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Supporting information for the article:

Water Soluble Cationic Porphyrin TMPipEOPP-induced G-quadruplex and Double-stranded DNA Photocleavage and Cell Phototoxicity

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1. Effects of KI on the absorption spectrum of TMPipEOPP

The effects of KI on the light absorption ability of TMPipEOPP were investigated. As shown in Fig. S1, free TMPipEOPP shows a strong Soret absorption band centered at 419 nm and four weak absorption bands centered at 521, 559, 593 and 650 nm, respectively. With the addition of Hum51, obvious hypochromicities were observed for these absorption bands, thus indicating that the presence of KI could greatly decrease the light absorption ability of TMPipEOPP.

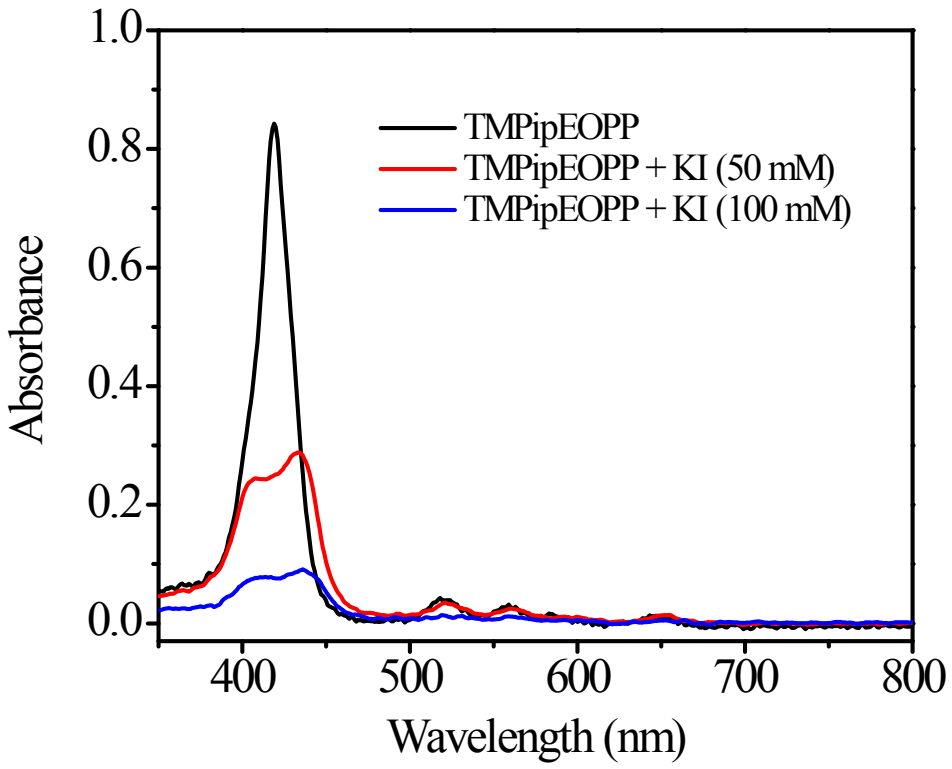

Fig. S1 UV-vis absorption spectra of TMPipEOPP in the absence or presence of KI.

2. Circular dichroism (CD) spectra of DS51 and Hum51 under different pH conditions

The effects of pH on secondary structures of DS51 and Hum51 were investigated by CD spectroscopy, a commonly used tool in DNA structure studies. To achieve this, 2 mL sample was prepared in 25 mM Tris-HCl buffer containing 1 μM DS51 or Hum51, 100 mM KCl and 10 mM Na_2EDTA. The sample was heated at 95 °C for 5 min, cooled slowly to 25 °C and incubated at this temperature for 30 min. After incubation at 4 °C overnight, CD spectra of the samples were recorded between 230 and 320 nm in 1 cm-path-length cuvettes on a Jasco J-715 spectropolarimeter. Spectra were averaged from 3 scans, which were recorded at 200 nm/min with a response time of 1 s and a bandwith of 1.0 nm.

As shown in Fig. S2, the CD spectrum of DS51 showed a positive peak at around 279 nm and a negative peak at around 243 nm, which is the characteristic of B-form duplex DNAs. Increasing pH from 4.0 to 10.0 almost had no effect on the CD spectrum of DS51, suggesting that the secondary structure of DS51 is not affected by pH. Similarly, Hum51 gave nearly overlapped CD spectra in the tested pH range. That is, a positive peak was observed at around 290 nm and a negative peak was given at around 240 nm, thus suggesting that Hum51 adopts a parallel/antiparallel-mixed G-quadruplex structure, and this secondary structure is unaffected by pH.

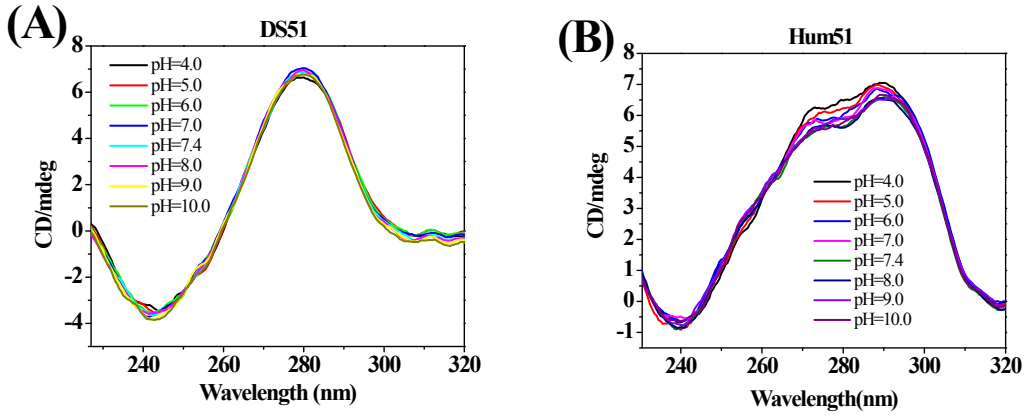

Fig. S2 Effects of pH on the CD spectra of DS51 or Hum51

3. Effects of K^+ concentration on the G-quadruplex structure of Hum51

Similar CD spectra were given by Hum51 under the two K^+ conditions (5 mM and 100 mM). That is, a positive peak and a negative peak were shown at around 290 nm and 240 nm, respectively (Fig. S3), indicating that Hum51 folded into similar parallel/antiparallel-mixed G-quadruplex structure under this two K^+ conditions.

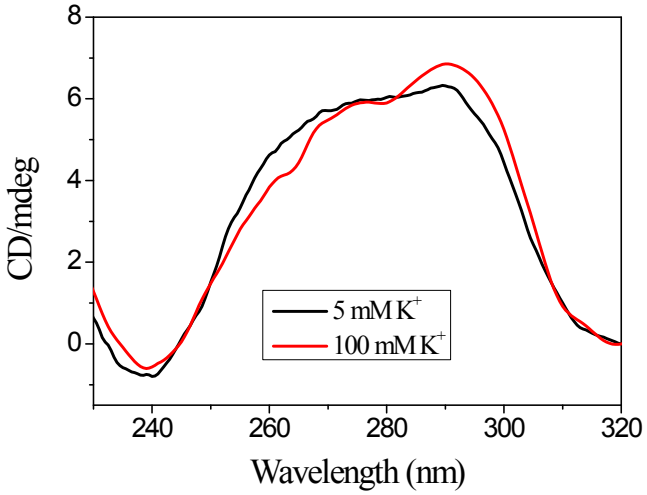

Fig. S3 CD spectra of Hum51 under different K^+ conditions