Structure-function study of peroxidase-like G-quadruplex-hemin complexes

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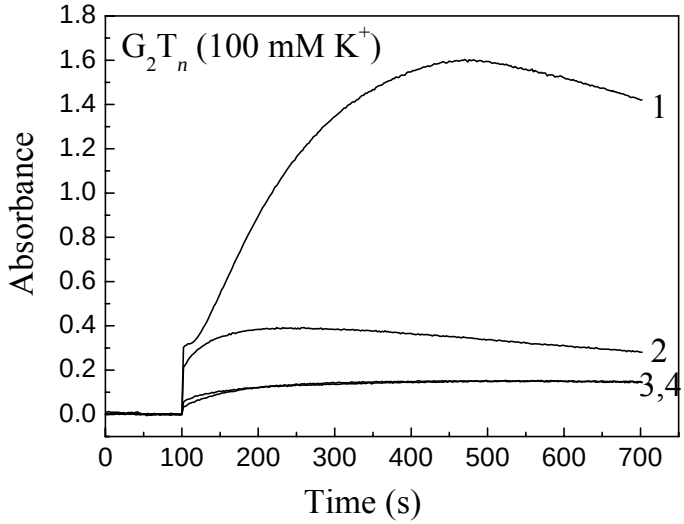
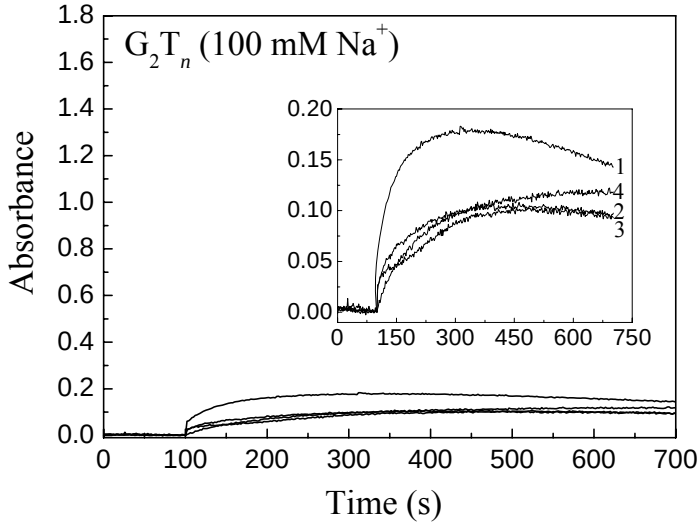
1. Detection of peroxidase activity of G_2T_n and G_3T_n by following the absorption intensity of the reaction mixture at λ = 414 nm





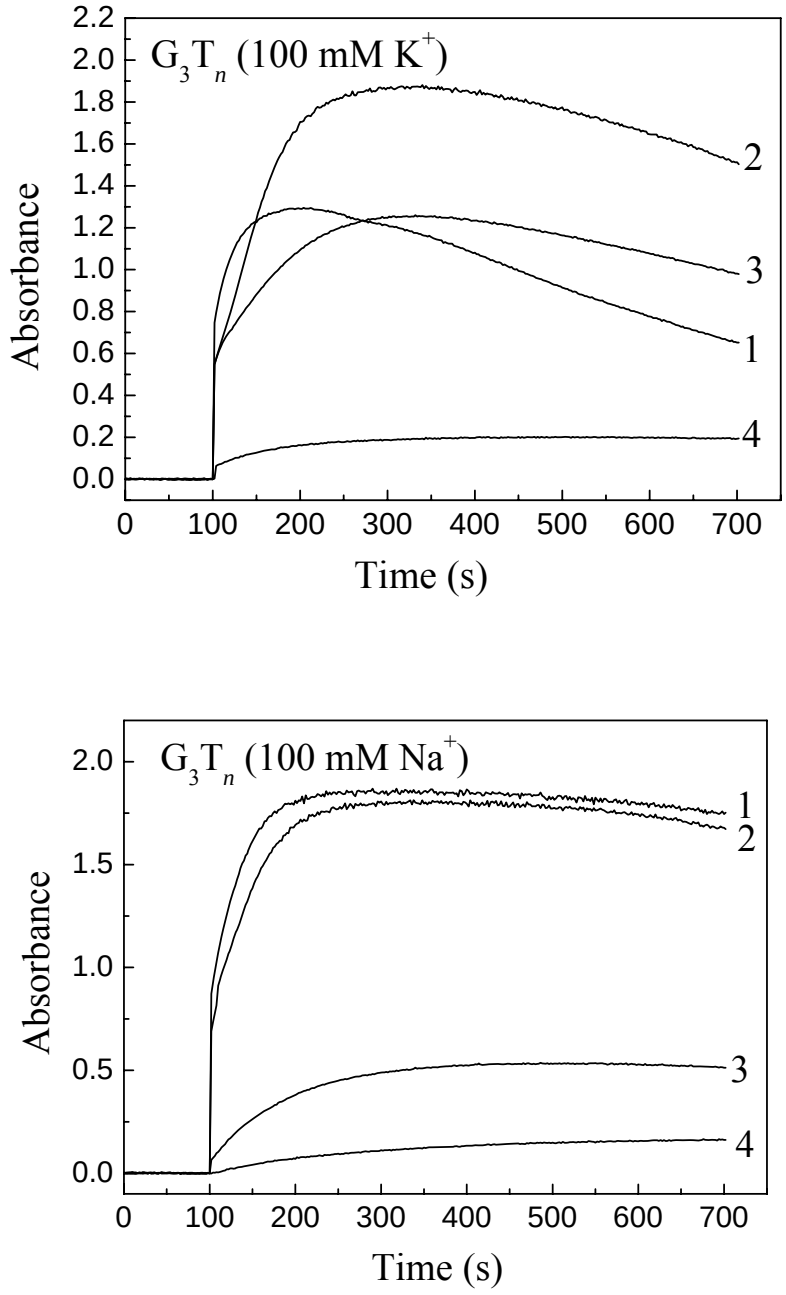
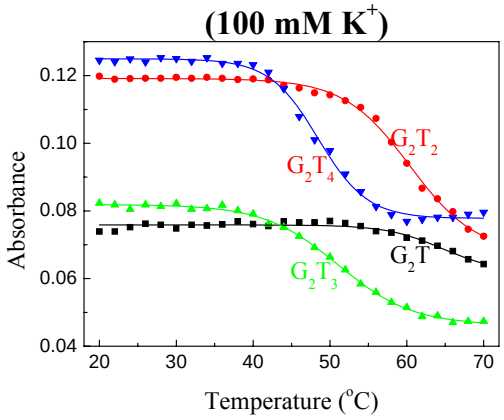
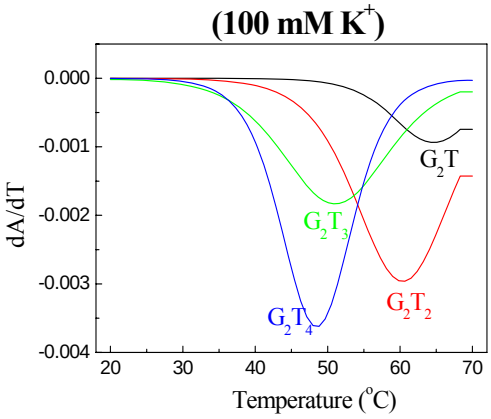
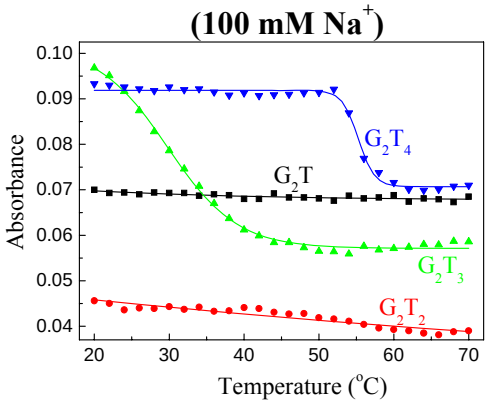


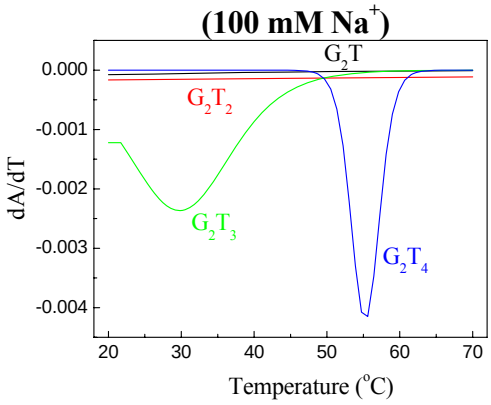
Fig. S1 Absorbance signal versus reaction time plots for the oxidative reaction of ABTS by H_2O_2 in the presence of hemin and the oligonucleotides with the sequence of $d(G_2T_n)_3G_2$ or $d(G_3T_n)_3G_3$ under different ionic conditions. The numbers labeled on the plots represent the values of *n*.

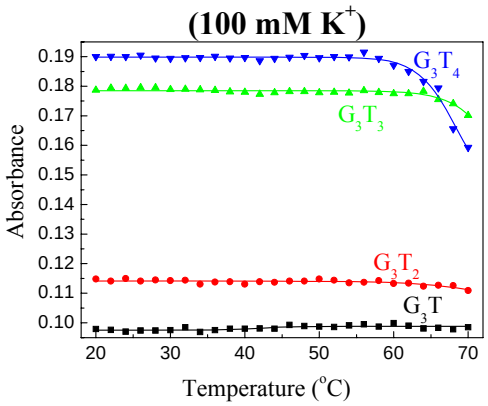
2. Thermal denaturation study of G_2T_n and G_3T_n

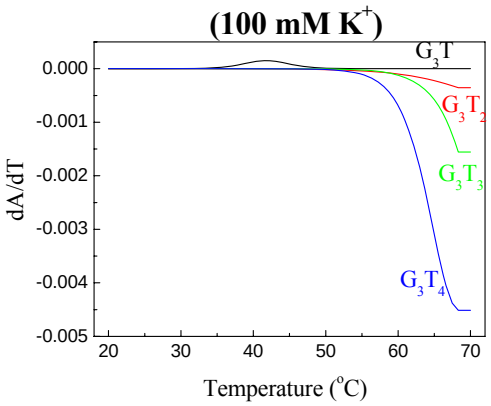












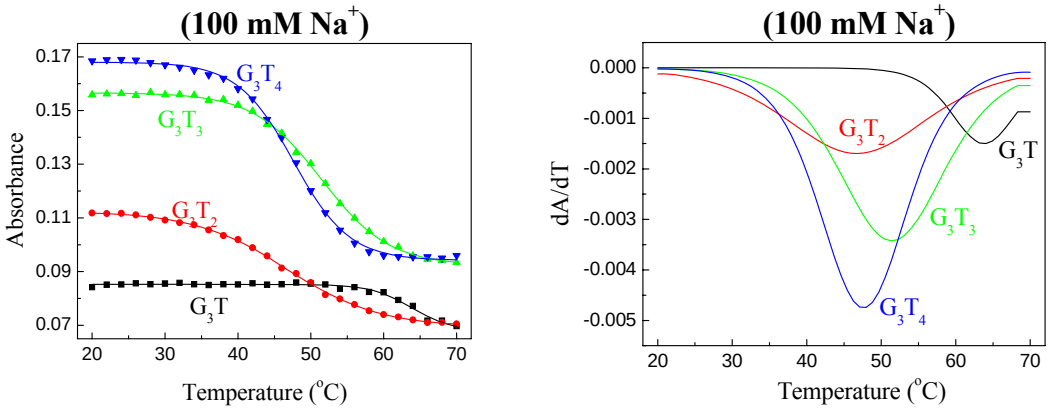
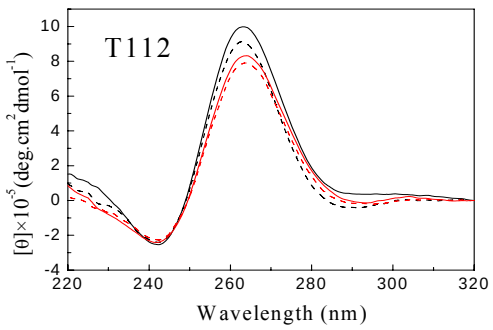
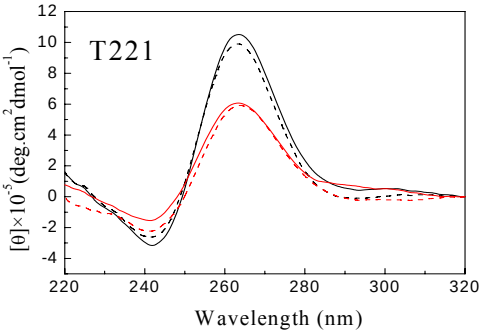
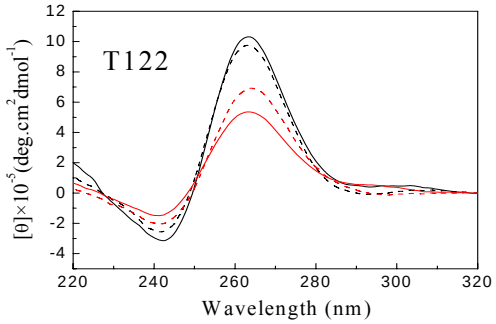


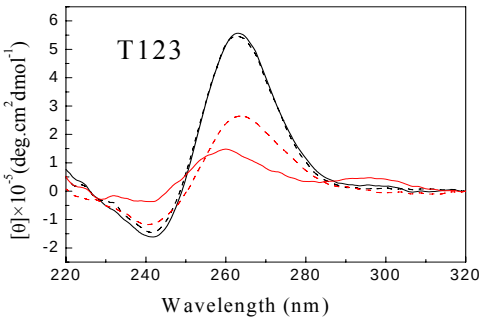
Fig. S2 Melting temperature (T_m) detection for the oligonucleotides with the sequence of $d(G_2T_n)_3G_2$ or $d(G_3T_n)_3G_3$. (**Left**) Denaturation profiles obtained by recording the absorbance change at 295 nm as a function of temperature. (**Right**) First derivative of the denaturation profiles.

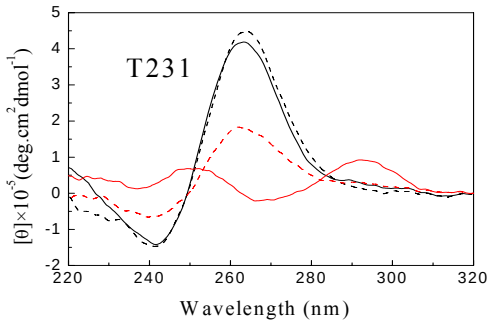
3. CD spectra of the oligonucleotides with the sequence of $dG_3T_iG_3T_jG_3T_kG_3$ in the absence or presence of hemin

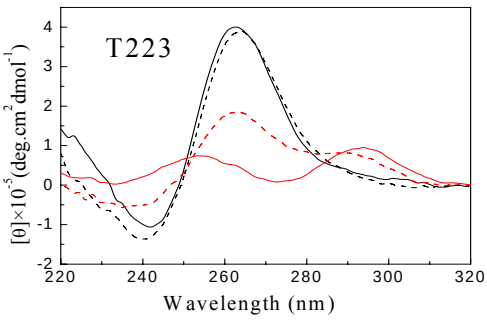


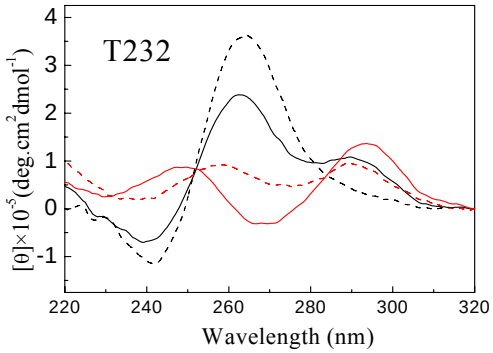


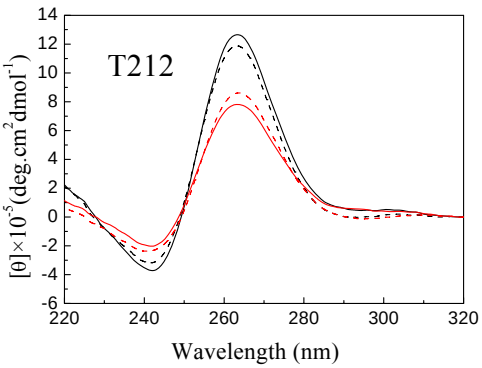












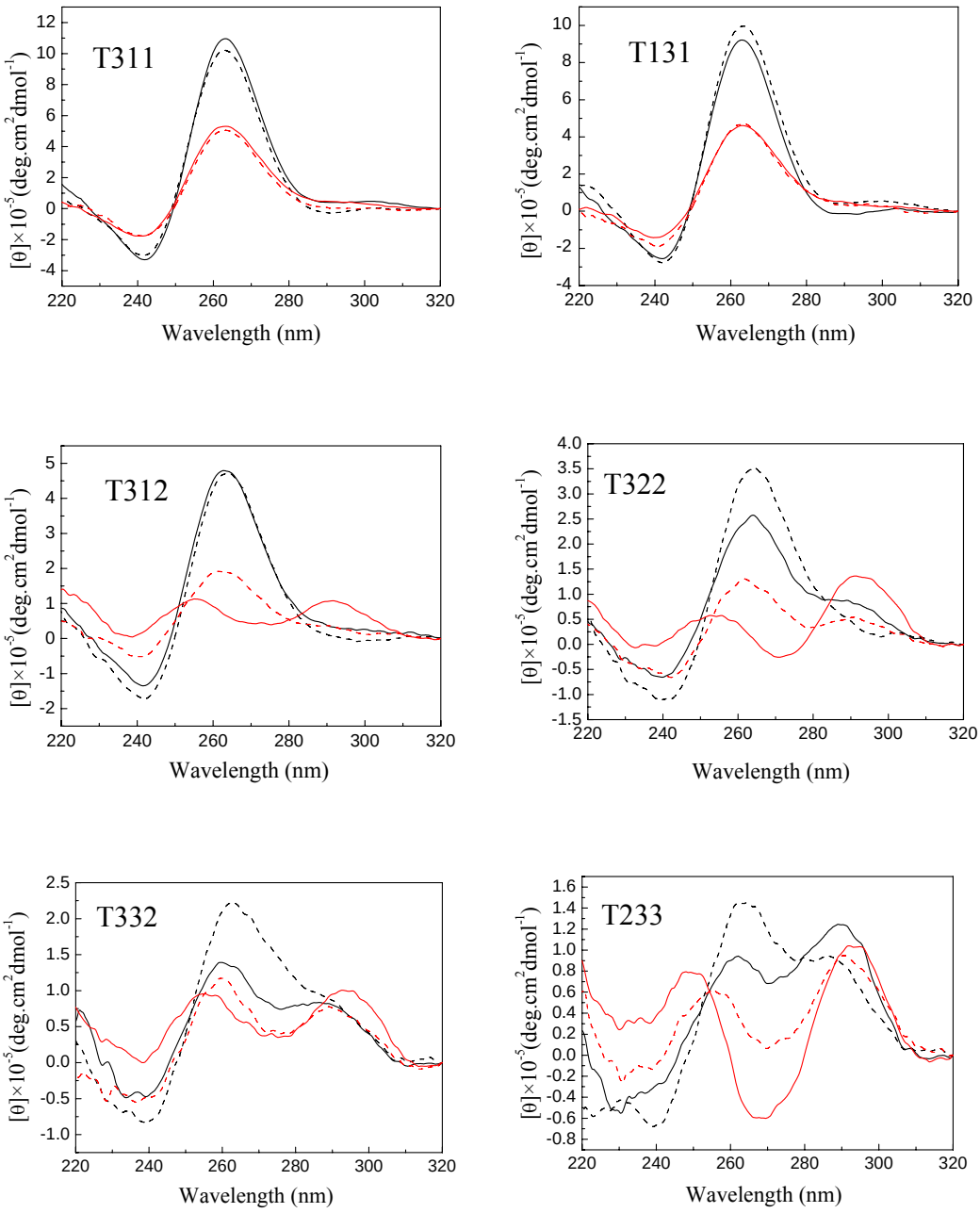


Fig. S3 CD spectra of the oligonucleotides with the sequence of $dG_3T_iG_3T_jG_3T_kG_3$ in the absence (solid lines) or presence (dotted lines) of hemin. The CD spectra were recorded in the presence of 100 mM K^+ (black lines) or 100 mM Na^+ (red lines).

4. Structure and peroxidase activity of the oligonucleotides with the sequence of $dG_3T_iG_3T_jG_3T_kG_3$

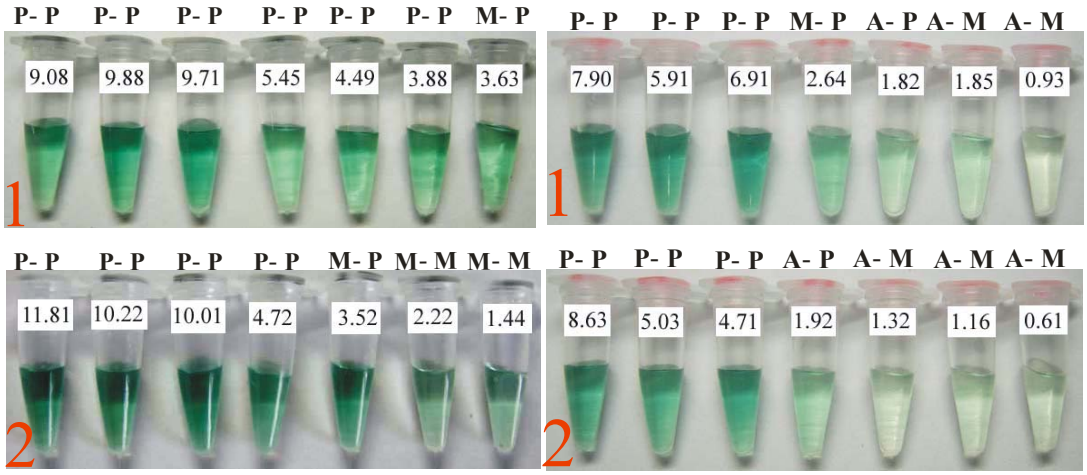


Fig. S4 Oxidation of ABTS by H_2O_2 in the presence of hemin and the oligonucleotides with the sequence of $dG_3T_iG_3T_jG_3T_kG_3$. The experiments were conducted in the presence of 100 mM K^+ (left 1 and 2) or 100 mM Na^+ (right 1 and 2). The letters on the top of each figure represent the G-quadruplex conformations in the absence (in the front of the short lines) or presence (behind the short lines) of hemin. The letters "P", "A" and "M" represent parallel, antiparallel and parallel/antiparallel mixture, respectively. The data in the figures represent the CD signal intensities of the oligonucleotides in the presence of hemin. The oligonucleotides are (left to right): T112, T221, T122, T123, T231, T223, T232 (left 1 and right 1); T212, T311, T131, T312, T322, T332, T233 (left 2 and right 2).

5. Absorbance signal versus K^+ concentration plots

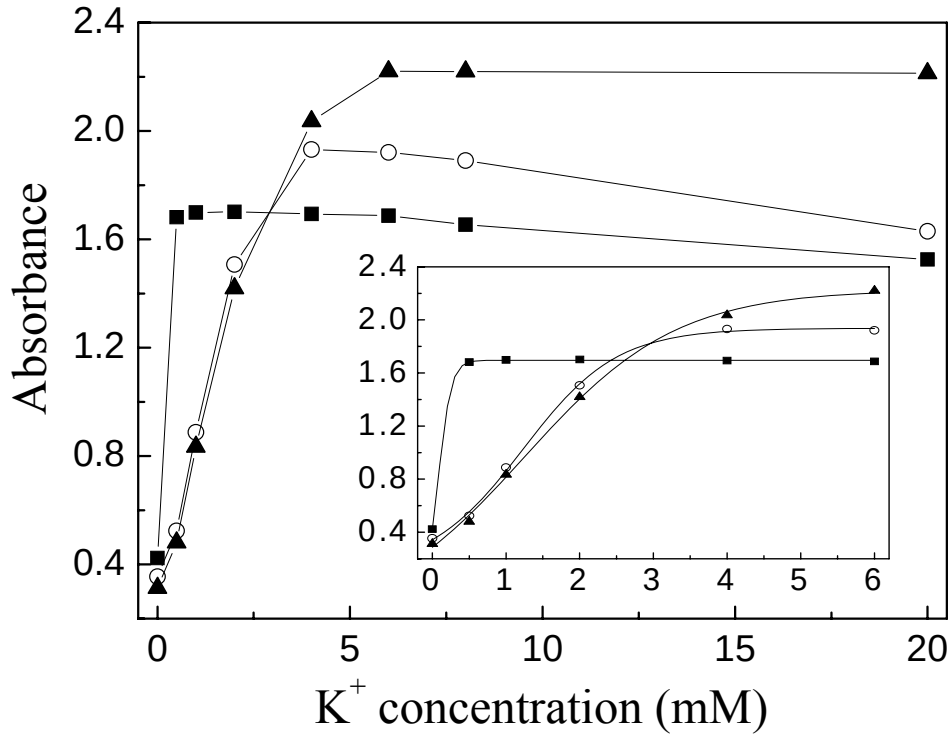


Fig. S5 Absorbance signal at 414 nm versus K^+ concentration plots for the oxidative reaction of ABTS by H_2O_2. The concentration of Na^+: 0 (■), 100 (○) and 300 mM (▲). The inserts show the normalized optical density versus K^+ concentration plots at low K^+ concentration ranges. The solid lines in the inserts represent nonlinear least-squares fit to the data. In this experiment, the oligonucleotide of T223 was used.