Supporting Information

Interaction of DNA and a series of aromatic donor-viologen acceptor molecules with and without the prescence of CB[8]

Tongyan Zhang,[a] Shiguo Sun,*[a] Fengyu Liu,[b] Jiangli Fan,[a] and Xiaojun Peng*[a]

a. State Key Laboratory of Fine Chemicals, Dalian University of Technology, No. 158-40 Zhongshan Road, Dalian 116012, China
b. State Key Laboratory of Fine Chemicals, School of Chemistry, Dalian University of Technology, No. 2 Linggong Road, Ganjingzi District, Dalian 116023, China

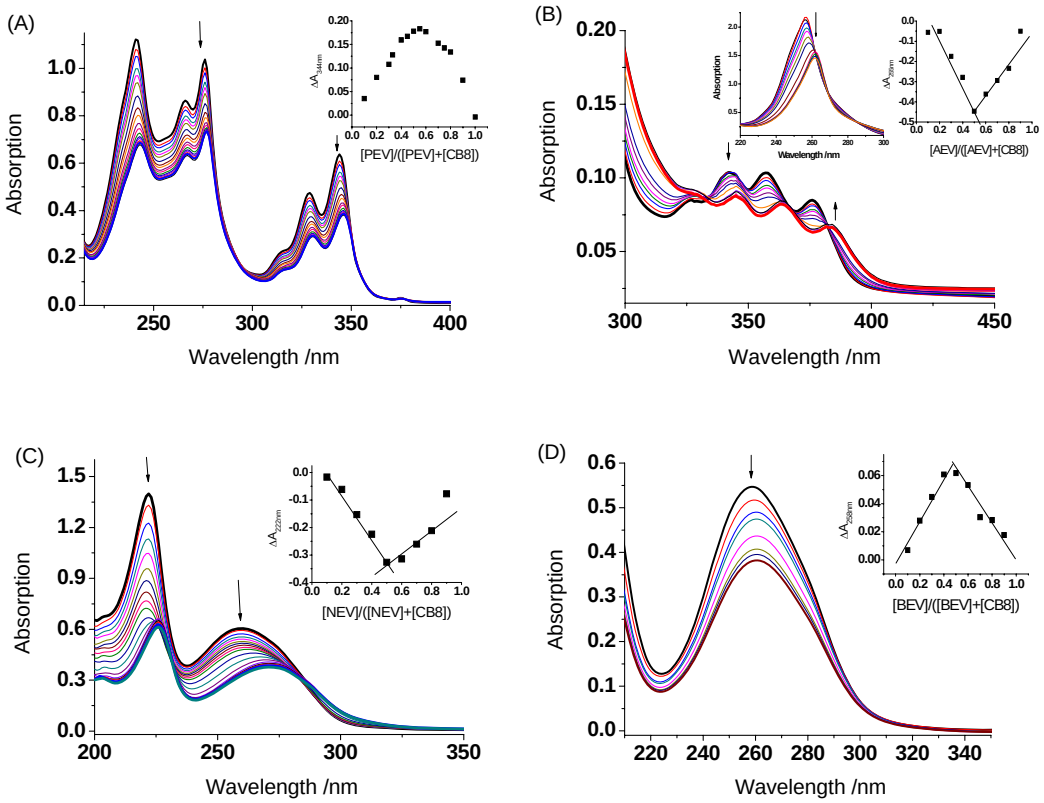

Fig. S1. The UV-vis absorption of compounds PEV(A), AEV(B), NEV(C) or BEV(D) with the addition of CB[8], the substrate concentration is 25 μM. Insert: The Job plot curves of compounds PEV(A), AEV(B), NEV(C) and BEV(D) with CB[8], the total concentration is 25 μM.

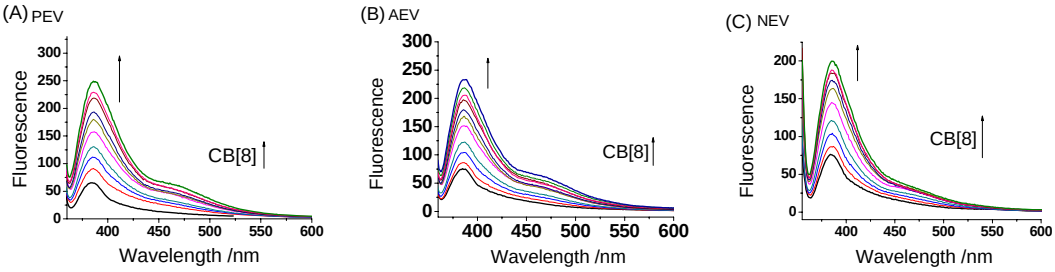

Fig. S2. The emission spectra of compounds PEV (A), AEV (B), NEV (C) with the addition of CB[8], the substrate concentration is 25 μM. (λ_{ex} = 340 nm)

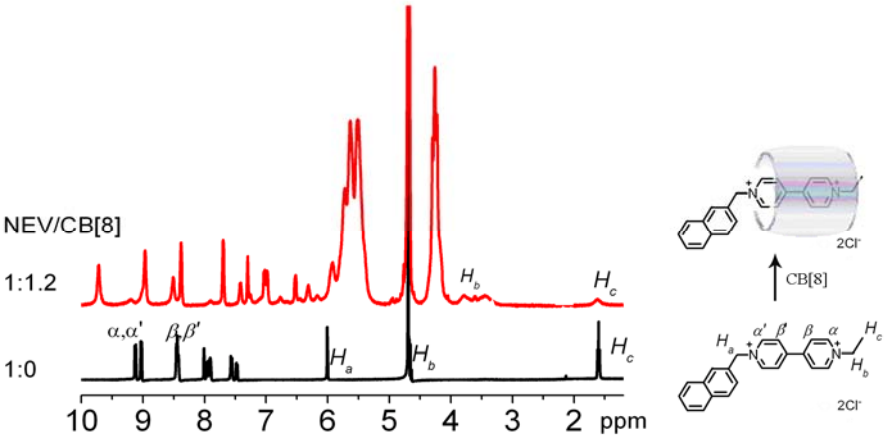

Fig. S3. ^{1}H NMR spectra and the schematic assembly of NEV and NEV/CB[8].

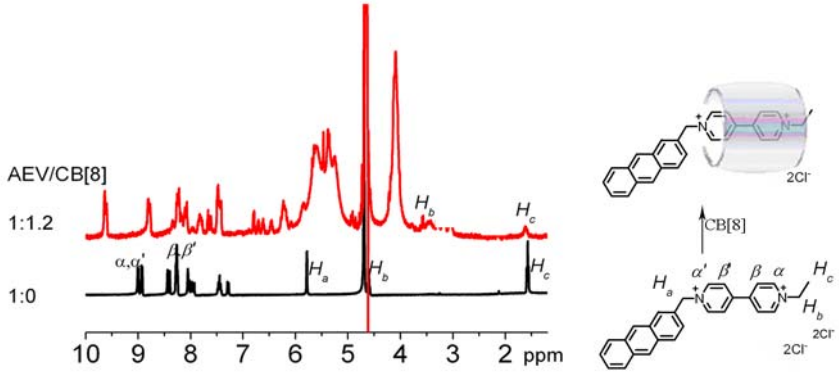

Fig. S4. ^{1}H NMR spectra and the schematic assembly of AEV and AEV/CB[8].

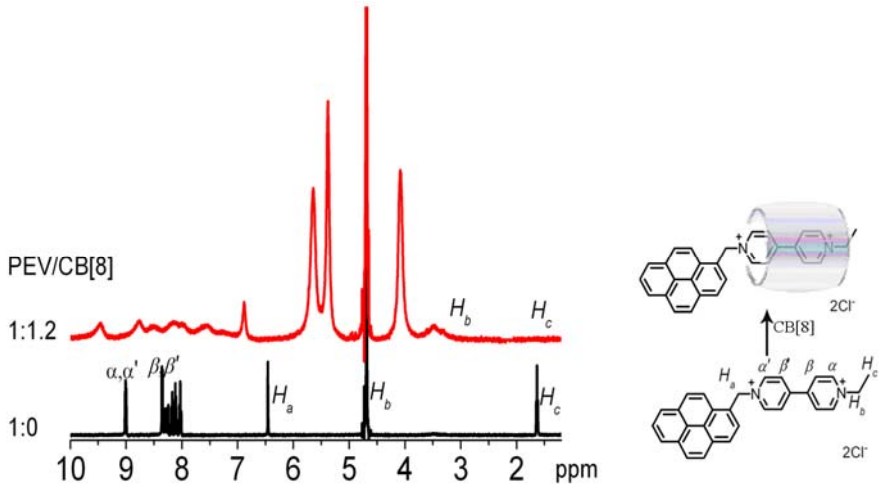

Fig. S5. ^{1}H NMR spectra and the schematic assembly of PEV and PEV/CB[8].

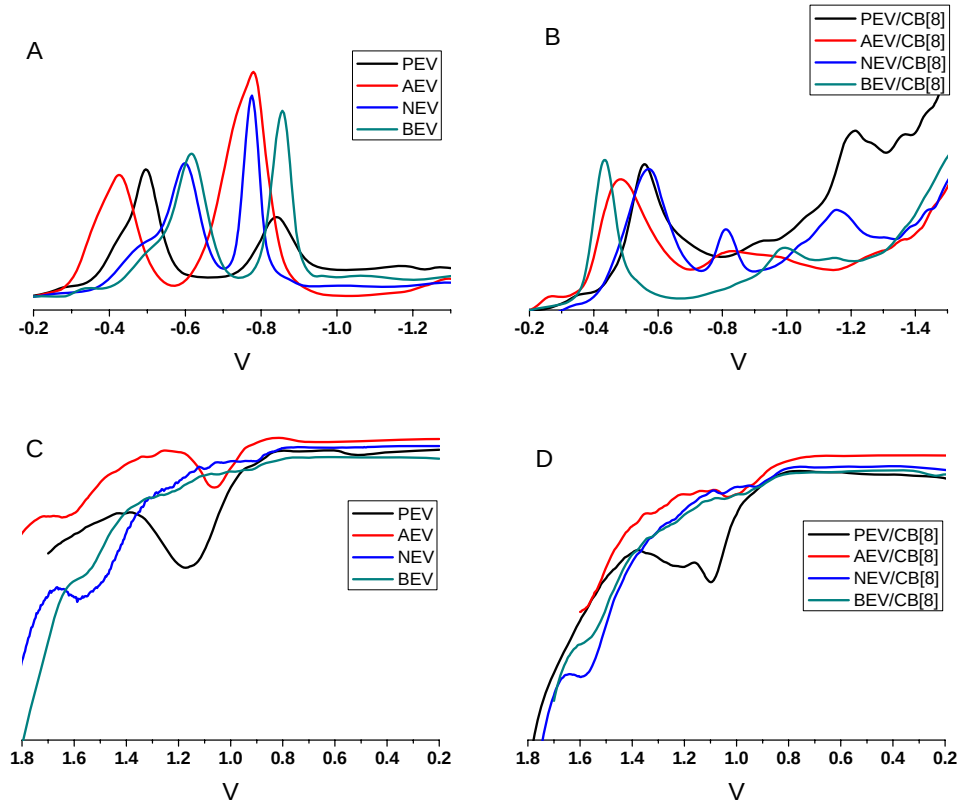

Fig. S6. Comparison of differential pulse voltammetric (DPV) responses for free PEV, AEV, NEV, BEV and their CB[8] complexes (1:1)

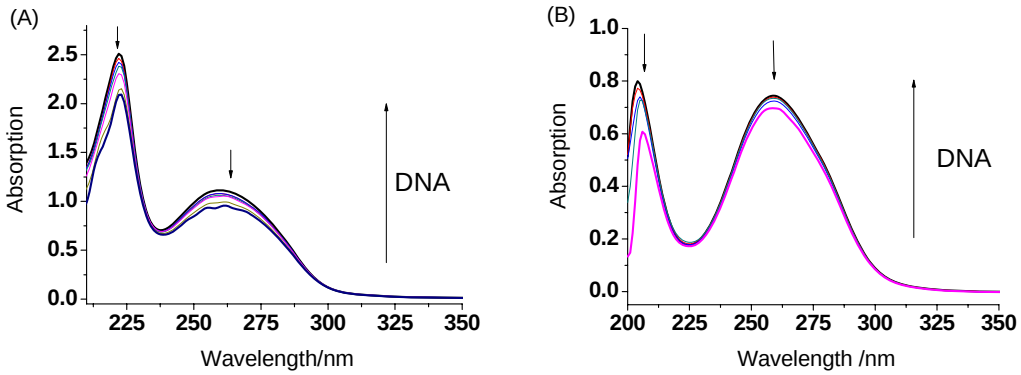

Fig. S7. The absorption spectra of NEV (A) and BEV (B) with the addition of CT DNA.

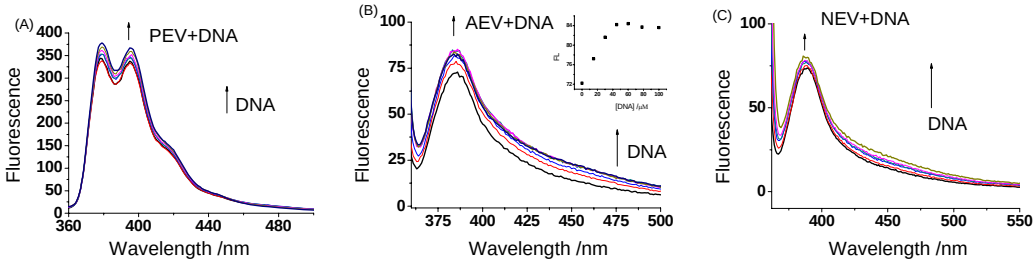

Fig. S8. The fluorescence spectra of PEV (A), AEV (B) and NEV (C) with the addition of CT DNA.

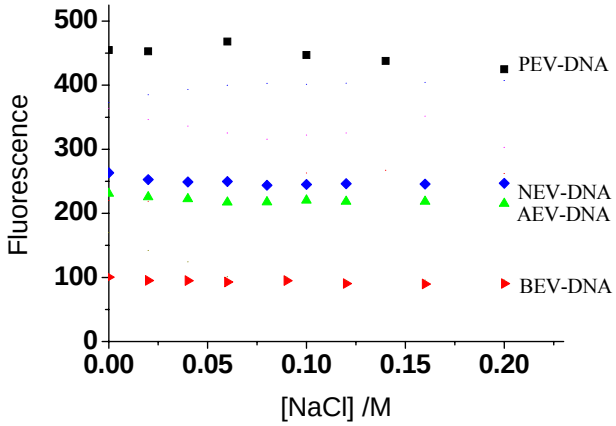

Fig. S9. The fluorescence spectra of PEV-DNA (black dot), AEV-DNA (green dot), NEV-DNA (blue dot) and BEV-DNA (red dot) with the addition of NaCl.

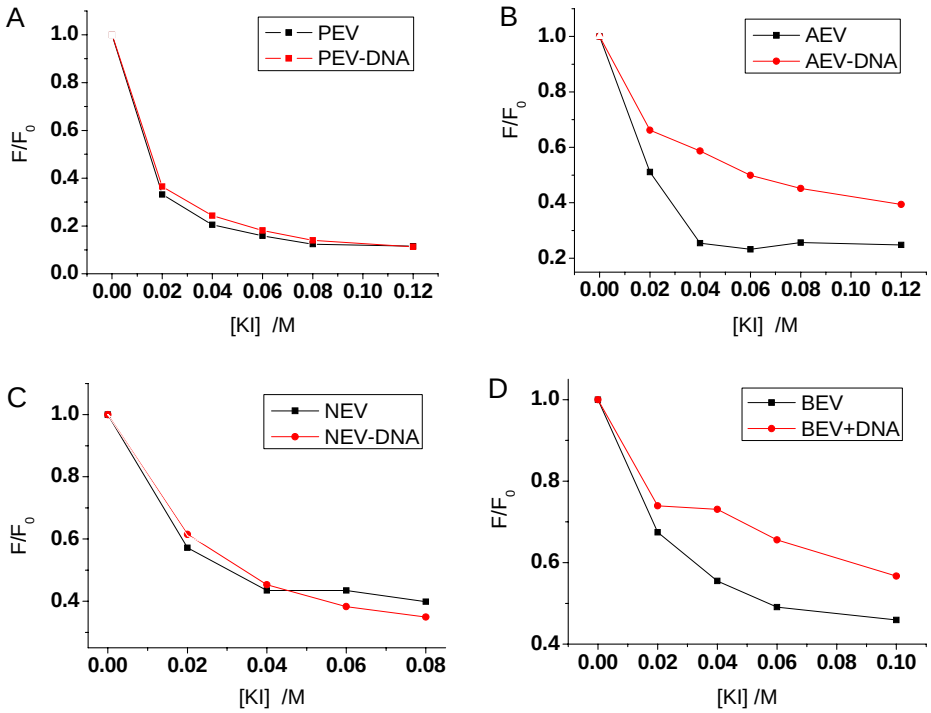

Fig. S10. The fluorescence spectra of PEV (A), AEV (B), NEV (C) and BEV (D) and their corresponding DNA solutions with the addition of KI.

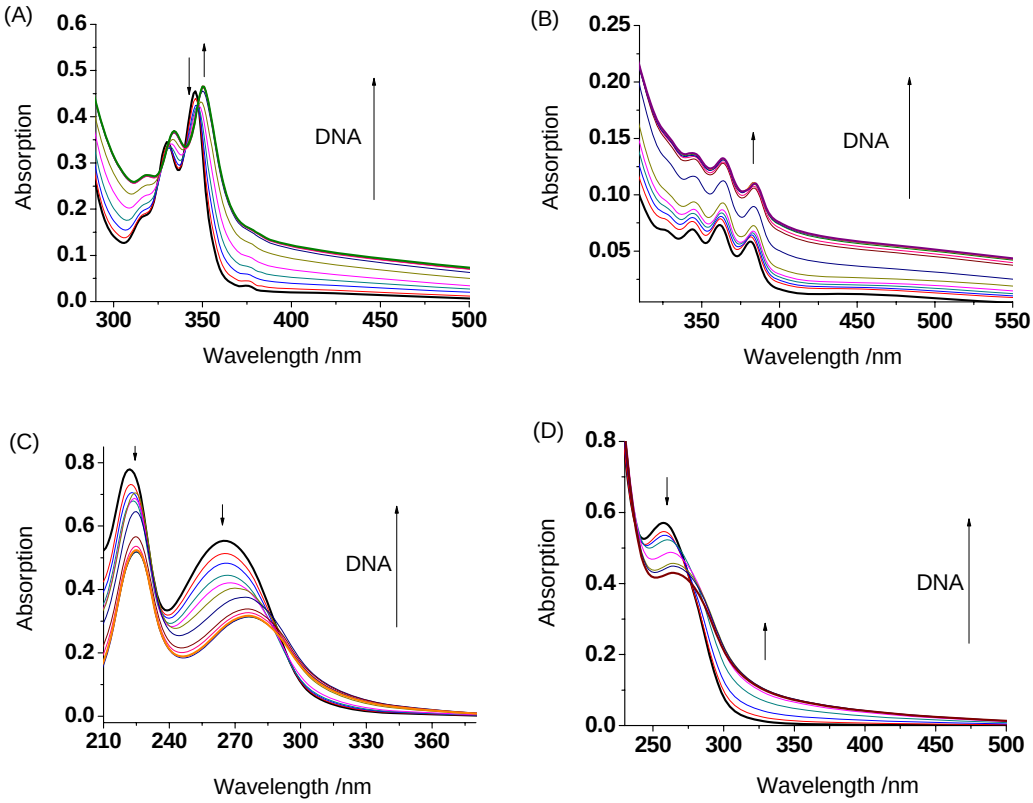

Fig. S11. The absorption spectra of PEV/CB[8] (A) and AEV/CB[8] (B), NEV/CB[8] (C) and BEV/CB[8] (D) with the addition of CT DNA.

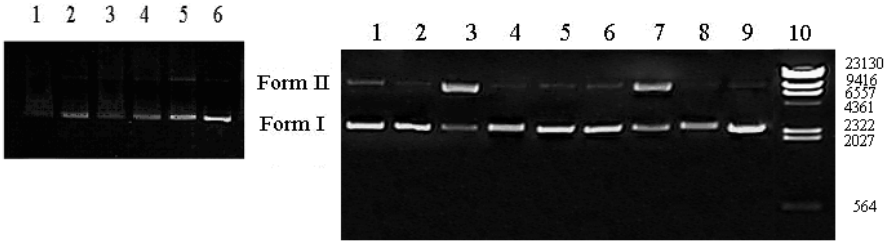

Fig. S12. Left: Gel electrophoresis diagram showing photoinduced oxidative cleavage of SC pBR322 DNA (0.15 μg, 3.44 μM) with different PEV concentration for 60 min irradiation under xenon arc lamp: lane 1-5, DNA + PEV, 100, 80, 60, 40, 20 μM, respectively; lane 6, DNA control. Right : The same DNA cleavage conditions by aromatic donor-viologen acceptor compounds (50 μM): lane 1-4, DNA + BEV, NEV, AEV and PEV, respectively, irradiation for 60 min; lane 5-8, DNA + BEV, NEV, AEV and PEV, respectively, irradiation for 30 min; lane 9, DNA control; lane 10: *λ-Hind* III digest DNA marker.

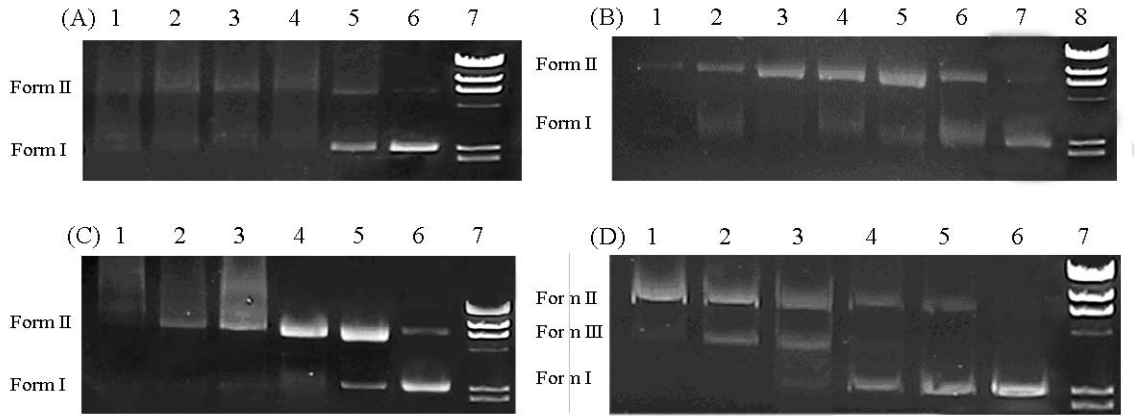

Fig. S13. Gel electrophoresis diagram showing the cleavage of SC pBR322 DNA (0.15 μg, 3.44 μM) by aromatic donor-viologen acceptor-CB[8] complexes irradiated under xenon arc lamp for 60 min. (A): lane 1-5, DNA + PEV/CB[8], 60, 50, 40, 30 and 20 μM, respectively; lane 6, DNA control; lane 7, *λ-Hind* III digest DNA marker. (B): lane 1-6, DNA + AEV/CB[8], 30, 25, 20, 15, 10 and 5 μM, respectively; lane 7, DNA control; lane 8, *λ-Hind* III digest DNA marker. (C): lane 1-5, DNA + NEV/CB[8], 60, 50, 40, 30 and 20 μM, respectively; lane 6, DNA control; lane 7, *λ-Hind* III digest DNA marker. (D): lane 1-5, DNA + BEV/CB[8], 60, 50, 40, 30 and 20 μM, respectively; lane 6, DNA control; lane 7, *λ-Hind* III digest DNA marker.

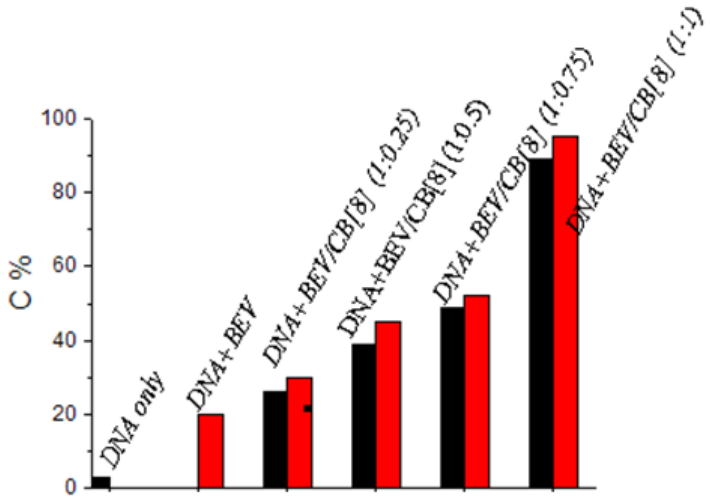

Fig. S14. SC pBR322 DNA (0.15 μg, 3.44 μM) cleavage by BEV (50 μM) in the presence of different equiv of CB[8] under xenon arc lamp: the first black column is DNA control, the other black columns are the percentages of cleavage (C %) with irradiation for 30 min and the red black columns are the percentages of cleavage with irradiation for 1 h. The C % is calculated according to Eq. (1).

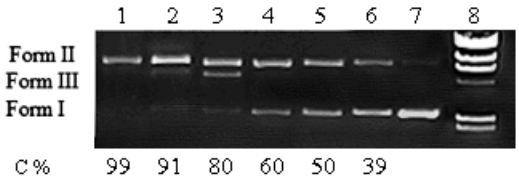

Fig. S15. Gel electrophoresis diagram showing photoinduced oxidative cleavage of SC pBR322 DNA (0.15 μg, 3.44 μM) by BEV/CB[8] (50 μM) for different exposure time: lane 1-6, DNA+ BEV/CB[8] irradiated for 60, 50, 40, 30, 20 and 10 min, respectively; lane 7, DNA control; lane 8, *λ-Hind* III digest DNA marker. The C % is the DNA cleavage yield which is calculated on Eq. (1).

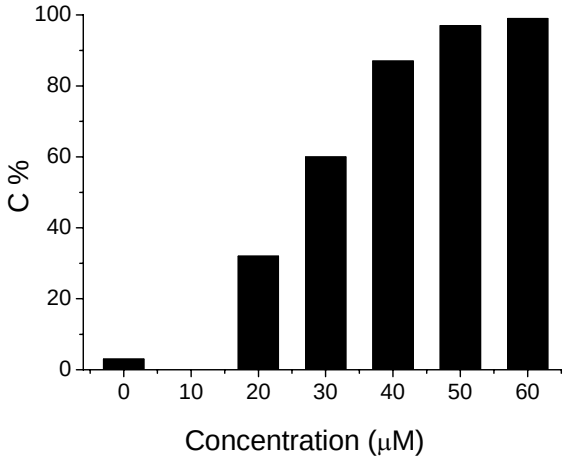

Fig. S16 SC DNA (0.15 μg, 3.44 μM) cleavage efficiency by different concentrations of BEV/CB[8] under the irradiation for 1 h at room temperature. The C% of DNA cleavage is calculated according to Eq. (1).

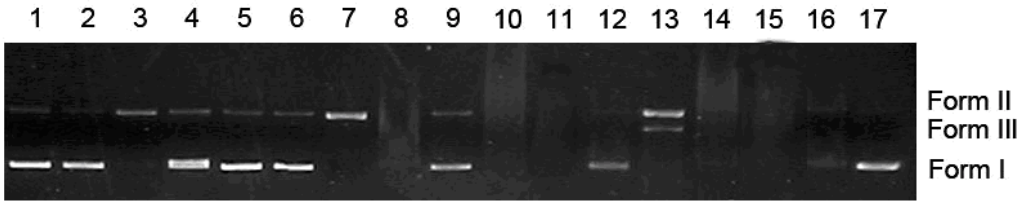

Fig. S17. Gel electrophoresis diagram showing photoinduced oxidative cleavage of SC pBR322 DNA (0.15 μg, 3.44 μM) by different complexes for 60 min: lane 1-4, DNA+ BEV, NEV, AEV and PEV (100 μM), irradiation under Ar; lane 5-8, the same samples to lane 1-4 but in air; lane 9-12, DNA+ BEV/CB[8], NEV/CB[8], AEV/CB[8] and PEV/CB[8] (30 μM), irradiation under Ar; lane 13-16, the same samples to lane 9-12 but in air; lane 17, DNA control; The C % is the DNA cleavage yield which is calculated on Eq. (1).

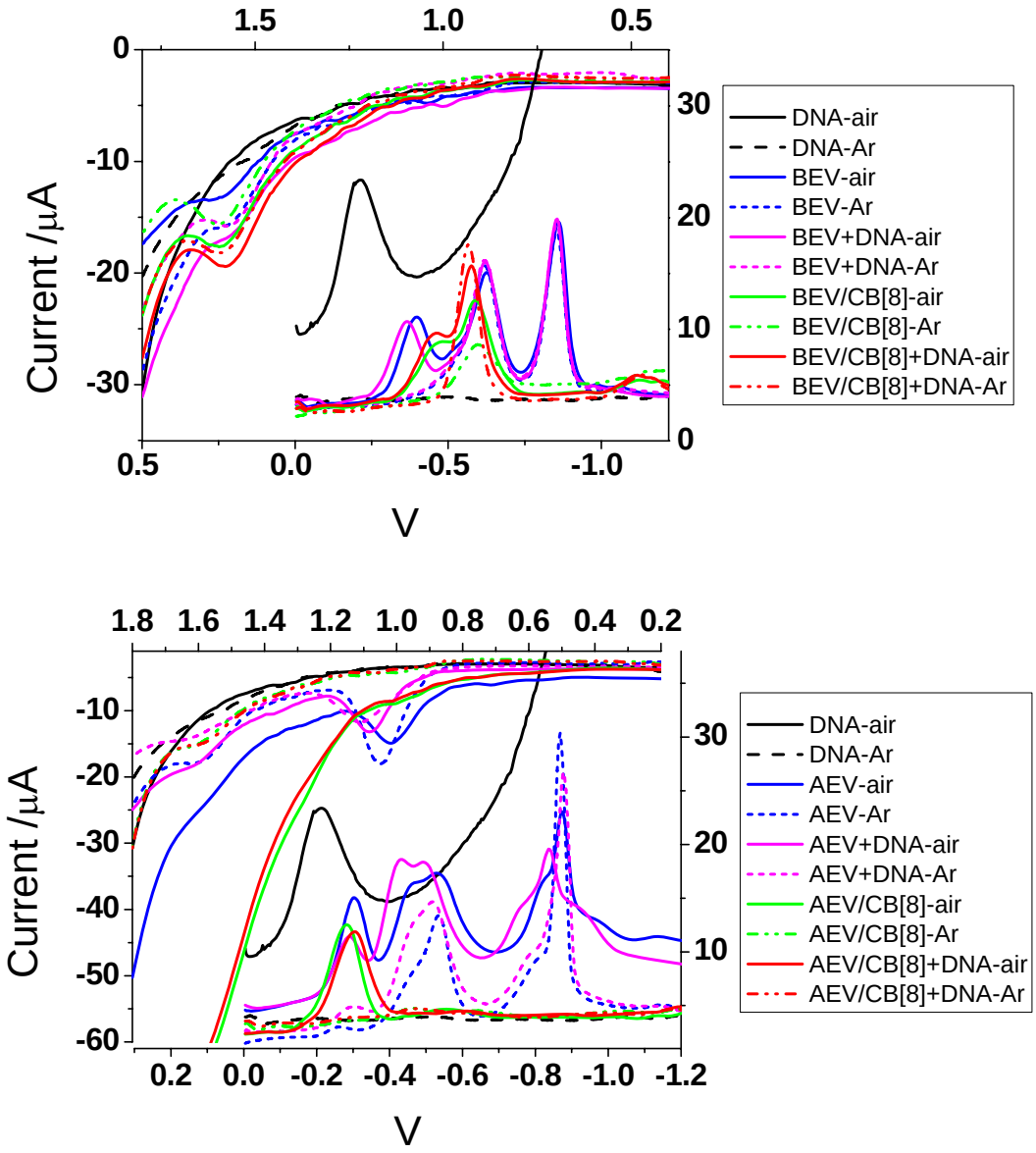

Fig. S18 Comparison of DPV of AEV, AEV/CB[8], BEV and BEV/CB[8] (0.5 mM) in phosphate sodium buffer (pH 7.0, 0.1M) with their pBR322 DNA (0.6 μM) solutions in the air and under Ar at room temperature. Top: compounds BEV and BEV/CB[8], bottom: compounds AEV and AEV/CB[8].