For Submission to *J. Chem. Soc. Dalton Trans.*

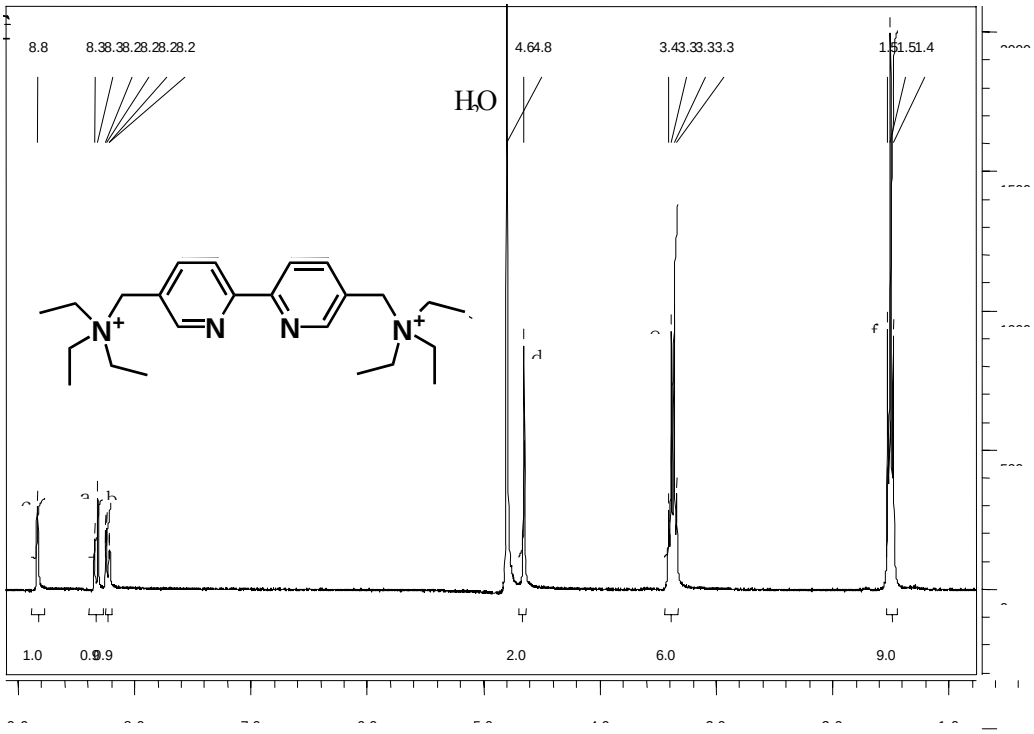
Double-strand DNA cleavage by copper complexes of 2,2'-dipyridyl with electropositive pendants

Yan An, Ming-Liang Tong, Liang-Nian Ji and Zong-Wan Mao*

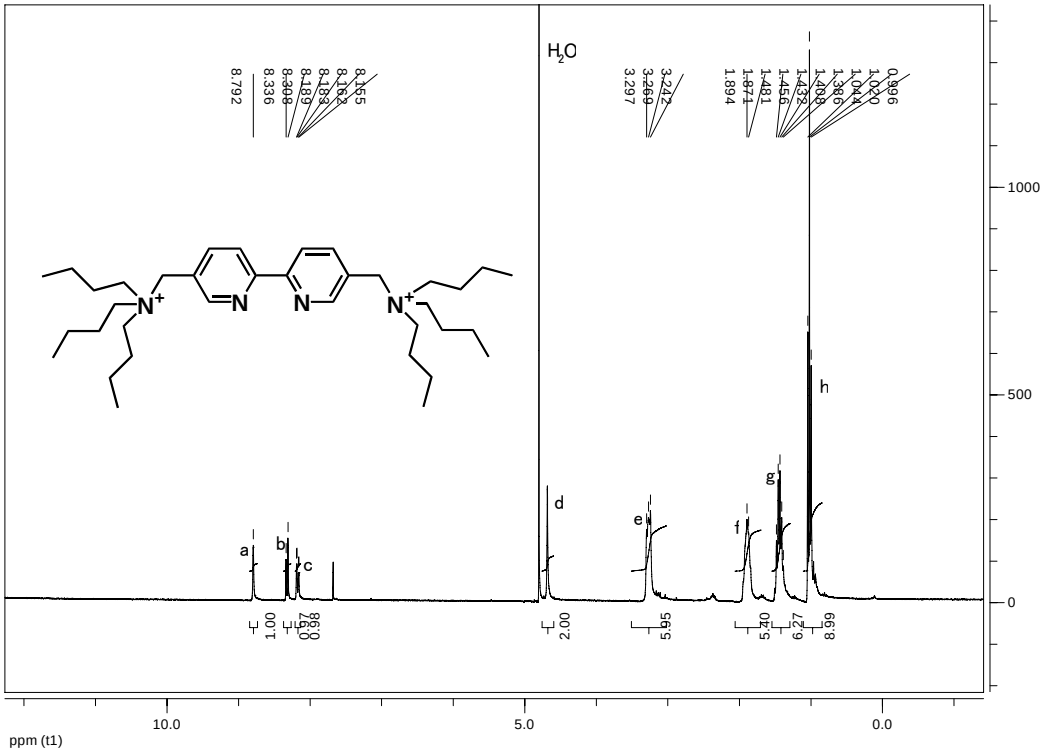
School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, China. Fax: (+86) 20 84112245; E-mail: cesmzw@zsu.edu.cn

Supporting information available: The ^{1}H-NMR and MS spectra of the ligands, the cif files of **1** and **2**, the T_m curves of DNA, the agarose gel electrophoresis and corresponding time course of DNA cleavage by the complexes.

1. **Fig. 1S** ^{1}H-NMR spectra of $\mathbf{L^1}$ (a) and $\mathbf{L^2}$ (b).
2. **Fig. 2S** ESI-MS spectra of $\mathbf{L^1}$ (a) and $\mathbf{L^2}$ (b)
3. **Fig. 3S** T_m curves of 100 μM CT DNA in 20 mM pH 8.0 HEPES buffer, 0.1 M $NaClO_4$, containing no Cu complex(■), 10 μM of **1**(▼), 20 μM of **1**(▲), 10 μM of **2**(◄) and 20 μM of **2**(►).
4. **Fig. 4S** Agarose gel showing cleavage of 38 μM pBR322 DNA incubated with 150 μM of complex in 20 mM HEPES, pH 7.2 at 37 ^{o}C for 1h for **1** and 24h for **2**. Lane C: DNA control, Lane 1: DNA + **1**, Lanes 2-4: DNA + **1** +100U/mL, 500U/mL, 1,000U/mL Catalase, Lane 5: DNA + **2**, Lanes 6-8: DNA + **2** +100U/mL, 500U/mL, 1,000U/mL Catalase.
5. **Fig. 5S** Agarose gel electrophoresis (a) and corresponding time course plots (b) showing cleavage of pBR322 DNA by complex **1** (30-300 μM) and **2** (30-210 μM) in 20 mM pH 7.2 HEPES buffer at 37 ^{o}C. In (a), lane C means DNA control, in (b), symbols ■ indicates the experimental data for the SC forms. The lines connecting them are single exponential fits.

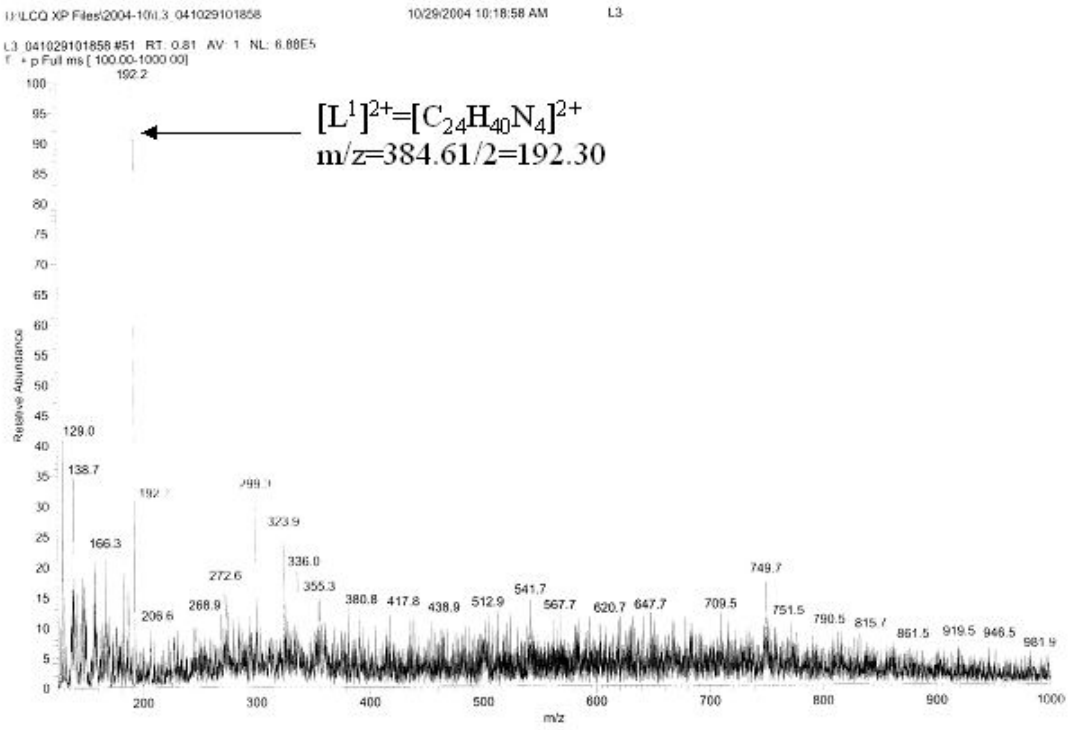


(a)

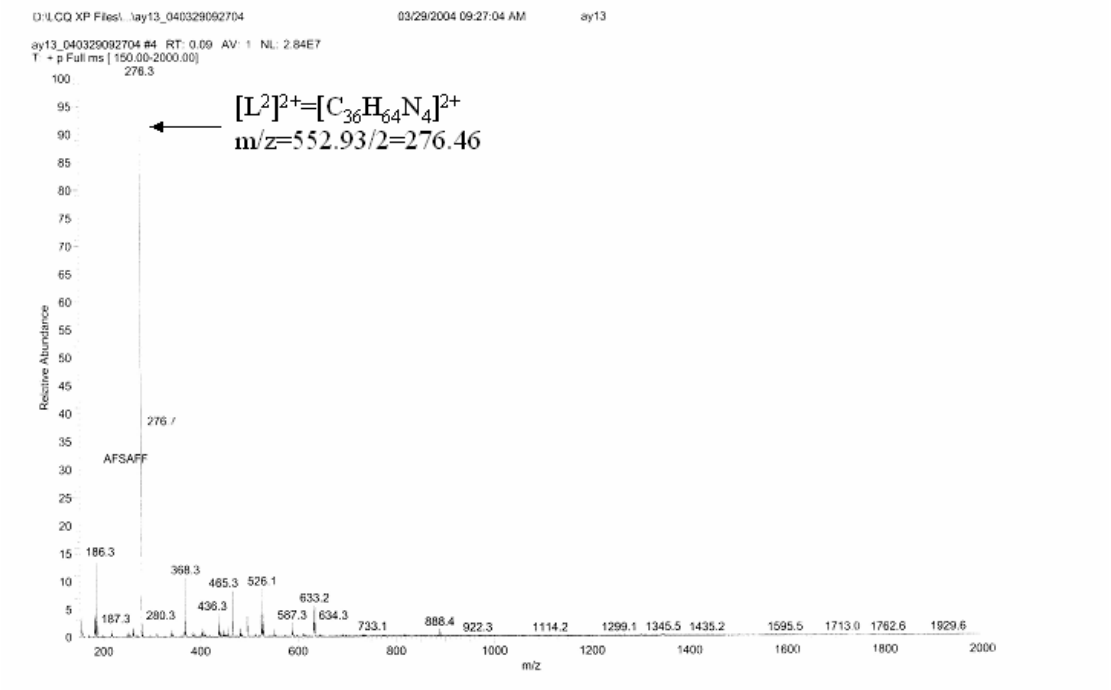


(b)

Fig. 1S ^{1}H-NMR spectra of $\mathbf{L^1}$ (a) and $\mathbf{L^2}$ (b).



(a)



(b)

Fig. 2S ESI-MS spectra of $\mathbf{L^1}$ (a) and $\mathbf{L^2}$ (b)

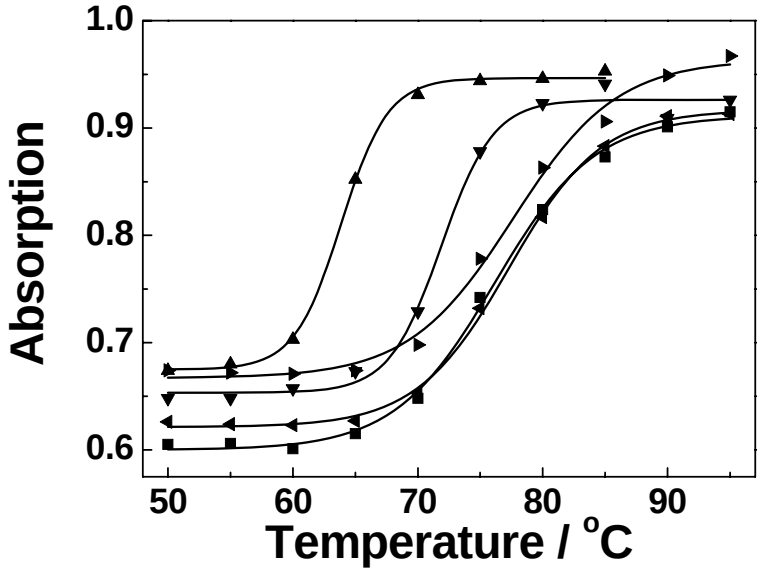


Fig. 3S T_m curves of 100 μM CT DNA in 20 mM pH 8.0 HEPES buffer, 0.1 M $NaClO_4$, containing no Cu complex(■), 10 μM of **1**(▼), 20 μM of **1**(▲), 10 μM of **2**(◄) and 20 μM of **2**(►).

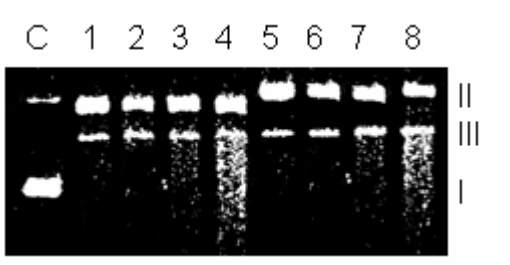
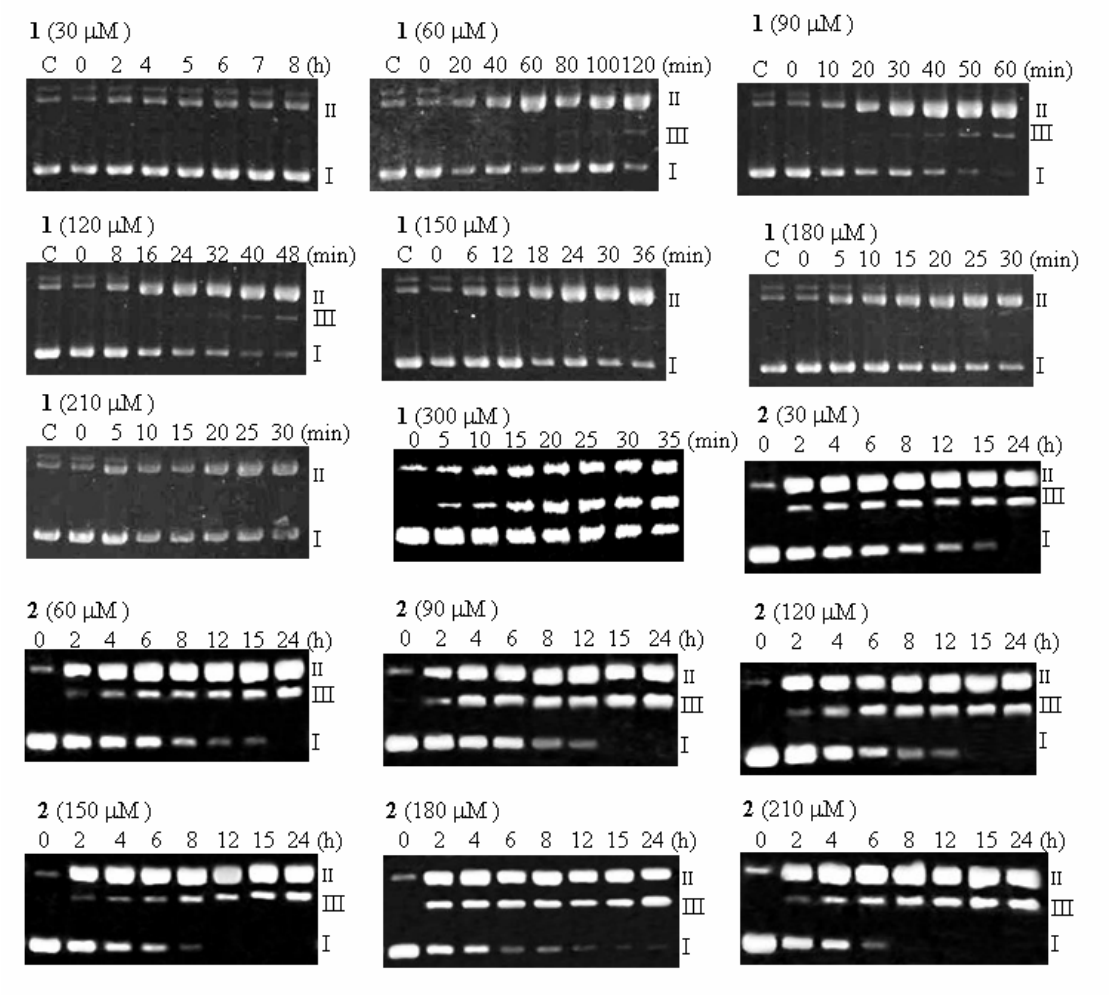
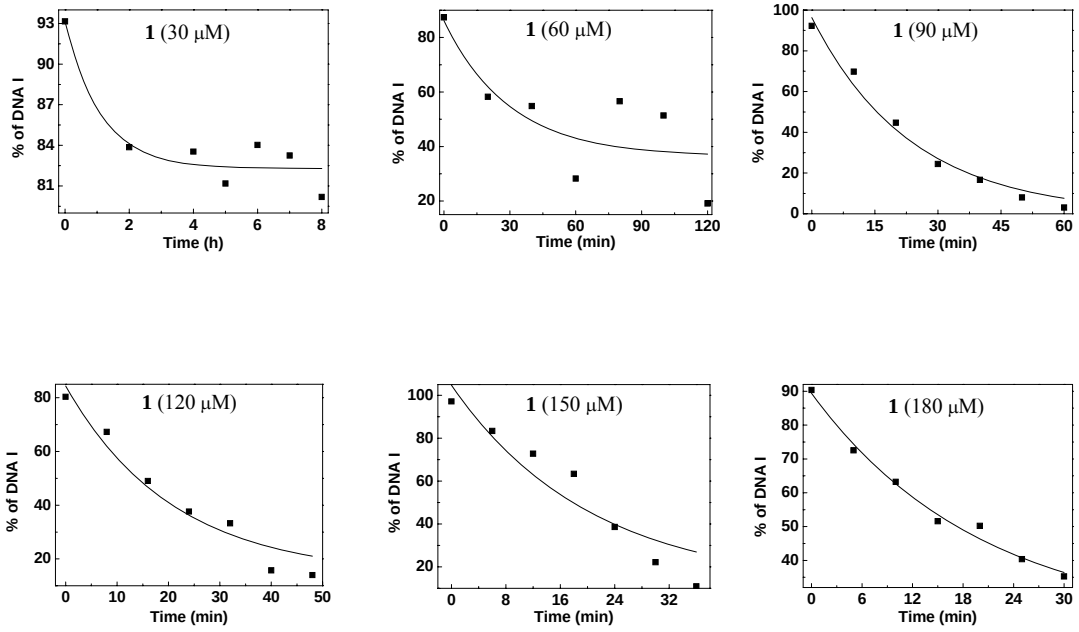
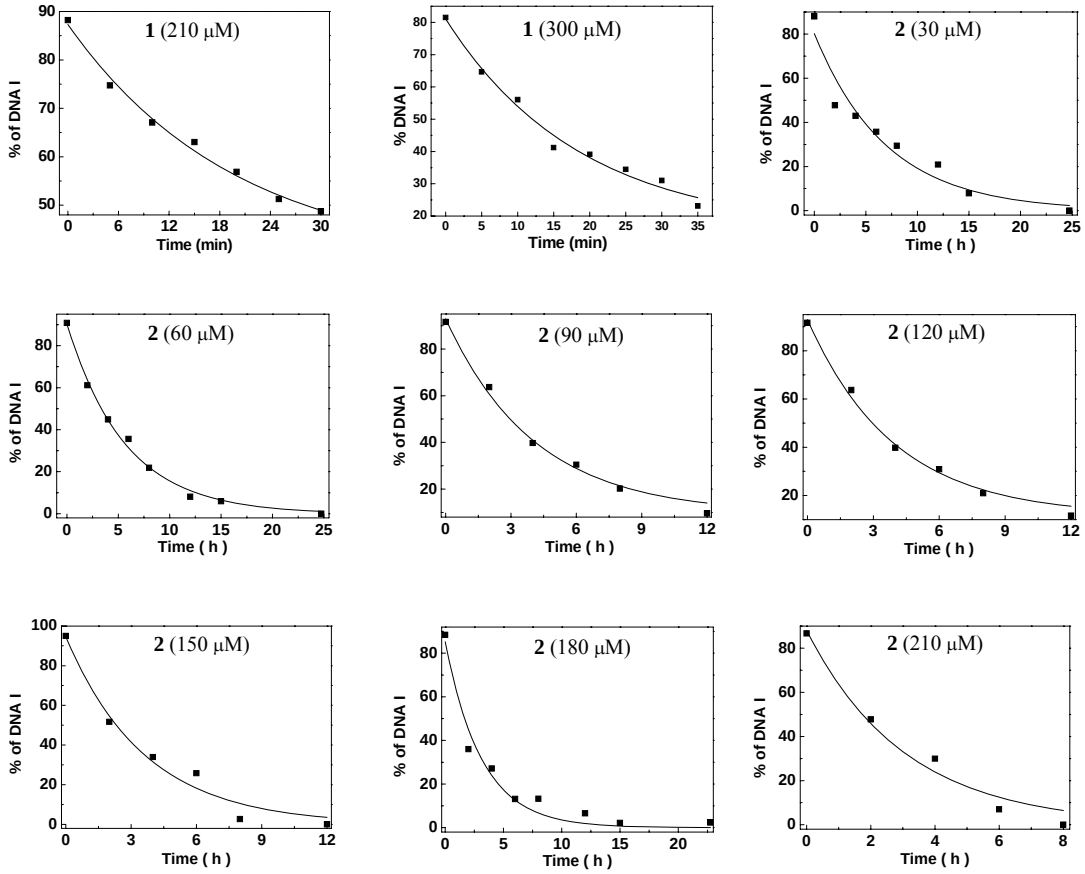


Fig. 4S Agarose gel showing cleavage of 38 μM pBR322 DNA incubated with 150 μM of complex in 20 mM HEPES, pH 7.2 at 37 °C for 1h for **1** and 24h for **2**. Lane C: DNA control, Lane 1: DNA + **1**, Lanes 2-4: DNA + **1** +100U/mL, 500U/mL, 1,000U/mL Catalase, Lane 5: DNA + **2**, Lanes 6-8: DNA + **2** +100U/mL, 500U/mL, 1,000U/mL Catalase.


1 (30 μM)
C 0 2 4 5 6 7 8 (h)
1 (60 μM)
C 0 20 40 60 80 100120 (min)
1 (90 μM)
C 0 10 20 30 40 50 60 (min)
1 (120 μM)
C 0 8 16 24 32 40 48 (min)
1 (150 μM)
C 0 6 12 18 24 30 36 (min)
1 (180 μM)
C 0 5 10 15 20 25 30 (min)
1 (210 μM)
C 0 5 10 15 20 25 30 (min)
1 (300 μM)
0 5 10 15 20 25 30 35 (min)
2 (30 μM)
0 2 4 6 8 12 15 24 (h)
2 (60 μM)
0 2 4 6 8 12 15 24 (h)
2 (90 μM)
0 2 4 6 8 12 15 24 (h)
2 (120 μM)
0 2 4 6 8 12 15 24 (h)
2 (150 μM)
0 2 4 6 8 12 15 24 (h)
2 (180 μM)
0 2 4 6 8 12 15 24 (h)
2 (210 μM)
0 2 4 6 8 12 15 24 (h)
II
III
I

(a)


1 (30 μM)
% of DNA I
Time (h)
1 (60 μM)
% of DNA I
Time (min)
1 (90 μM)
% of DNA I
Time (min)
1 (120 μM)
% of DNA I
Time (min)
1 (150 μM)
% of DNA I
Time (min)
1 (180 μM)
% of DNA I
Time (min)



(b)

Fig. 5S Agarose gel electrophoresis (a) and corresponding time course plots (b) showing cleavage of pBR322 DNA by complex **1** (30-300 μM)and **2** (30-210 μM) in 20 mM pH 7.2 HEPES buffer at 37 ^{o}C. In (a), lane C means DNA control, in (b), symbols ■ indicates the experimental data for the SC forms. The lines connecting them are single exponential fits.