Supporting Information

The G-triplex DNA could function as a new variety of DNA peroxidase

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General information: All the oligonucleotides were purchased from Takara Co. (Dalian, China). Hemin was purchased from Acros Inc., HEPES and ABTS were purchased from Sigma, H_2O_2 was purchased from Sinopharm Chemical Reagent Co. Ltd. $Ca(H_2PO_4)_2$, KCl and NaCl were purchased from Alfa Aesar Inc.

Circular Dichroic Studies. CD experiments utilizing a Jasco-810 spectropolarimeter (Jasco, Easton, MD, USA) were measured at room temperature using a quartz cell with a 0.1 cm path length, CD spectra were collected from 220 to 330 nm and with a scanning speed of 200 nm/min. The bandwidth was 5 nm, and the response time was 2 s. All CD spectra were baseline-corrected for signal contributions due to the buffer and were the average of at least two runs.

Absorbance Spectroscopy of DNA-Hemin Complexes. Different concentrations of DNA were prepared and heated at 95 °C for 5 min in a buffer containing 10 mM $Ca(H_2PO_4)_2$ (pH 4.0), 70 mM KCl. Samples were incubated at room temperature, and then hemin was added, making sure the final concentration was at 0.5 μM. The detection was then done in the Spectrum mode of the Shimadzu UV-2550 UV-vis spectrophotometer using a quartz cell with a 1 cm path length.

Kinetic Measurements of Peroxidase Reactions. Different concentrations of oligomer were prepared and heated at 95 °C for 5 min in a buffer containing 10 mM $Ca(H_2PO_4)_2$ (pH 4.0), 70 mM KCl; samples were then incubated at room temperature, and then hemin was added, making sure that the final concentration was 500 nM. Samples were incubated at room temperature for another 20 mins, and then $ABTS^{2-}$ and H_2O_2 were added. The detection was done in the Kinetics mode of a Shimadzu UV-2550 UV-vis spectrophotometer using a quartz cell with a 1 cm path length.

Table S1 Sequences of oligomers used in the study.

Oligomer	Sequence(from 5'to 3')
T1	GGTTGGTGTGG
T2	TGTTGGTGTGG
T3	GTTTGGTGTGG
TBA	GGTTGGTGTGGTTGG

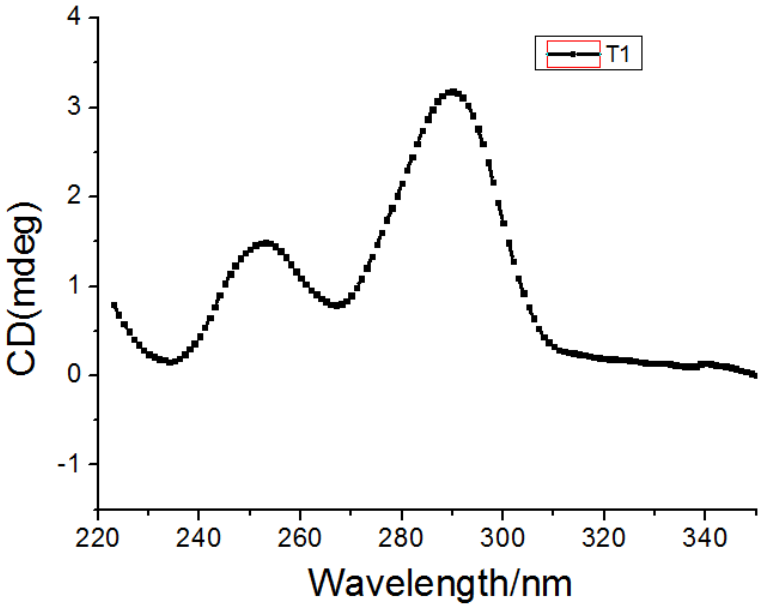

Figure S1. CD spectra of T1 (black dot-line) was measured at 10 °C. The experiments were performed in a buffer solution containing 10 mM $Ca(H_2PO_4)_2$, 70 mM KCl (pH 4.0) and 10 μM T1. CD spectra (220 nm-350 nm) were recorded in a quartz cuvette of 0.1 cm path length at a scan speed of 50 nm/min.

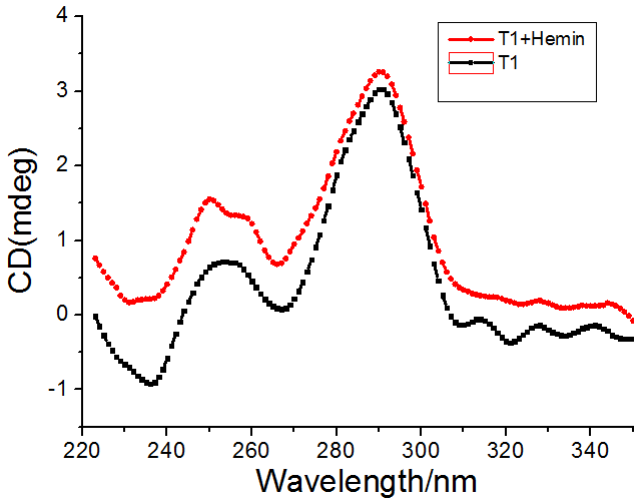

Figure S2. CD spectra of T1 (black dot-line) or T1 incubated with hemin (red dot-line) were measured at 10 °C. The experiments were performed in a buffer solution containing 10 mM $Ca(H_2PO_4)_2$, 70 mM KCl (pH 4.0), 10 μM T1, and 0.5 μM hemin. CD spectra (220 nm-350 nm) were recorded in a quartz cuvette of 0.1 cm path length at a scan speed of 50 nm/min.

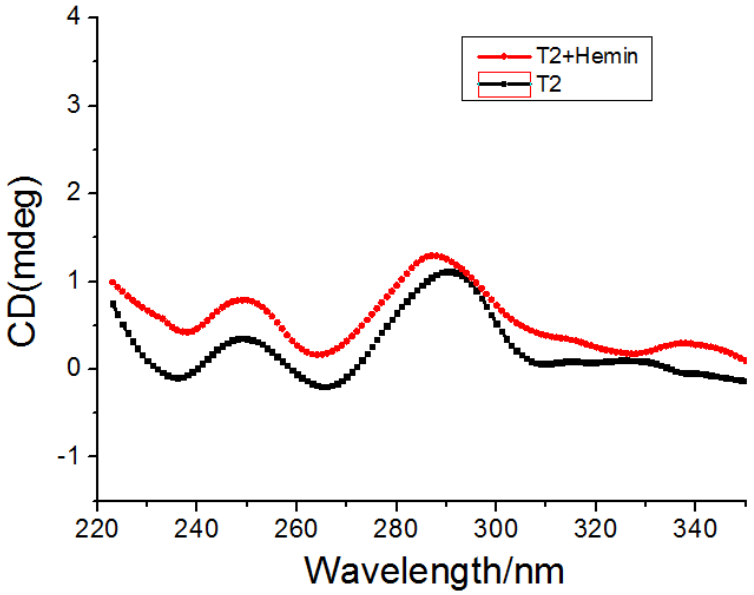

Figure S3. CD spectra of T2 (black dot-line) or T2 incubated with 0.5 μM hemin (red dot-line) were measured at 10 ^{o}C. The experiments were performed in a buffer solution containing 10 mM $Ca(H_2PO_4)_2$, 70 mM KCl (pH 4.0), 10 μM T2, in the presence or absence of 0.5 μM hemin. CD spectra (220 nm-350 nm) were recorded in a quartz cuvette of 0.1 cm path length at a scan speed of 50 nm/min.

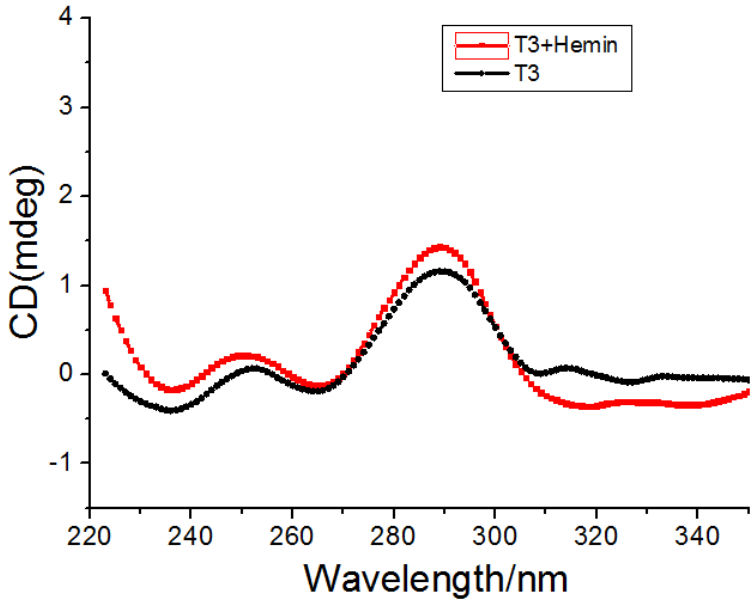

Figure S4. CD spectra of T3 (black dot-line) or T3 incubated with 0.5 μM hemin (red dot-line) were measured at 10 ^{o}C. The experiments were performed in a buffer solution containing 10 mM $Ca(H_2PO_4)_2$, 70 mM KCl (pH 4.0), 10 μM T3, in the presence or absence of 0.5 μM hemin. CD spectra (220 nm-350 nm) were recorded in a quartz cuvette of 0.1 cm path length at a scan speed of 50 nm/min.

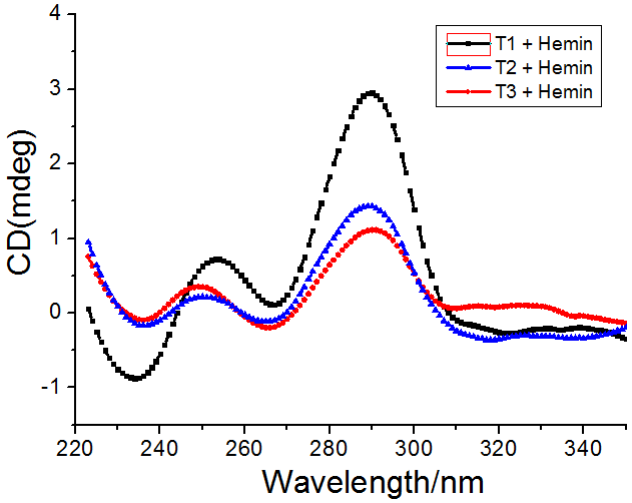

Figure S5. Overlay of CD spectra of T1, T2 or T3 when incubated with hemin. The experiments were performed in a buffer solution containing 10 mM $Ca(H_2PO_4)_2$, 70 mM KCl (pH 4.0), 10 μM oligomer, 0.5 μM hemin and the spectra were measured at 10 ^oC. CD spectra (220 nm-350 nm) were recorded in a quartz cuvette of 0.1 cm path length at a scan speed of 50 nm/min.

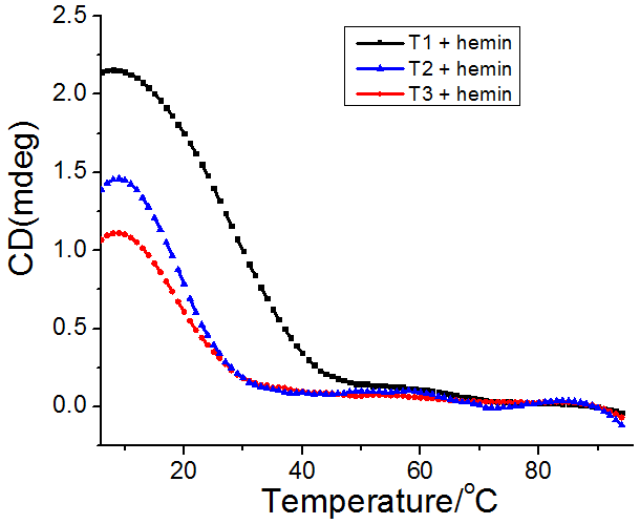

Figure S6. Normalized CD melting curves of T1, T2 or T3 recorded at 289 nm at a scan rate of 0.5 ^oC/min. T2 and T3 were used as the control. The experiments were performed in a buffer solution containing 10 mM $Ca(H_2PO_4)_2$, 70 mM KCl (pH 4.0), 8 μM oligomer, 0.5 μM hemin. T1 was found to have a much larger Tm than the one of T2 or T3, which indicated a stable secondary structure of T1. CD absorbance at 289 nm was recorded in a quartz cuvette of 0.1 cm path length.

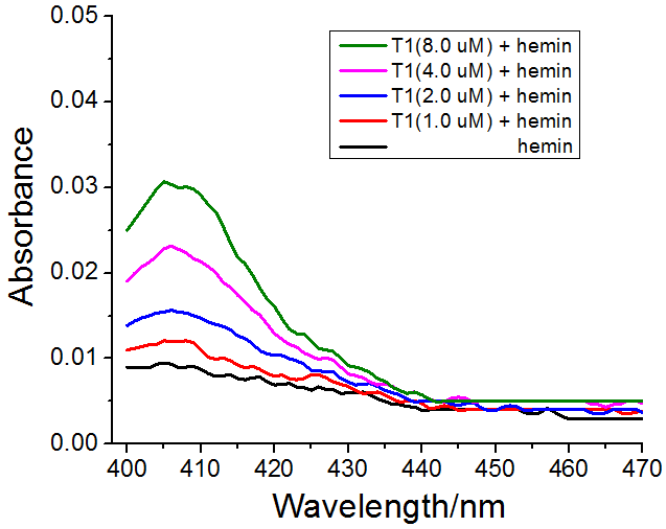

Figure S7. UV titration study of hemin (0.5 μM) upon increasing concentrations of T1. The experiments were performed in a buffer solution containing 10 mM $Ca(H_2PO_4)_2$ and 70 mM KCl (pH 4.0), with indicated amounts of T1 in the graph. A concentration-dependent manner of the Soret absorbence increase could be observed. UV spectra were recorded in a quartz cuvette of 1 cm path length.

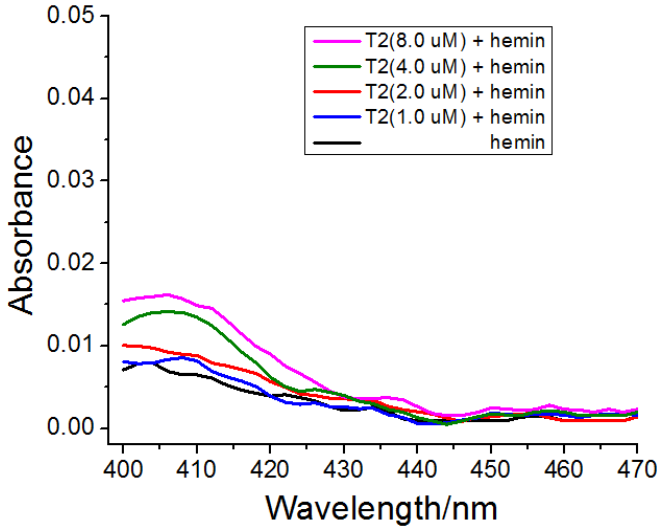

Figure S8. UV titration study of hemin (0.5 μM) upon increasing concentrations of T2. The experiments were performed in a buffer solution containing 10 mM $Ca(H_2PO_4)_2$ and 70 mM KCl (pH 4.0), with indicated amounts of T2 in the graph. UV spectra were recorded in a quartz cuvette of 1 cm path length.

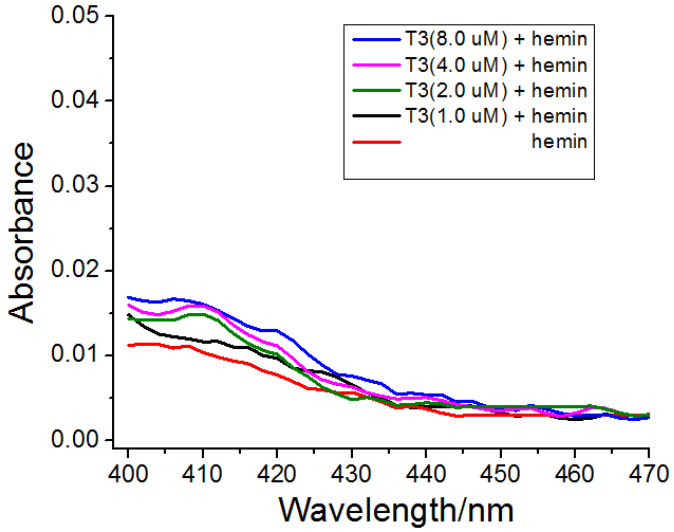

Figure S9. UV titration study of hemin (0.5 μM) upon increasing concentrations of T3. The experiments were performed in a buffer solution containing 10 mM $Ca(H_2PO_4)_2$ and 70 mM KCl (pH 4.0), with indicated amounts of T3 in the graph. UV spectra were recorded in a quartz cuvette of 1 cm path length.

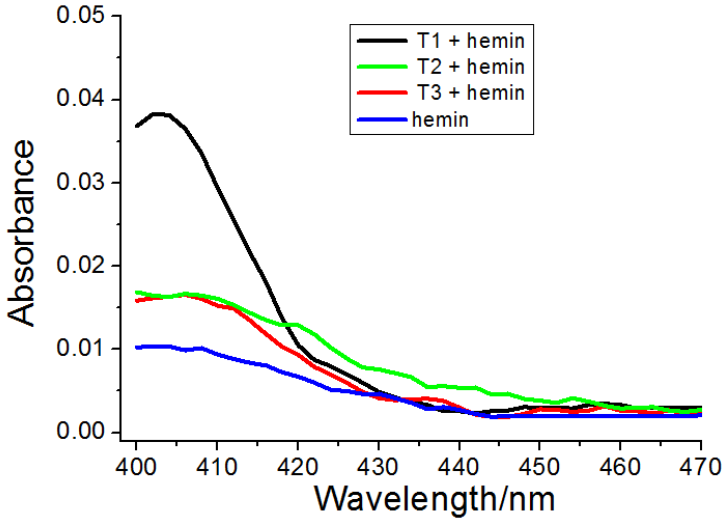

Figure S10. Comparative UV titration studies of hemin (0.5 μM) upon 8.0 μM T1 (black line), 8.0 μM T2 (green line) or 8.0 μM T3 (red line). The experiments were performed in a buffer solution containing 10 mM $Ca(H_2PO_4)_2$ and 70 mM KCl (pH 4.0). UV spectra were recorded in a quartz cuvette of 1 cm path length.

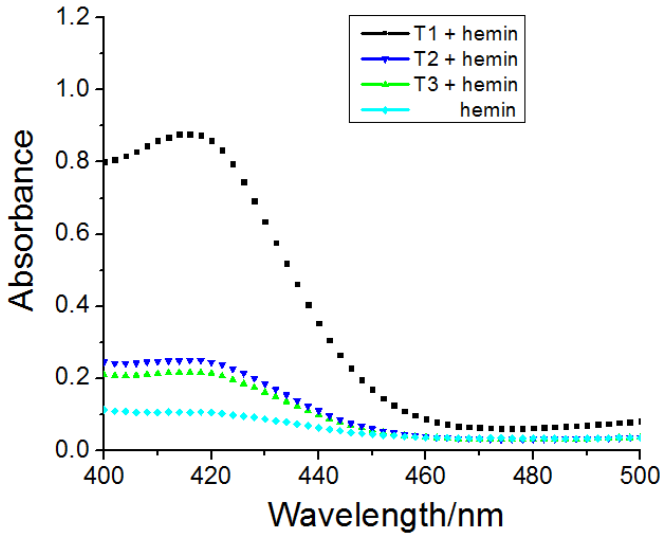

Figure S11. The activity of the peroxidatic system was dependent on the existence of G-triplex. The UV spectra after 1200 s of the oxygenation product $ABTS^{\bullet-}$ in buffer consisting of 10 mM $Ca(H_2PO_4)_2$, 70 mM KCl (pH 4.0), 0.50 μM oligomers, 0.5 μM hemin, H_2O_2 (1.6 mM) and $ABTS^{2-}$ (2.0 mM). UV spectra were recorded in a quartz cuvette of 1 cm path length.