DNA Cleavage by the Cu(II) Complex of the DNA-intercalating 9-Bis(pyridin-2-ylmethyl)aminobenzo[*b*]quinolizinium

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Supporting Information

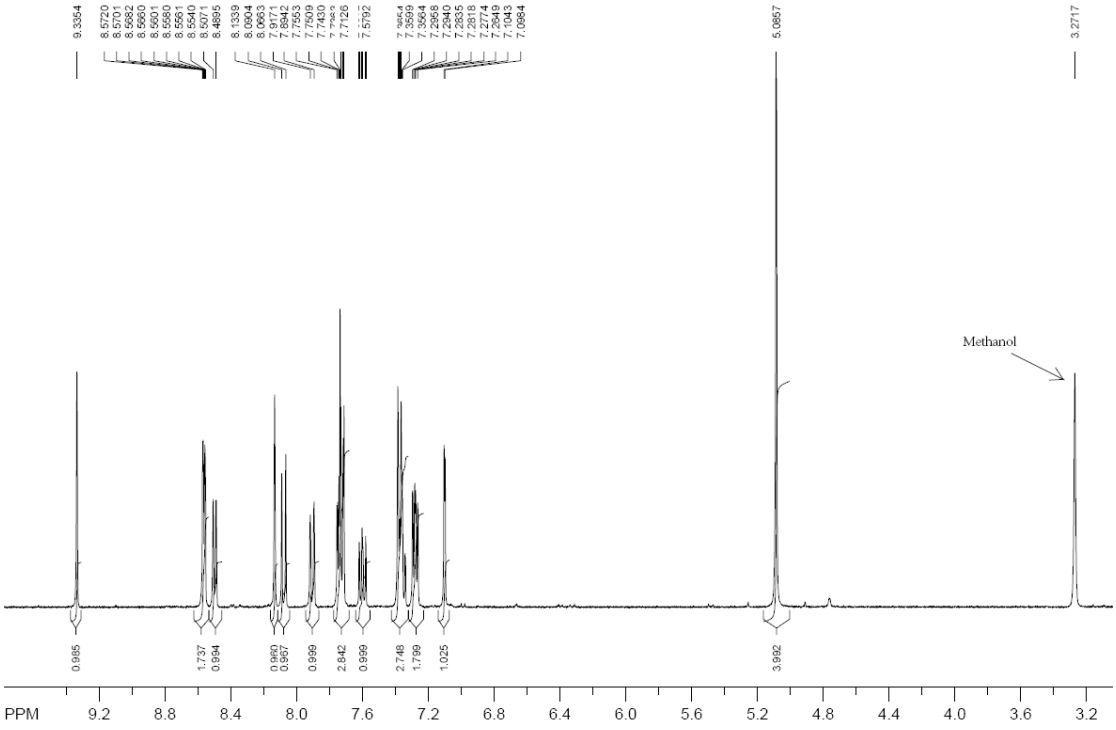

Figure S1. ^{1}H-NMR spectrum of **1a** in CD_3CN.

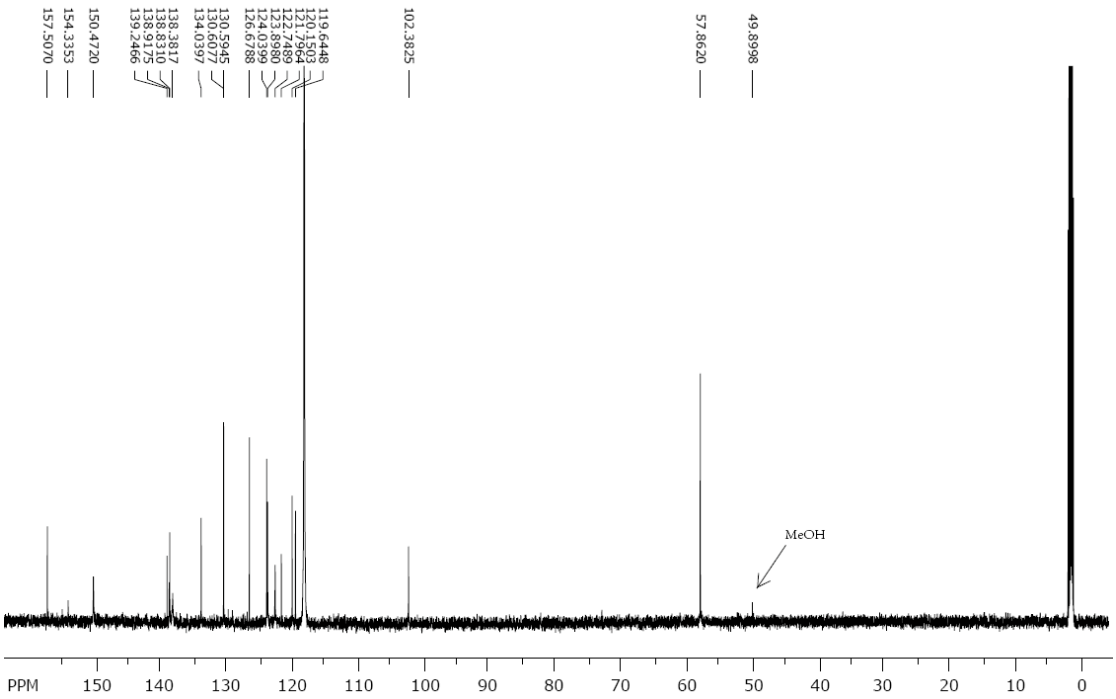

Figure S2. ^{13}C-NMR spectrum of **1a** in CD_3CN.

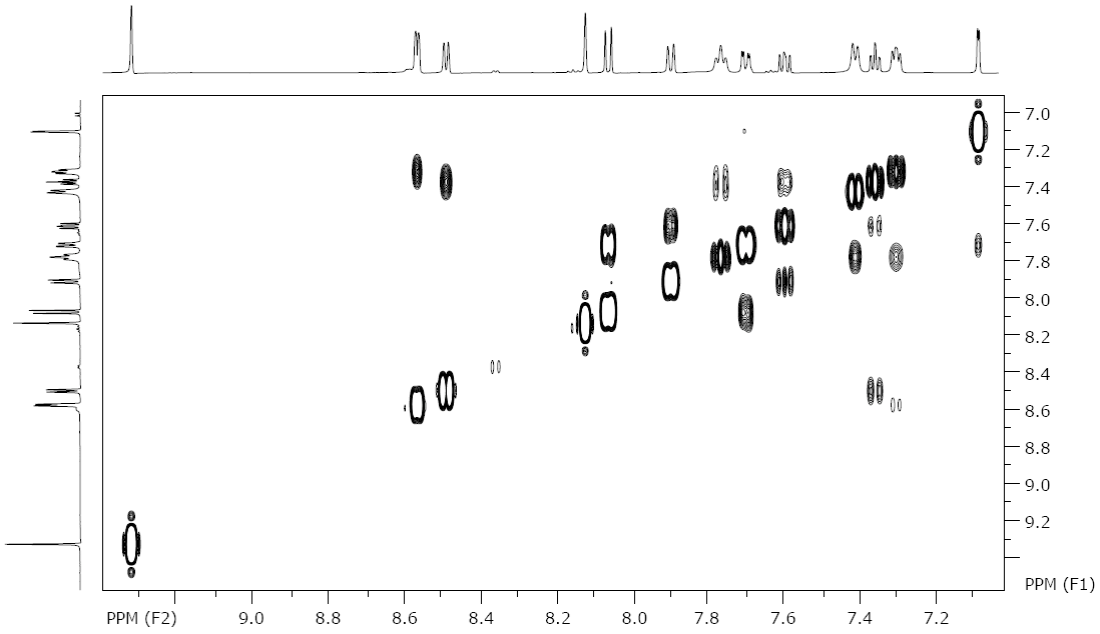

Figure S3. {1H, 1H}-COSY spectrum of **1a** in CD_3CN.

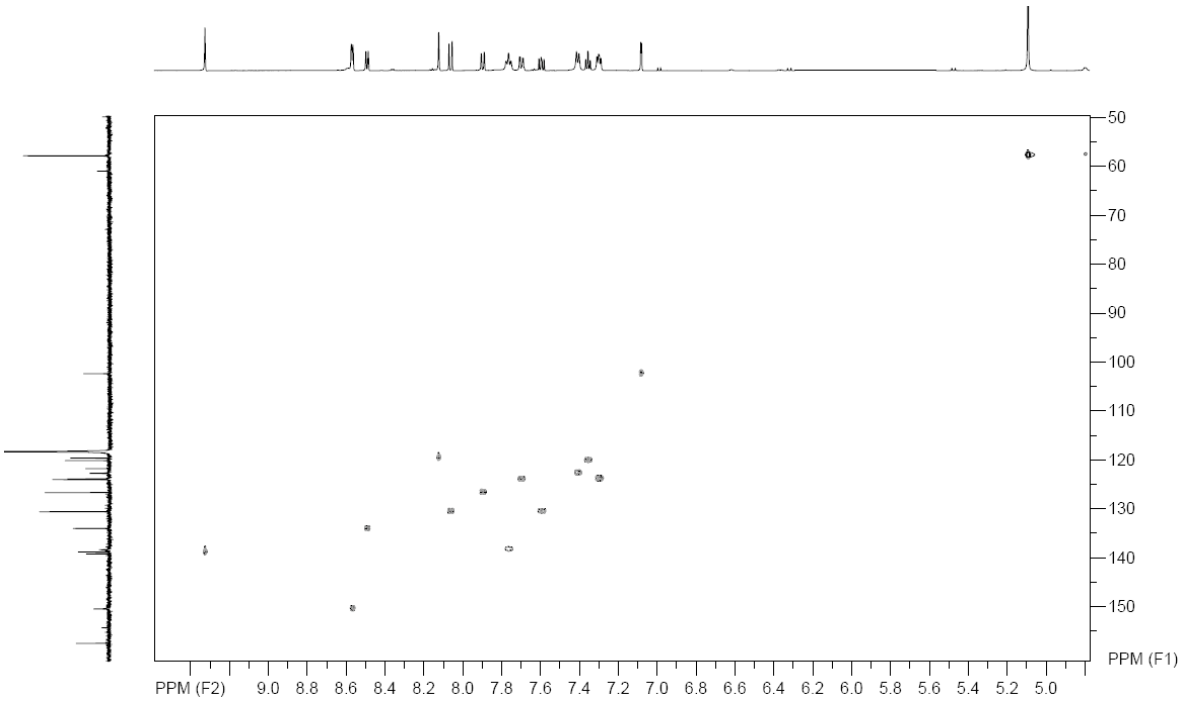

Figure S4. HSQC spectrum of **1a** in CD_3CN

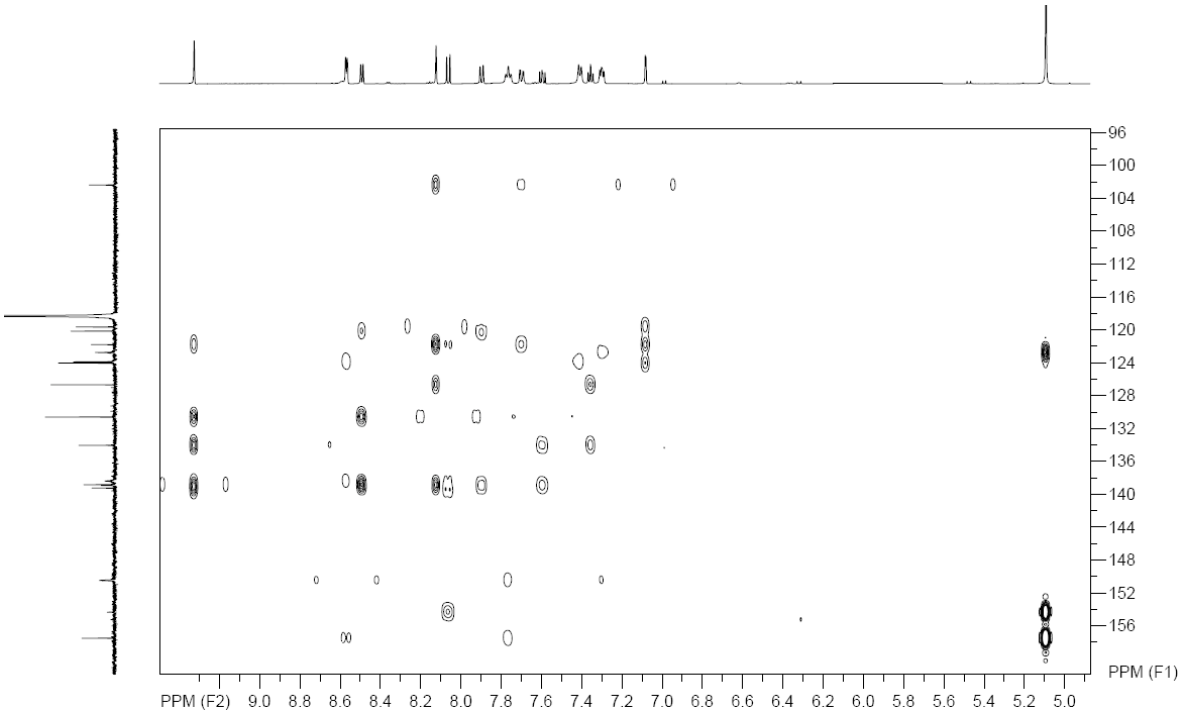

Figure S5. HMBC spectrum of **1a** in CD_3CN.

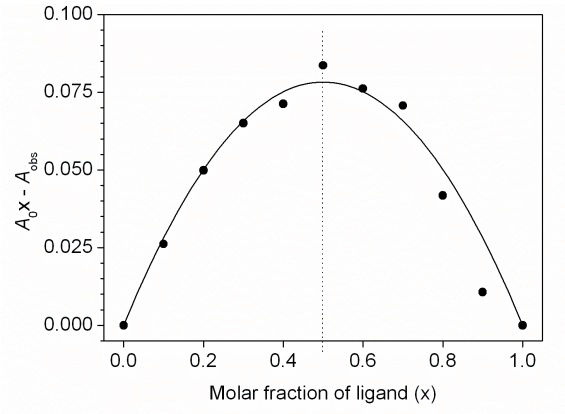

Figure S6. Job' plot of **1a** with Cu^{2+} in water (HEPES, 50 mM, pH 7.30). The total concentration of **1a** and Cu^{2+} is 50 μM. The absorption was measured at λ = 440 nm.

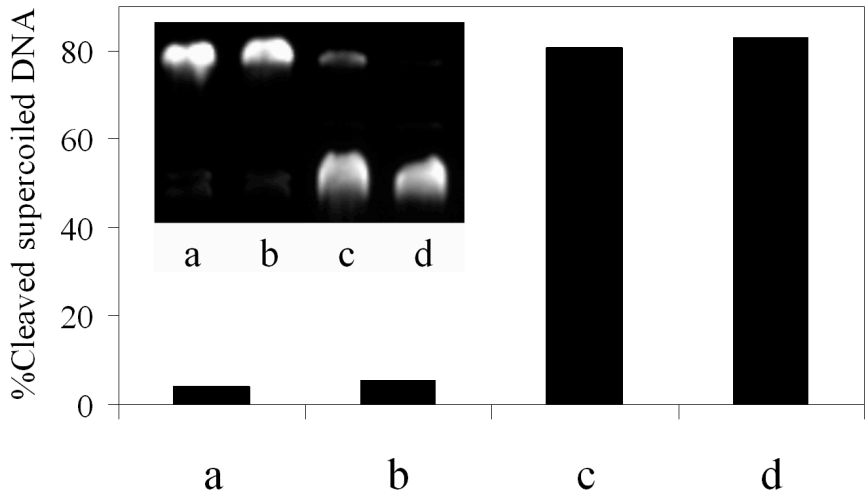

Figure S7. Formation of single-strand breaks in plasmid pBR322 (0.03 mM in bp) in the absence of **1a**-Cu(II) complex under aerobic (a) and anaerobic (b) conditions, and in the presence of **1a**-Cu^{2+} complex (0.04 mM) under aerobic (c) and anaerobic (d) conditions. T = 37 ^{o}C, t = 2 h, pH = 7.3 buffer (50 mM Tris-HCl/10 mM NaCl).

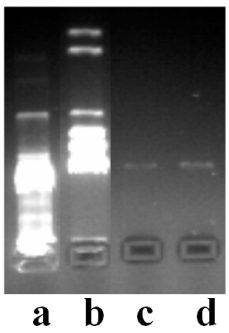

Figure S8. T4 ligase enzymatic assay: a: Religated Lambda DNA/HindIII after incubation with T4 ligase; b: Lambda DNA/HindIII after incubation without T4 ligase; c: relaxed plasmid pBR322 after treatment with the **1a**-Cu(II) complex; d: plasmid pBR322 after treatment with the **1a**-Cu(II) complex and subsequent incubation with T4 ligase.

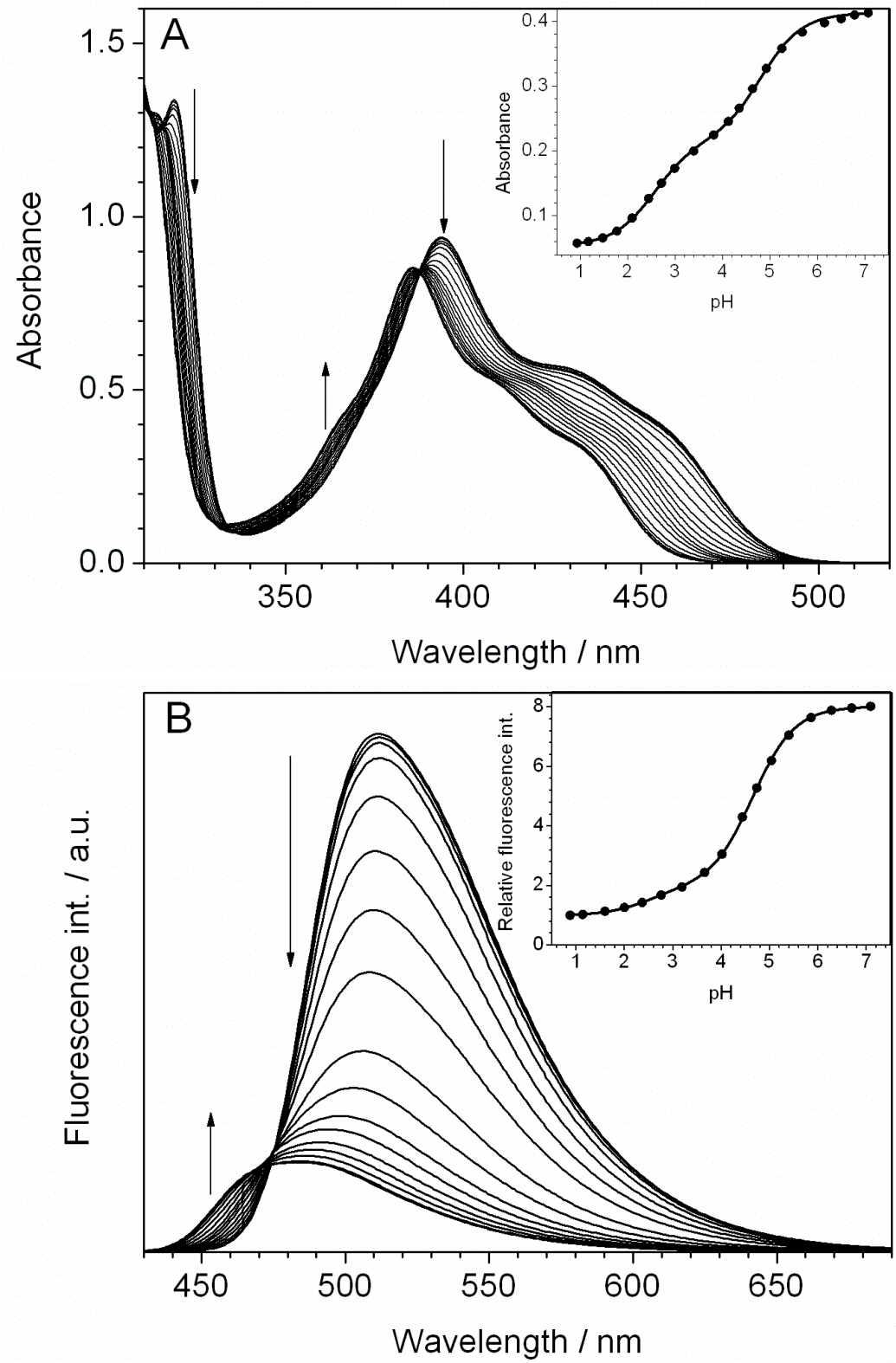

Figure S9. Spectrophotometric (A) and spetrofluorimetric titration (B) of aq. HCl (2 M) to **1a** (A: c = 50 μM; B: c = 10 μM) in Britton-Robinson buffer (pH = 0.9–7.1). The arrows indicate the changes of the bands upon acidification. Insets: Plot of the absorption at 454 nm (A) and emission intensity at 512 nm (B) versus pH of the solution, numerical fits calculated for pK_a = 2.5 ± 0.1 and 4.7 ± 0.2 from photometric titration.

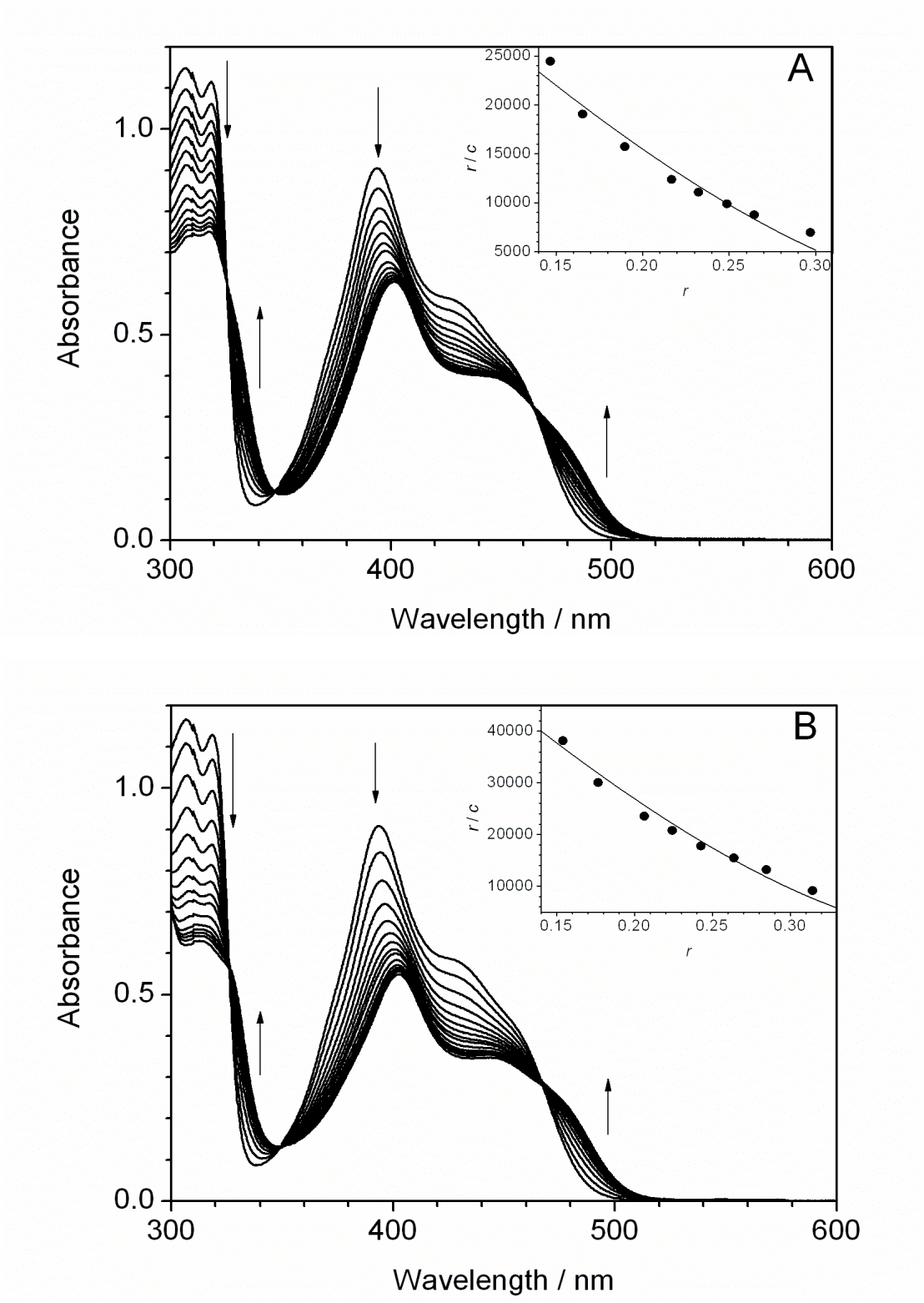

Figure S10. Spectrophotometric titration of poly(dAdT)$_2$ (A) and poly(dCdG)$_2$ (B) to **1a** (c = 50 μM) in BPE buffer; pH = 7.0. The arrows indicate the changes of the bands upon addition of polynucleotides DNA. Insets: the Scatchard plot (r/c vs c; r = ligand-to-DNA ratio r) fitted to the neighbor-exclusion model of McGhee and von Hippel to give the binding constants K_b = (1.5 ± 0.1) × 10^4 M^{-1} (A) and K_b = 3.1 ± 0.1 × 10^4 M^{-1} (B), binding site sizes n = 2.0 ± 0.1 (A) and n = 2.3 ± 0.1 (B).

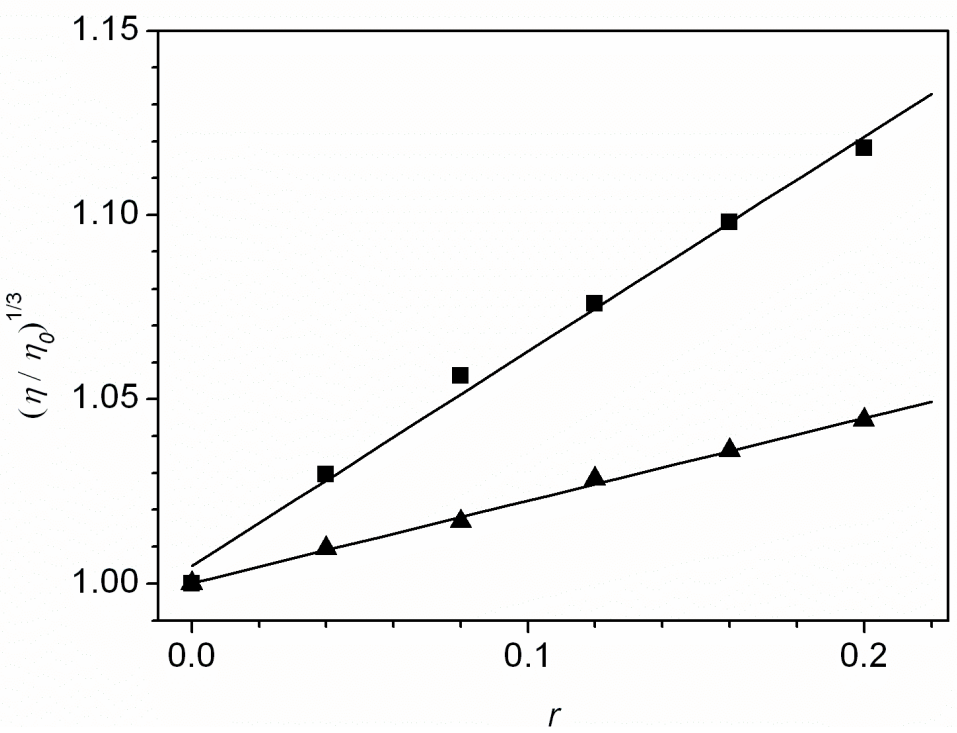

Figure S11. The relative specific viscosity of ct DNA solutions in the presence of ethidium bromide (■) and **1a** (▲) versus ligand-to-DNA ratio *r*.