Supporting Information for

Self-activating nuclease and anticancer activities of copper(II) complexes with aryl-modified 2,6-di(thiazol-2-yl)pyridine

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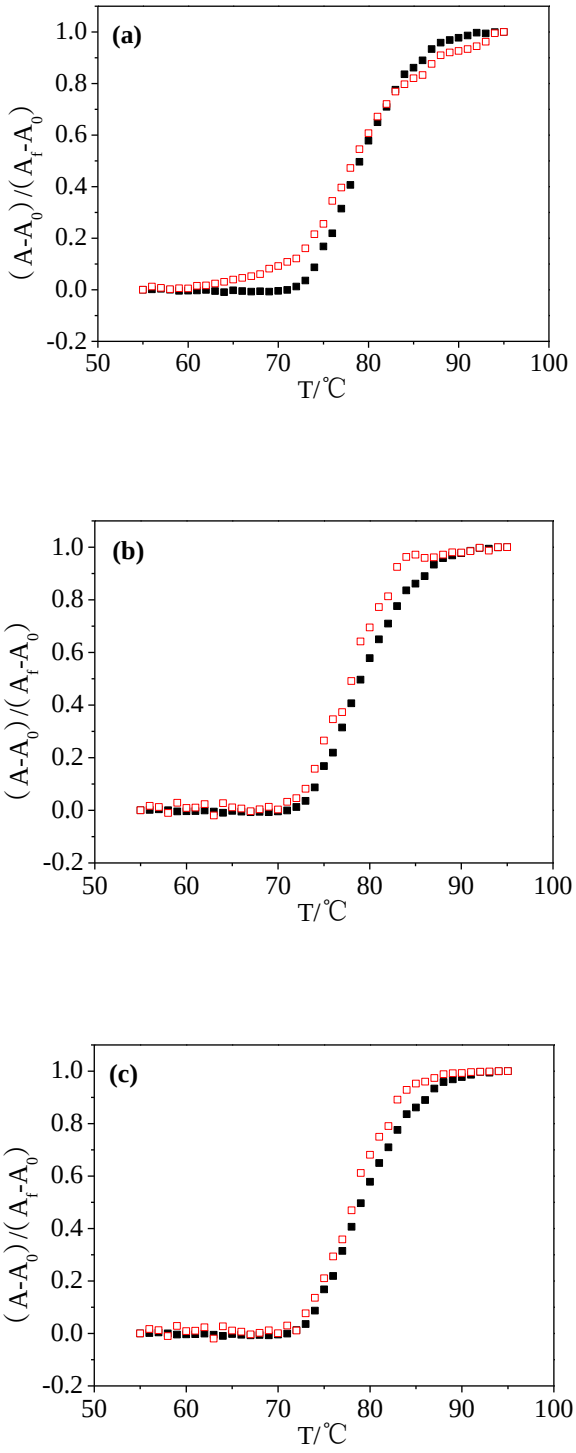

Figure S1. The thermal melt curves of calf thymus DNA (100 μM, ■) incubated with different concentration of complexes **CuPDTP** (a), **CuADTP** (b), **CuBFDTP** (c). The ratio of [Cu]/[DNA] is 0.2 (□). The data was determined by measuring the absorbance of DNA at 260 nm.

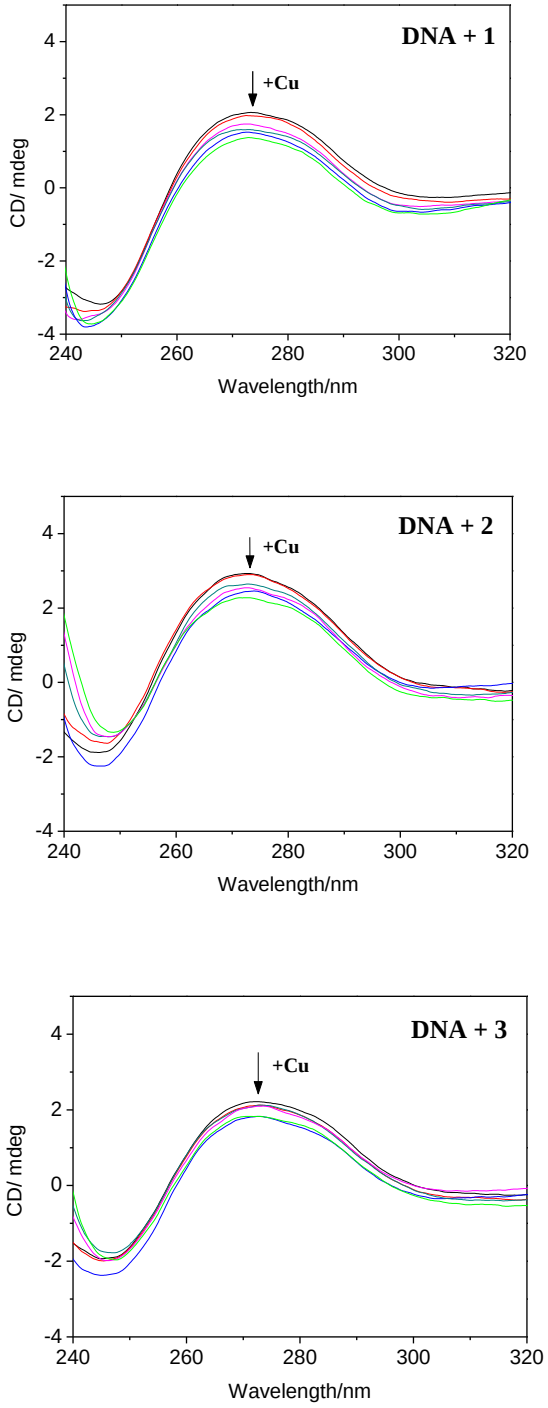

Figure S2. CD spectra of pBR322 DNA (50 μM bp) in the presence of copper complexes **CuPDTP** (**1**), **CuADTP** (**2**) and **CuBFDTP** (**3**). [Cu]/[DNA] = 0, 0.1, 0.2, 0.3, 0.4, 0.5.

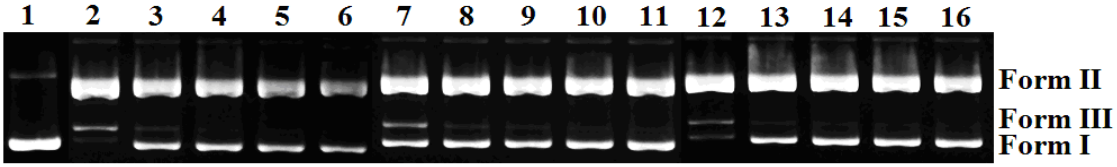

Figure S3. Agarose gel of plasmid DNA cleavage by Cu(II) complexes at different salt concentrations. Lane 1: DNA control (40 μM), Lane 2-6: **CuPDTP** (100 μM) + NaCl (18, 50, 100, 150, 200 mM), Lane 7-11: **CuADTP** (100 μM) + NaCl (18, 50, 100, 150, 200 mM), Lane 12-16: **CuBFDTP** (100 μM) + NaCl (18, 50, 100, 150, 200 mM).

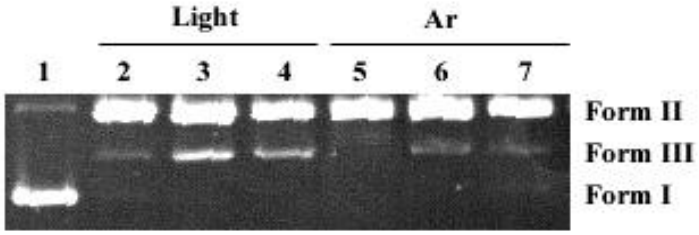

Fig. S4. Gel electrophoresis of pBR 322 DNA cleavage catalyzed by **CuPDTP-CuBFDTP** in phosphate buffer at 37 ^{o}C for 1.5 h. (a) Lane 1: DNA control, Lane 2: DNA + **CuPDTP** (100 μM), Lane 3: DNA + **CuADTP** (100 μM), Lane 4: DNA + **CuBFDTP** (100 μM), Lane 5: DNA + **CuPDTP** (100 μM), Lane 6: DNA + **CuADTP** (100 μM), Lane 7: DNA + **CuBFDTP** (100 μM).

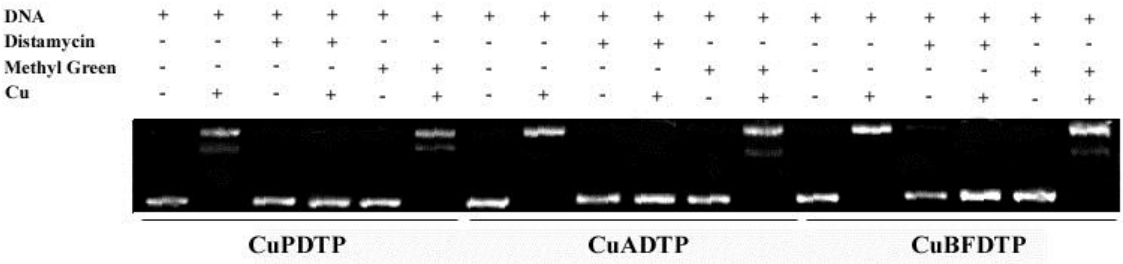

Figure S5. The DNA groove binding preference of the Cu(II) complexes. [DNA] = 40 μM, [Cu] = 100 μM, [Distamycin] = 200 μM, [Methyl Green] = 200 μM.

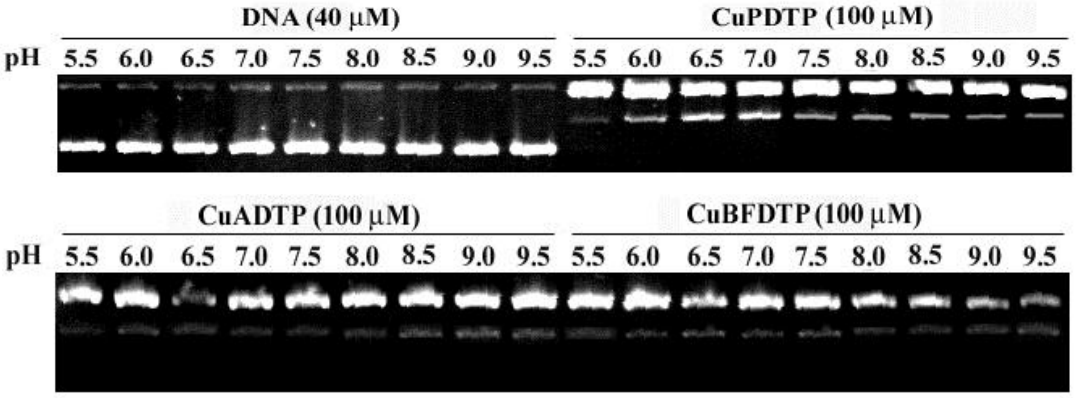

Figure S6. The pH effect on the DNA cleavage activity of Cu(II) complexes.

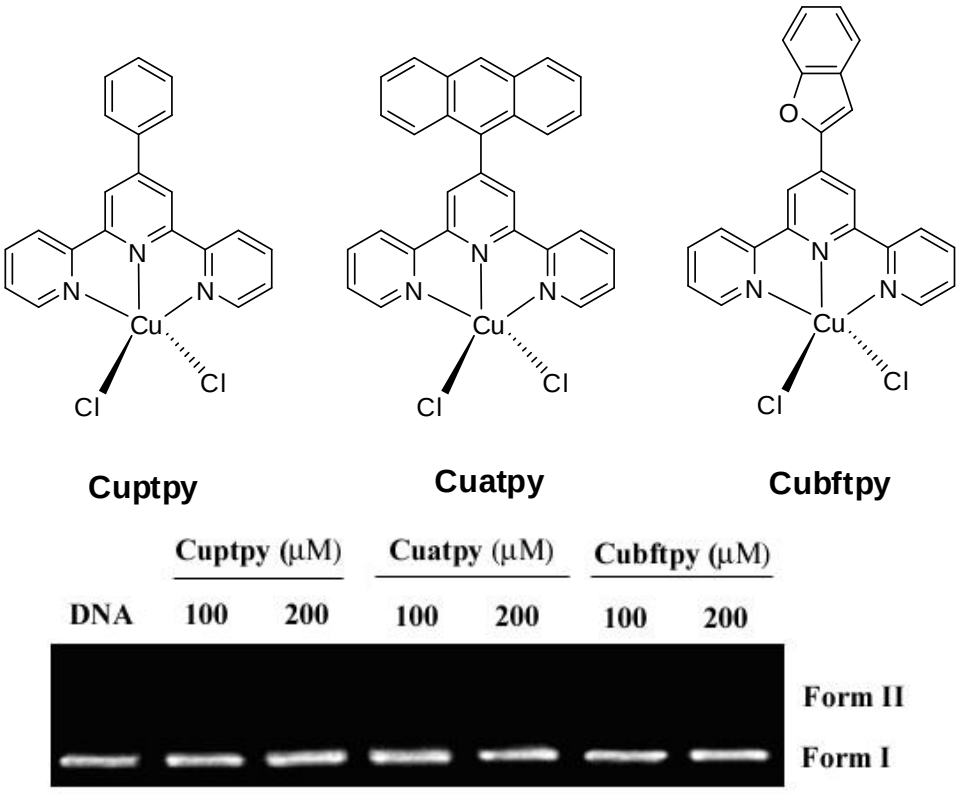

Fig. S7. Gel electrophoresis of pBR 322 DNA cleavage catalyzed by Cuptpy-Cubftpy in phosphate buffer at 37 ^{o}C for 1.5 h. DNA control (40 μM).

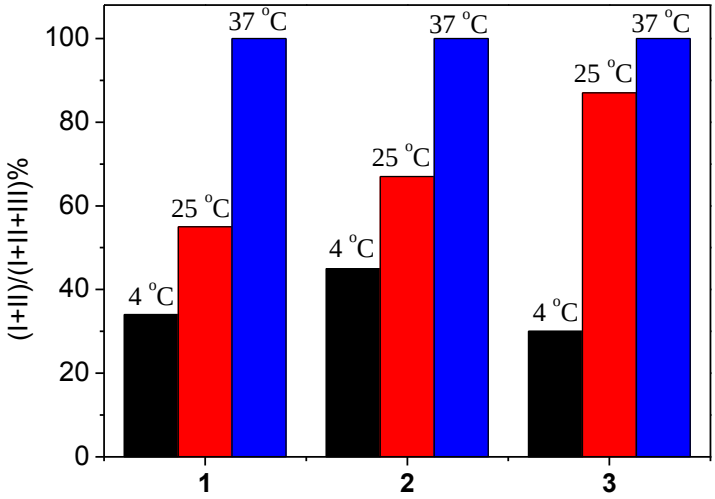

Figure S8. Plasmid DNA cleavage by **CuPDTP** (**1**), **CuADTP** (**2**) and **CuBFDTP** (**3**) (200 μM) at different temperature incubated 20 min in phosphate buffer. The nuclease activity showing a temperature-dependent manner.

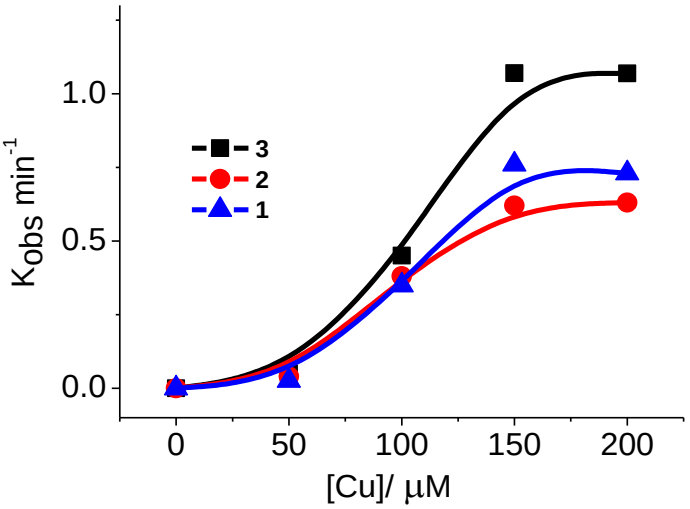

Figure S9. Kinetics for the cleavage of plasmid pBR322 DNA by **CuPDTP** (▲), **CuADTP** (●) and **CuBFDTP** (■) in a 10 mM phosphate buffer (pH 7.2) at 37 ◦C.

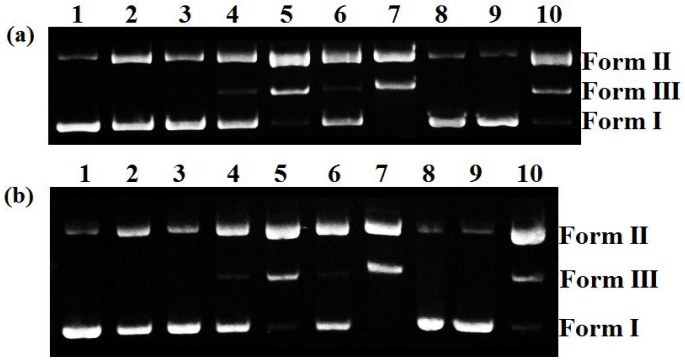

Figure S10. Agarose gel electrophoresis of pBR 322 DNA (40 μM in bp) with complex **CuPDTP** (a) and **CuADTP** (b) (100 μM) in the presence of various radical scavengers for 1.5 h at 37 ^{o}C. Lane 1: DNA control, Lane 2: DNA + complex (100 μM); Lane 3: +NaN_3 (100 mM); Lane 4: + Histidine (100 mM); Lane 5: + DMSO (100 mM); Lane 6: + Mannitol (50 mM); Lane 7: + SOD (500 U/mL); Lane 8: + Catalase (1000 U/mL); Lane 9: + EDTA (10 mM); Lane 10: + TEMPO (20 mM).

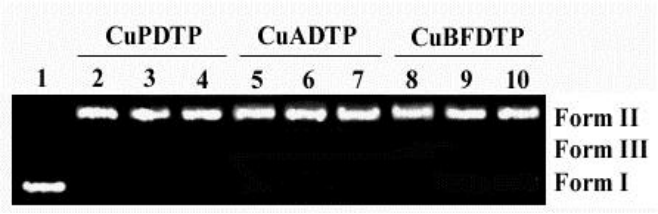

Figure S11. Agarose gel electrophoresis of pBR 322 DNA (40 μM in bp) with Cu(II) complexes in the presence of various radical scavengers for 1.5 h in the dark at 37 ^{o}C. Lane 1: DNA control, Lane 2: DNA + **CuPDTP** (100 μM); Lane 3: DNA + **CuPDTP** (100 μM) +NaN_3 (100 mM); Lane 4: DNA + **CuPDTP** (100 μM) + Histidine (100 mM); Lane 5: DNA + **CuADTP** (100 μM); Lane 6: DNA + **CuADTP** (100 μM) +NaN_3 (100 mM); Lane 7: DNA + **CuADTP** (100 μM) + Histidine (100 mM); Lane 8: DNA + **CuBFDTP** (100 μM); Lane 9: DNA + **CuBFDTP** (100 μM) +NaN_3 (100 mM); Lane 10: DNA + **CuBFDTP** (100 μM) + Histidine (100 mM).

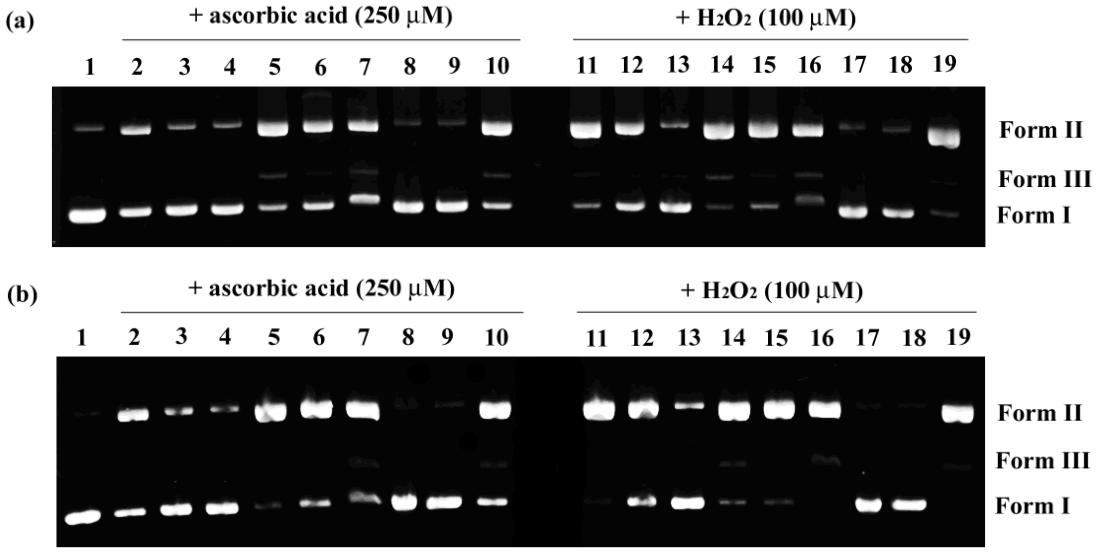

Figure S12. Agarose gel electrophoresis of **CuPDTP** (a) and **CuADTP** (b) (10 μM) oxidative cleaving DNA in the prescence of radical inhibitors under redox condition. Lane 1: DNA control, Lane 2 and 11: DNA + Cu (100 μM) ; Lane 3 and 12: Cu + NaN_3 (100 mM); Lane 4 and 13: Cu + Histidine (100 mM); Lane 5 and 14: Cu + DMSO (100 mM); Lane 6 and 15: Cu + Mannitol (50 mM); Lane 7 and 16: Cu + SOD (500 U/mL); Lane 8 and 17: Cu + Catalase (1000 U/mL); Lane 9 and 18: Cu + EDTA (10 mM); Lane 10 and 19: Cu + TEMPO (20 mM).

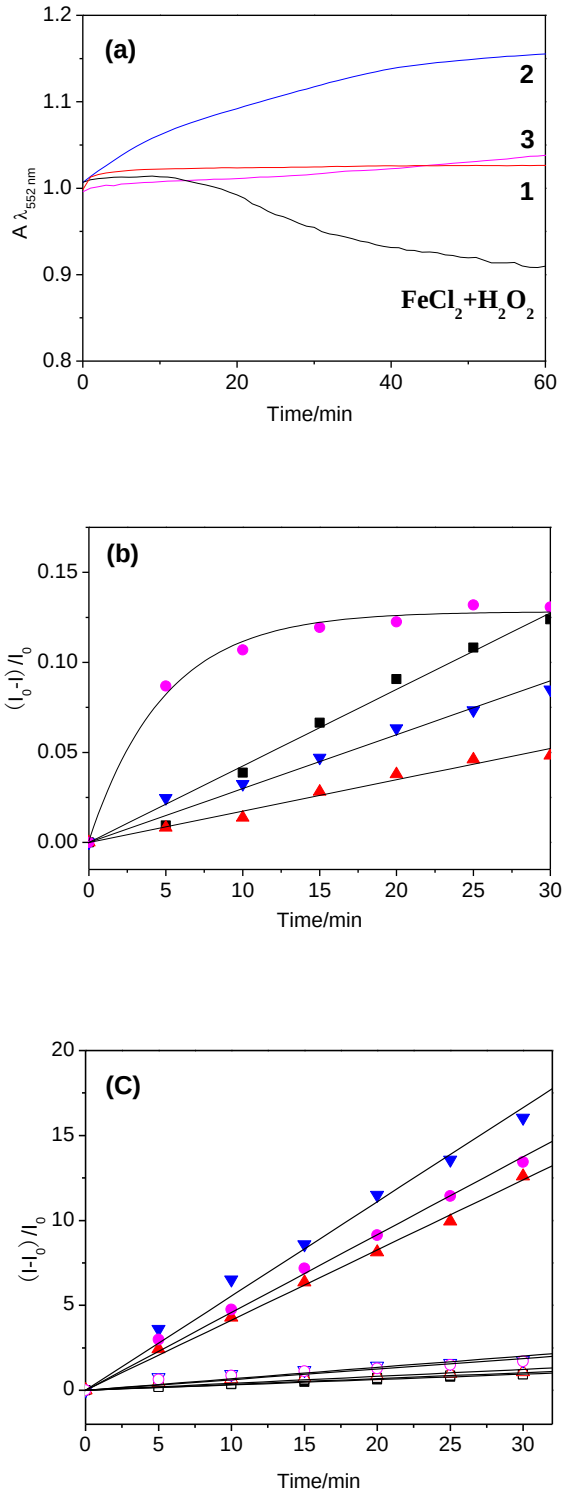

Figure S13. (a) UV absorbance of Rhodamine B (10 μM)in the presence of Cu(II) complexes (100 μM) in phosphate buffer under aerobic condition. $FeCl_2$ (100 μM) and H_2O_2 mixture (Fenton conditions) as a control experiment. (b) The DPBF (10 μM) consumption percentage as a function of time in the CH_3OH solution of $[Ru(bpy)_3]^{2+}$ (■,

30 μM), **CuPDTP** (▲, 30 μM), **CuADTP** (▼, 30 μM), **CuBFDTP** (●, 30 μM). (c) Dye degration of DCFH (0.2 μM) incubated with $[Ru(bpy)_3]^{2+}$ (■, 30 μM), **CuPDTP** (▲, 30 μM), **CuADTP** (▼, 30 μM), **CuBFDTP** (●, 30 μM), and with $[Ru(bpy)_3]^{2+}$ (□, 30 μM), **CuPDTP** (Δ,30 μM), **CuBDTP** (∇, 30 μM), **CuBFDTP** (o, 30 μM) in the presence of Catalase (1000 U/mL).