Study of an unusual charge-transfer inclusion complex with NIR absorption, and its application for DNA photocleavage

Shiguo Sun,* Wenyan Gao, Fengyu Liu, Jiangli Fan and Xiaojun Peng*

Supporting information

Figure S1 $^1$H NMR spectra (400 MHz, D$_2$O) of MV$^{2+}$ alone (a), addition of 1 equiv of CB[8] (b), addition of 0.5 equiv of PTZ (c), addition of 1 equiv of PTZ (d).
Figure S2 ESI-MS spectra of the 1:1:1 inclusion complex of PTZ, MV$^{2+}$ and CB[8]. Inserts are enlarged parts of the MS spectrum for the 1:1:1 inclusion complex (bottom) and computer simulation result (top).

Figure S3 Absorption spectra change for 0.1 mM MV$^{2+}$-CB[8] in 1:1 ratio in water solution along with gradually addition of PTZ (0-1.0 equiv).

Figure S4 Cyclic voltammograms of MV$^{2+}$ and CB[8] with and without the presence of PTZ in 0.1 M (pH = 7) phosphate buffer solution, red) 0.1 mM MV$^{2+}$ +1.0 equiv CB[8], black) 0.1 mM MV$^{2+}$+1.0 equiv CB[8]+1.0 equiv PTZ. The scan rate is 100 mVs$^{-1}$. 
Figure S5 Photocleavage of pBR322 DNA (10 μL, 3.44 μM) in the presence of 40 μM different complexes under 60 min light irradiation, Lane 1, DNA alone; Lane 2, DNA and PTZ; Lane 3, DNA and 1:1 PTZ+MV²⁺; Lane 4, DNA and 1:1:1 ternary complex PTZ-MV²⁺-CB[8]; Lane 5-7, DNA and 1:1:1 ternary complex PTZ-MV²⁺-CB[8] under irradiation of NEC NP60+ digital projector (200 W, 20 cm in distance) for 20, 40, 60, 90 min, respectively.