2)

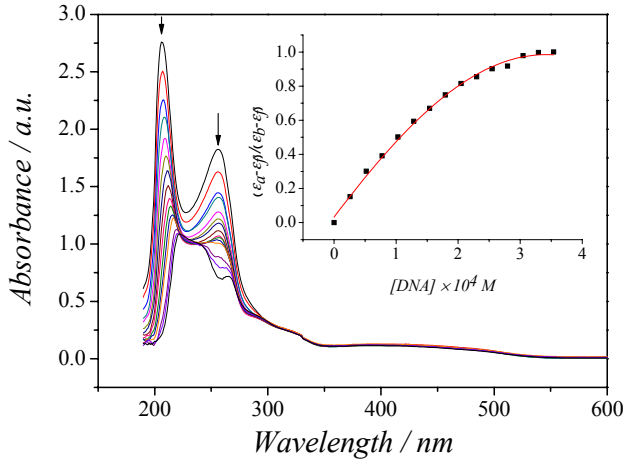


(4)

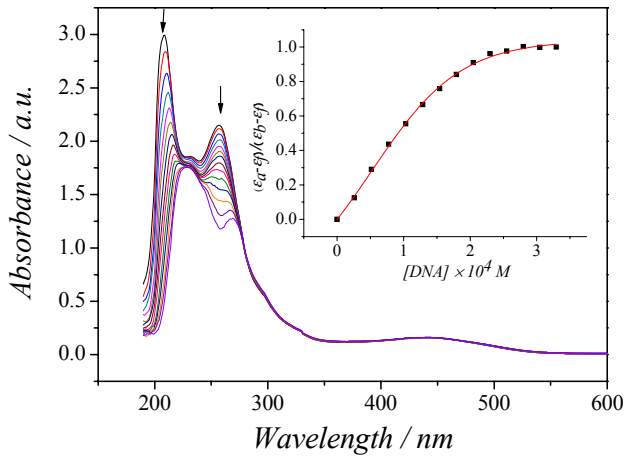
Fig. 1S X-Band ESR spectra of complexes **1, 2,** and **4** in the solid state at room temperature


Absorbance / a.u.
Wavelength / nm
(εa-εf)/(εb-εf)
[DNA] ×10⁴ M

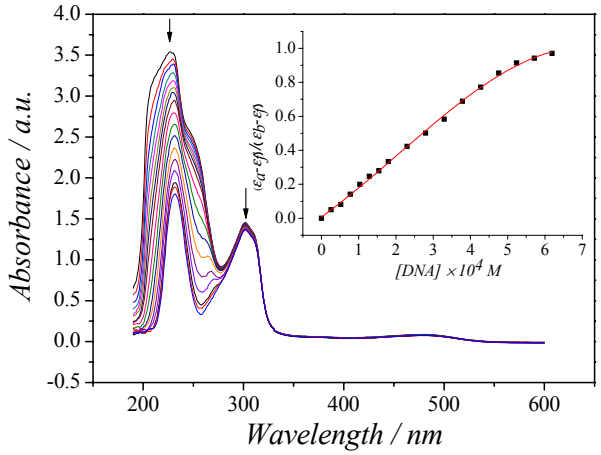
(1)


Absorbance / a.u.
Wavelength / nm
(εa-εf)/(εb-εf)
[DNA] ×10⁴ M

(2)


Absorbance / a.u.
Wavelength / nm
(εa-εf)/(εb-εf)
[DNA] ×10⁴ M

(3)



(4)

Fig. 2S Absorption spectra of 3.85×10^{-5} M complexes **1**, **2**, **3** and **4** in the presence of increasing amounts of CT-DNA at room temperature in Tris-HCl / NaCl buffer (pH = 7.2). Arrows indicate the change in absorbance upon increasing the DNA concentration. Insert: Plot of $(\epsilon_a-\epsilon_f) / (\epsilon_b-\epsilon_f)$ versus [DNA] for the titration of DNA to Cu(II) complexes.

Table 1S Absorption spectral properties of copper (II) complexes bound to CT-DNA.

complex		λ_{max} (nm)	change in absorbance	$\Delta\varepsilon$ (%)	red shift (nm)
$[Cu(1,4\text{-tpbd})Br_2]$	**1**	205	hypochromism	55	16
$[Cu_2(1,4\text{-tpbd})(H_2O)_4]^{4+}$	**2**	206	hypochromism	61	16
$[Cu_2(1,4\text{-tpbd})(1,10\text{-phen})_2(DMF)_2]^{4+}$	**3**	208	hypochromism	41	19
$[Cu_2(1,4\text{-tpbd})(2,2'\text{-bpy})_2(ClO_4)_2]^{2+}$	**4**	227	hypochromism	49	5

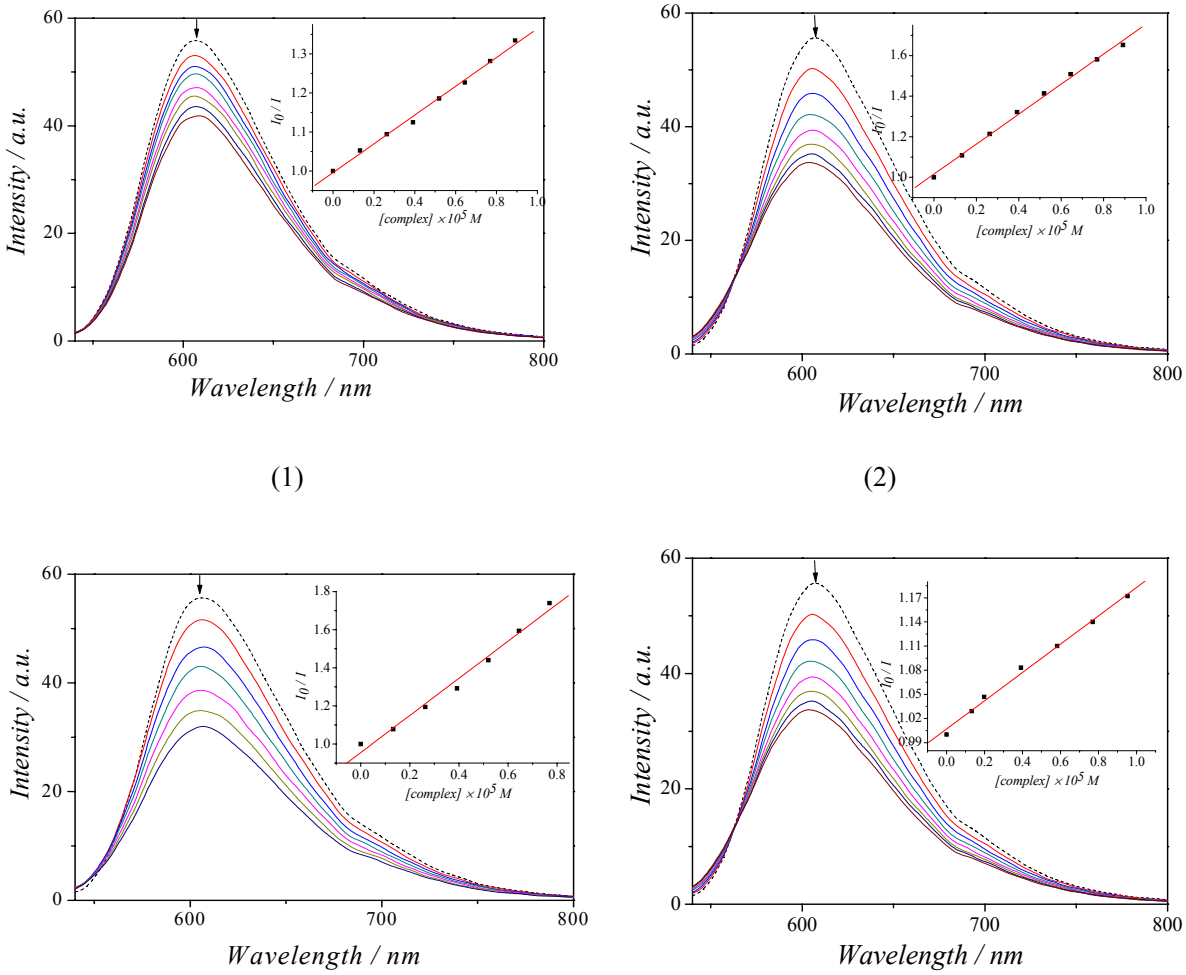


Fig. 3S Fluorescence quenching curves of EB bound to CT-DNA by complexes **1** (0-4.46 × 10^{-5} M), **2** (0-4.46 × 10^{-5} M), **3** (0-3.85 × 10^{-5} M) and **4** (0-4.76 × 10^{-5} M). The dash line shows the intensity in the absence of complexes. Inset: Plot of I_0 / I versus [complex].

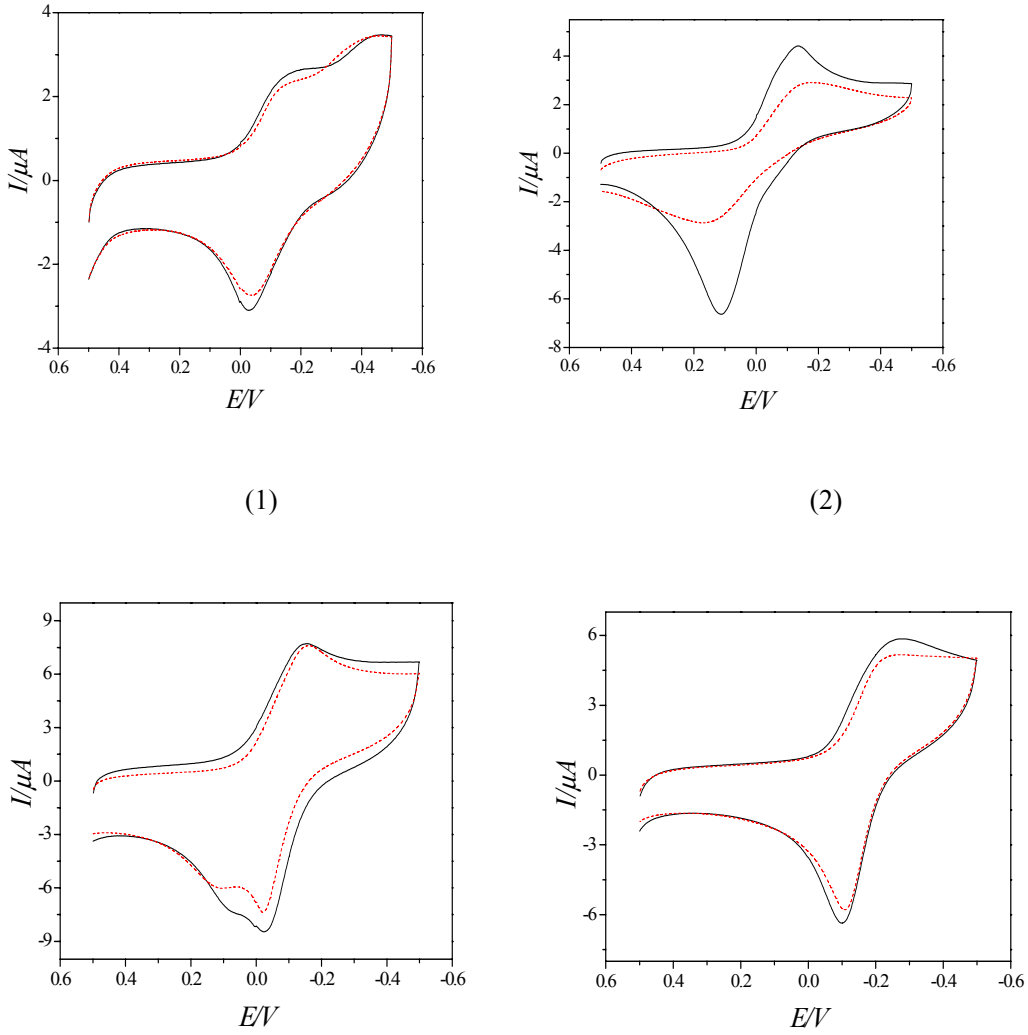


Fig. 4S Cyclic voltammograms of complexes **1, 2, 3** and **4** in absence (solid line) and presence (dash line) of CT-DNA in 10 mM Tris–HCl / 50 mM NaCl buffer (pH = 7.2). Scan rate: 100 $mV \cdot s^{-1}$.

Table 2S Electrochemical data for complexes **1, 2, 3, 4** in the absence and presence of CT-DNA

Complex	E_{pa} (mV)	E_{pc} (mV)	$E_{1/2}$ (mV)	ΔE (mV)*
1	–28, –39	–160, –137	–94, –88	6.0
2	113, 166	–135, –181	–11, –7.5	3.5
3	–24, –20	–157, –159	–90.5, –89.5	1.0
4	–99, –109	–281, –268	–190, –188.5	1.5

*ΔE indicates the positive shifts for the four copper(II) complexes in the absence and presence of CT-DNA. ΔE = (E_{pa} + E_{pc}) / 2, where E_{pa} and E_{pc} are anodic and cathodic peak potentials. $\Delta E = E_{pa}$- E_{pc}, i_{pa} and i_{pc} are anodic and cathodic peak currents.

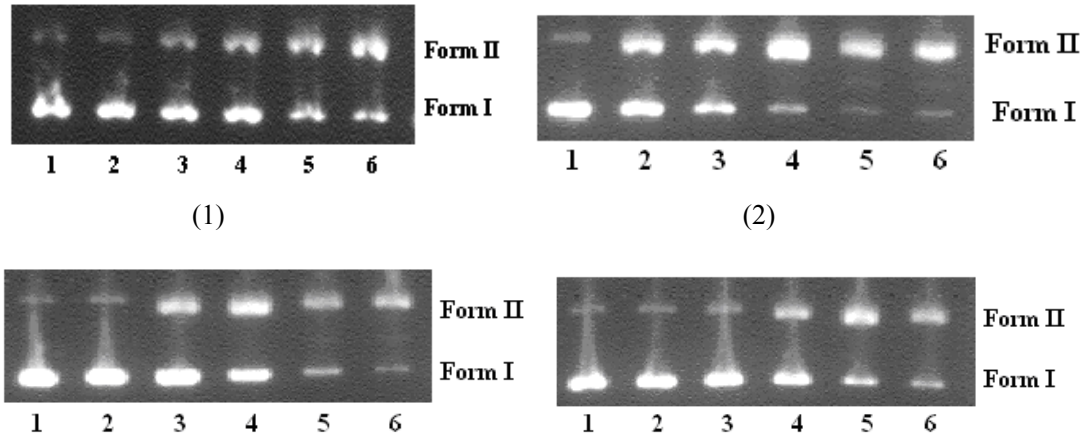


Fig. 5S Gel electrophoresis diagrams showing the cleavage of pBR322 DNA (0.1 μg / μL) at different complex concentrations in Tris-HCl / NaCl buffer (pH = 7.2) and 37 □ for 3 h. (1) Lane 1: DNA control; Lane 2-6: DNA + **1** (0.005, 0.02, 0.035, 0.1, 0.2 mM), respectively; (2) Lane 1: DNA control; Lane 2-6: DNA + **2** (0.005, 0.02, 0.035, 0.1, 0.15 mM), respectively; (3) Lane 1: DNA control; Lane 2-6: DNA + **3** (0.005, 0.02, 0.035, 0.1, 0.2 mM), respectively; (4) Lane 1: DNA control; Lane 2-6: DNA + **4** (0.005, 0.02, 0.035, 0.1, 0.2 mM), respectively.

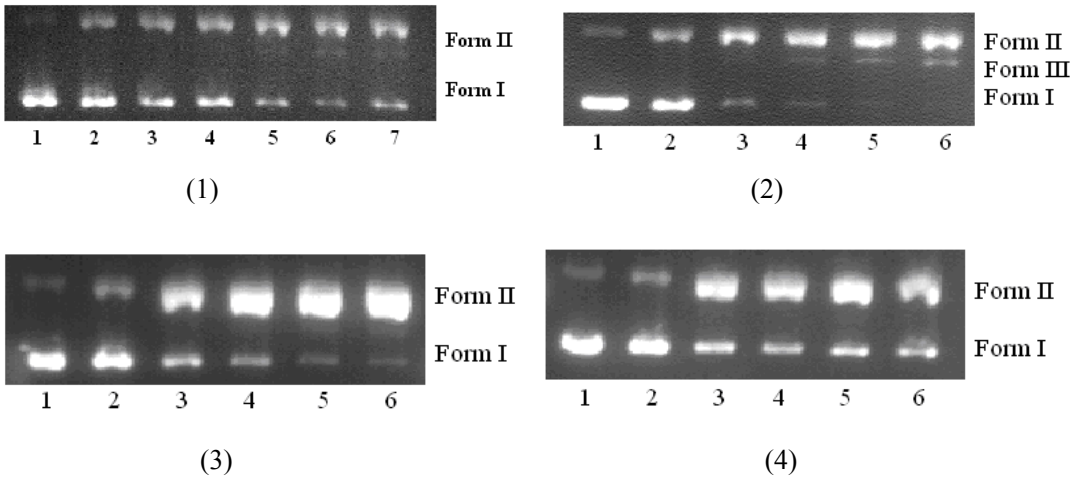


Fig. 6S Time-dependence of pBR322 DNA cleavage by complexes in Tris-HCl / NaCl buffer (pH = 7.2) at 37 □. (1) Lane 1: DNA control (4 h); Lane 2-7: DNA + 0.4 mM **1** (0, 0.5, 1, 2, 3, 4 h), respectively; (2) Lane 1: DNA control (3 h); Lane 2-6 DNA + 0.15 mM **2** (0 h, 0.5 h, 1 h, 2 h, 3 h), respectively; (3) Lane 1: DNA control (3 h); Lane 2-6 DNA + 0.15 mM **3** (0 h, 0.5 h, 1 h, 2 h, 3 h), respectively; (4) Lane 1: DNA control (3 h); Lane 2-6 DNA + 0.1 mM **4** (0 h, 0.5 h, 1 h, 2 h, 3 h), respectively.

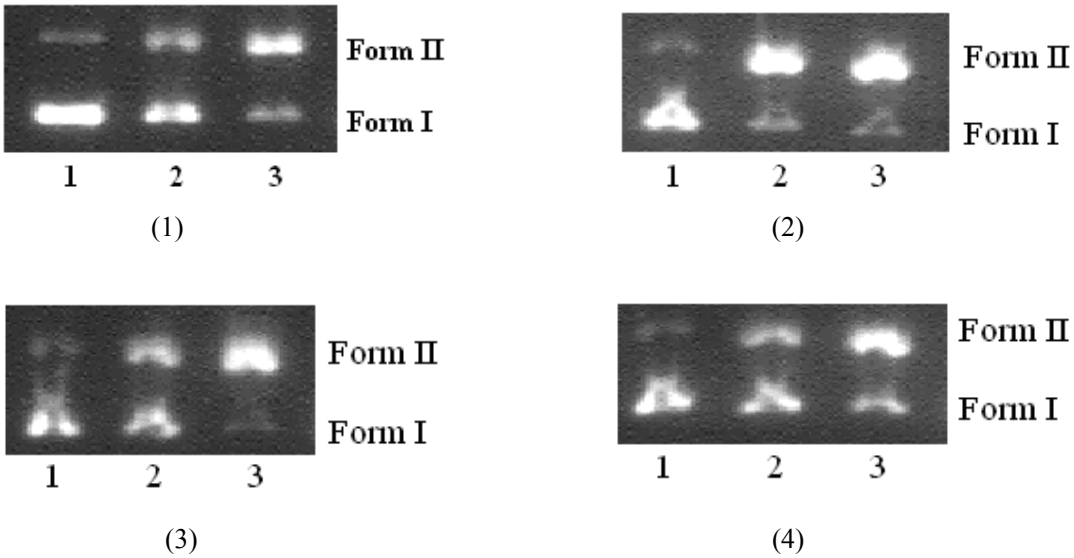


Fig. 7S Cleavage of pBR322 DNA (0.1μg / μL) at room temperature for 3 h. (1) Lane 1: DNA control; Lane 2: DNA + 0.4 mM **1** in nitrogen atmosphere; Lane 3: DNA + 0.4 mM **1** in air; (2) Lane 1: DNA control; Lane 2: DNA + 0.035 mM **2** in N_2 atmosphere; Lane 3: DNA + 0.035 mM **2** in air; (3) Lane 1: DNA control; Lane 2: DNA + 0.05 mM **3** in N_2 atmosphere; Lane 3: DNA + 0.05 mM **3** in air; (4) Lane 1: DNA control; Lane 2: DNA + 0.05 mM **4** in N_2 atmosphere; Lane 3: DNA + 0.05 mM **4** in air.

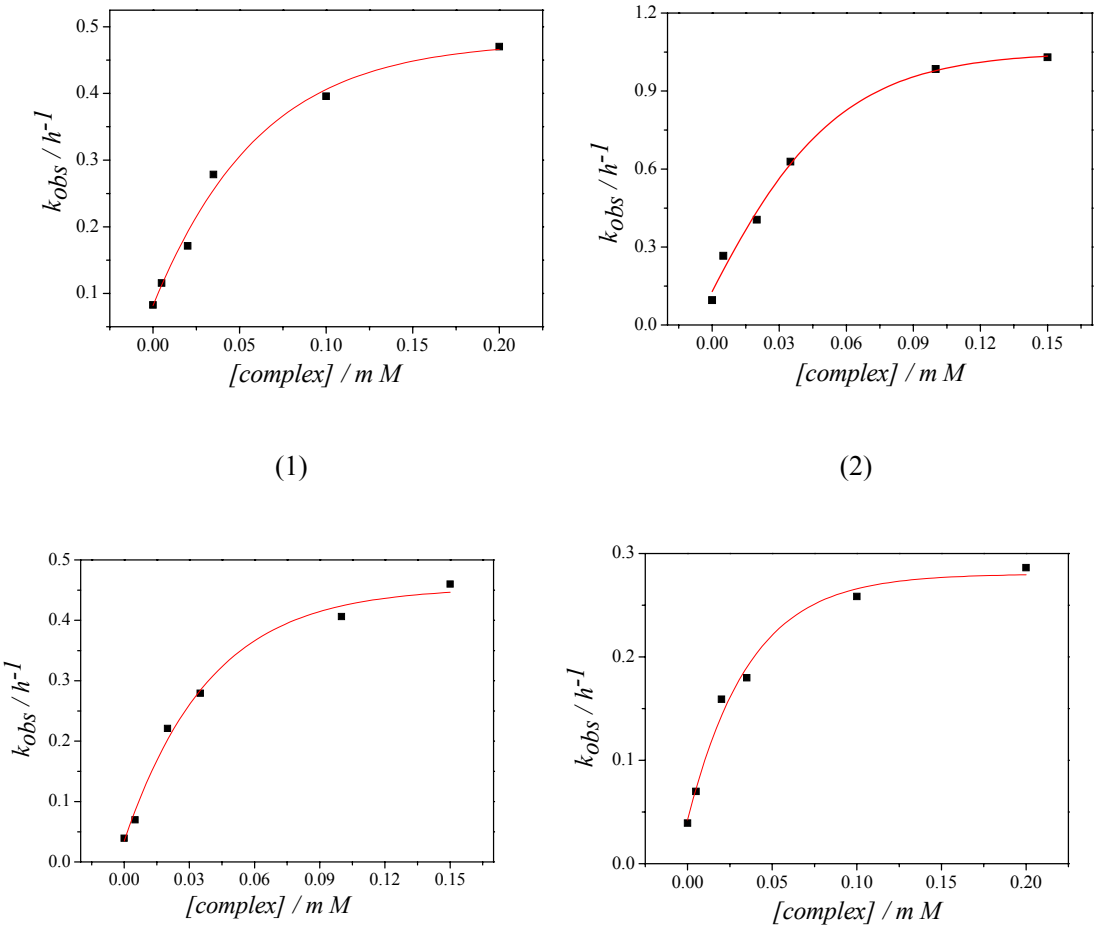


Fig. 8S Kinetics for the cleavage of plasmid pBR322 DNA by **1, 2, 3** and **4** in Tris-HCl / NaCl buffer (pH = 7.2) at 37 □ for 3h.