Supporting Information

Duplex and Quadruplex DNA Binding and Photocleavage by Trioxatriangulenium Ion†

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DMS footprinting. DMS footprinting reactions were carried out essentially as described (*1S*) with the exception that parallel reactions were carried out in the presence of 10 μM TOTA. Briefly, reaction mixtures (20 μL) containing 3 μL 5'-labeled DNA substrates in the presence or absence of 10 μM TOTA perchlorate at room temperature in 50 mM sodium phosphate buffer containing 10 or 100 mM KCl, pH 7 were treated with 1 μL of a 20% DMS solution in water. After a period of 5 to 30 min, the reaction was quenched by the addition of 100 μL stop buffer (1.0 M □-mercaptoethanol, 1.5 M sodium acetate and 1 μg glycogen). The samples were precipitated by cold EtOH, and washed twice with 70 % EtOH. Samples were subjected to piperidine heat treatment (1 M piperidine, 90 °C, 15 min), dried in a vacuum concentrator, and subjected to electrophoresis on a 12% denaturing polyacrylamine gel.

Reference

1S. Tuntiwechapikul, W., Lee, J. T., and Salazar, M. (2001) Design and synthesis of the G-quadruplex-specific cleavage reagent perylene-EDTA•Iron(II), *J. Am. Chem. Soc. 123*, 5606–5607.

Figure Legends

Figure 1S. Phosphorimage of DMS footprinting of the 5'-labeled TAG strand of the duplex (D) and quadruplex (DQ) substrates in the presence and absence of 10 μM TOTA. Each group of lanes corresponds to a time-course exposure to DMS for 5, 10, 20, and 30 min. Lanes 1: TAG•T6 quadruplex (DQ) in 100 mM KCl after heat treatment (90 °C, 5

min) and rapid annealing; Lanes 2: TAG•T6 quadruplex (DQ) in 100 mM KCl after annealing overnight; Lanes 3: TAG•T6 quadruplex (DQ) in 100 mM KCl in the presence of 10 μM TOTA; Lane 4: TAG•T6 quadruplex (DQ) in 10 mM KCl; Lanes 5: TAG•T6 quadruplex (DQ) in 10 mM KCl in the presence of 10 μM TOTA; Lanes 6: TAG•CTA duplex (D) in 100 mM KCl. Lanes G and GA: Maxam-Gilbert G and GA sequencing.

Figure 2S. Phosphorimage of DMS footprinting of the 5'-labeled TG strand of the duplex (D) and quadruplex (DQ) substrates in the presence and absence of 10 μM TOTA. Each group of lanes corresponds to a time-course exposure to DMS for 5, 10, and 20 min. Lanes 1: TG•T6 quadruplex (DQ) in 100 mM KCl after heat treatment (90 °C, 5 min) and rapid annealing; Lanes 2: TG•T6 quadruplex (DQ) in 100 mM KCl after annealing overnight; Lanes 3: TG•T6 quadruplex (DQ) in 100 mM KCl in the presence of 10 μM TOTA; Lane 4: TG•T6 quadruplex (DQ) in 10 mM KCl; Lanes 5: TG•T6 quadruplex (DQ) in 10 mM KCl in the presence of 10 μM TOTA; Lanes 6: TG•CT duplex (D) in 100 mM KCl. Lanes G and GA: Maxam-Gilbert G and GA sequencing.

Figure 3S. Phosphorimage of the cleavage product for duplex (D) and quadruplex (DQ) substrates in the presence of 10 μM TOTA. A. Photocleavage of 5'-labeled TAG duplex (lanes 6 and 12) and quadruplex (all other lanes) substrates: Lanes 2, 4–6, 8, and 10–12 were irradiated (350 nm, 30 min), all other lanes are dark controls; Lanes 3–6 and 9–12 are in the presence of 10 μM TOTA; Lanes 7–12 were subjected to piperidine heat treatment prior to electrophoresis, Lanes 5 and 11 are in 10 mM KCl, all other lanes are in 100mM KCl phosphate buffer pH 7.0. B. Photocleavage of 5'-labeled TG duplex (lanes 6 and 12) and quadruplex (all other lanes) substrates: Lanes 2, 4–6, 8, and 10–12 were irradiated (350 nm, 30 min), all other lanes are dark controls; Lanes 3–6 and 9–12

are in the presence of 10 μM TOTA; Lanes 7–12 were subjected to piperidine heat treatment prior to electrophoresis, Lanes 5 and 11 are in 10 mM KCl, all other lanes are in 100mM KCl phosphate buffer pH 7.0. Lanes G and GA: Maxam-Gilbert G and GA sequencing.

Figure 4S: Histogram of phosphorimage in Figure 3S-A. A. TOTA photocleavage of TAG•CTA duplex (D), lane 12; B. TOTA photocleavage of TAG•T6 quadruplex (DQ) in 10 mM KCl, lane 11; C. TOTA photocleavage of TAG•T6 quadruplex (DQ) in 100 mM KCl, lane 10.

Figure 5S. Histogram of phosphorimage in Figure 3S-B. A. TOTA photocleavage of TG•CA duplex (D), lane 12; B. TOTA photocleavage of TG•T6 quadruplex (DQ) in 10 mM KCl, lane 11; C. TOTA photocleavage of TG•T6 quadruplex (DQ) in 100 mM KCl, lane 10.

Figure 1S.

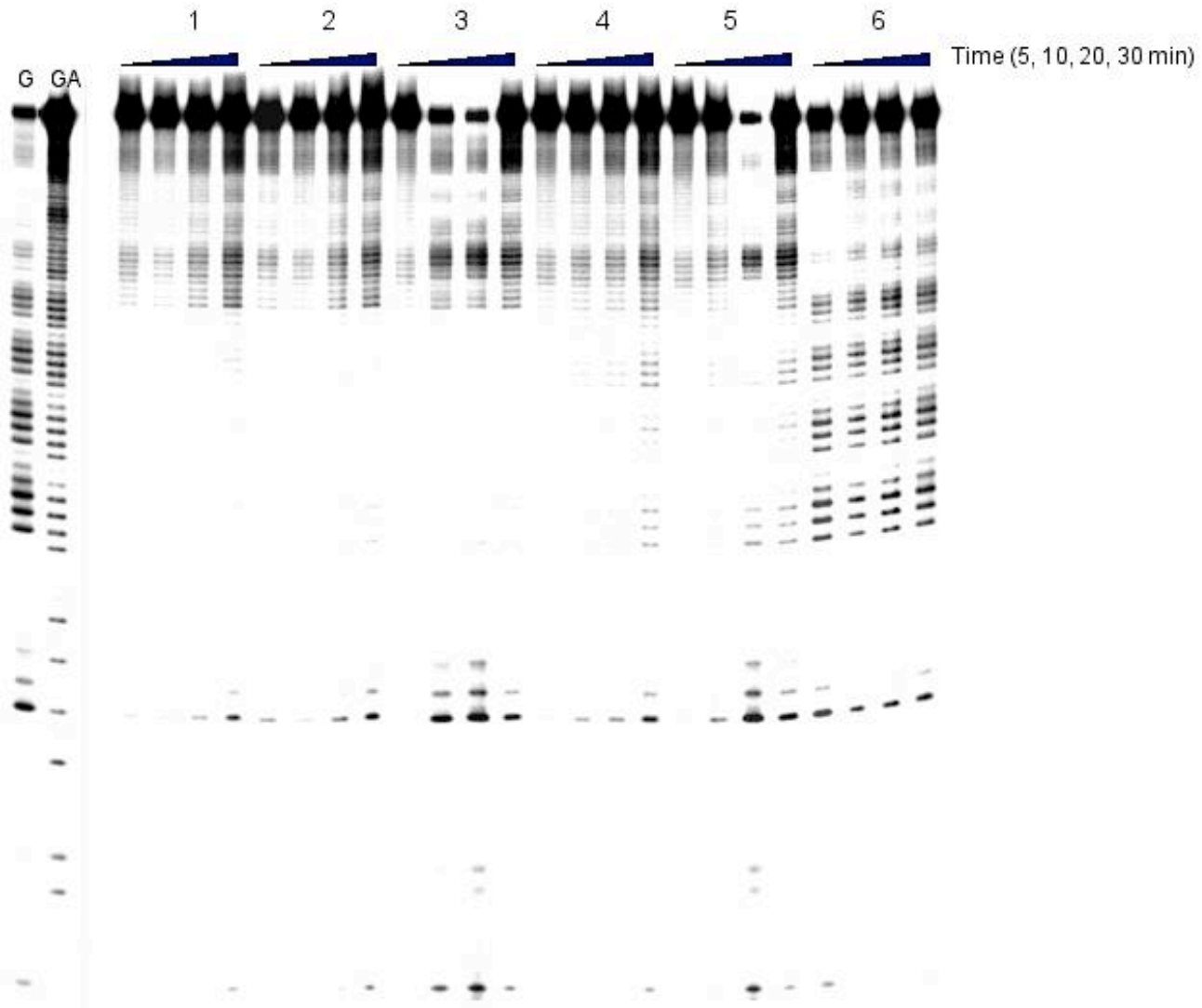


Figure 2S.

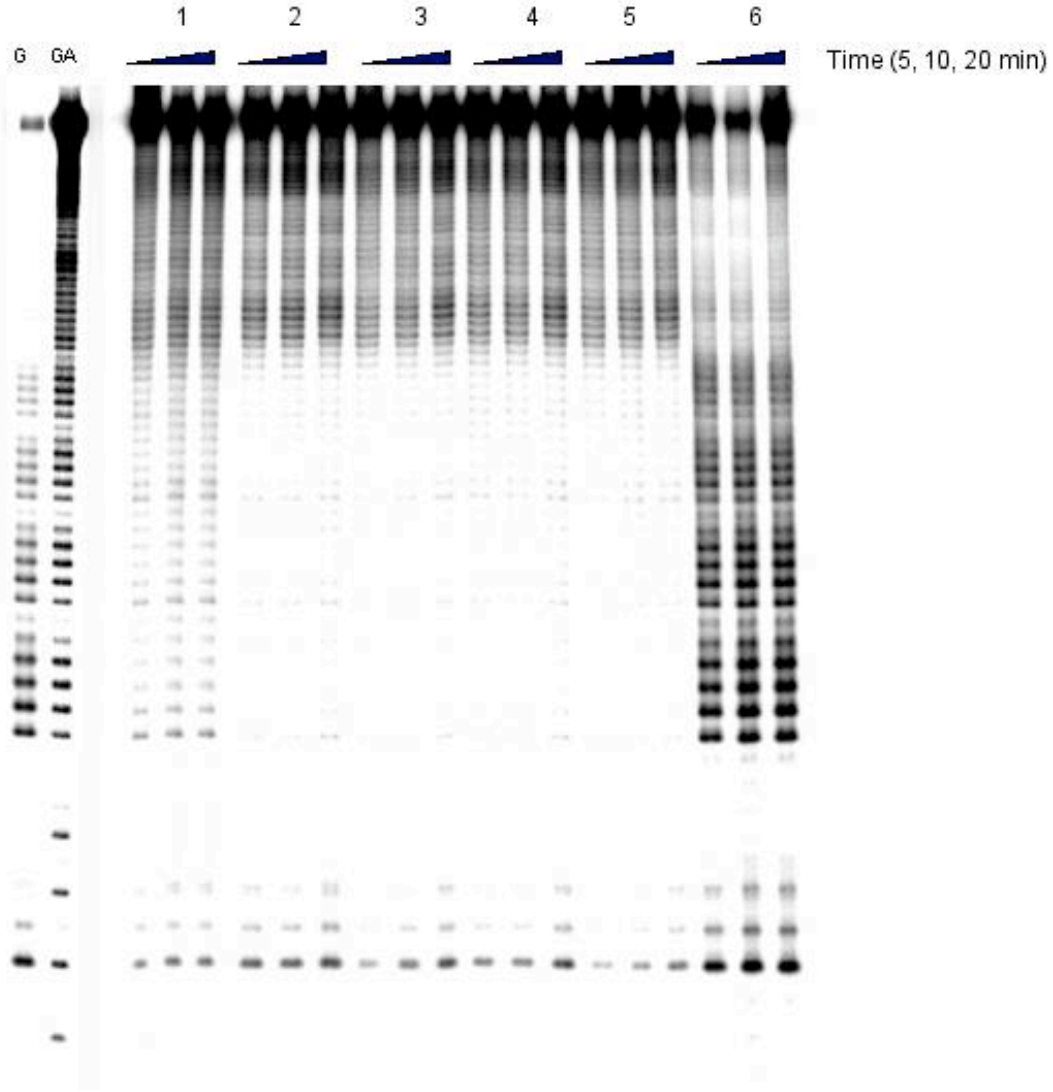


Figure 3S.

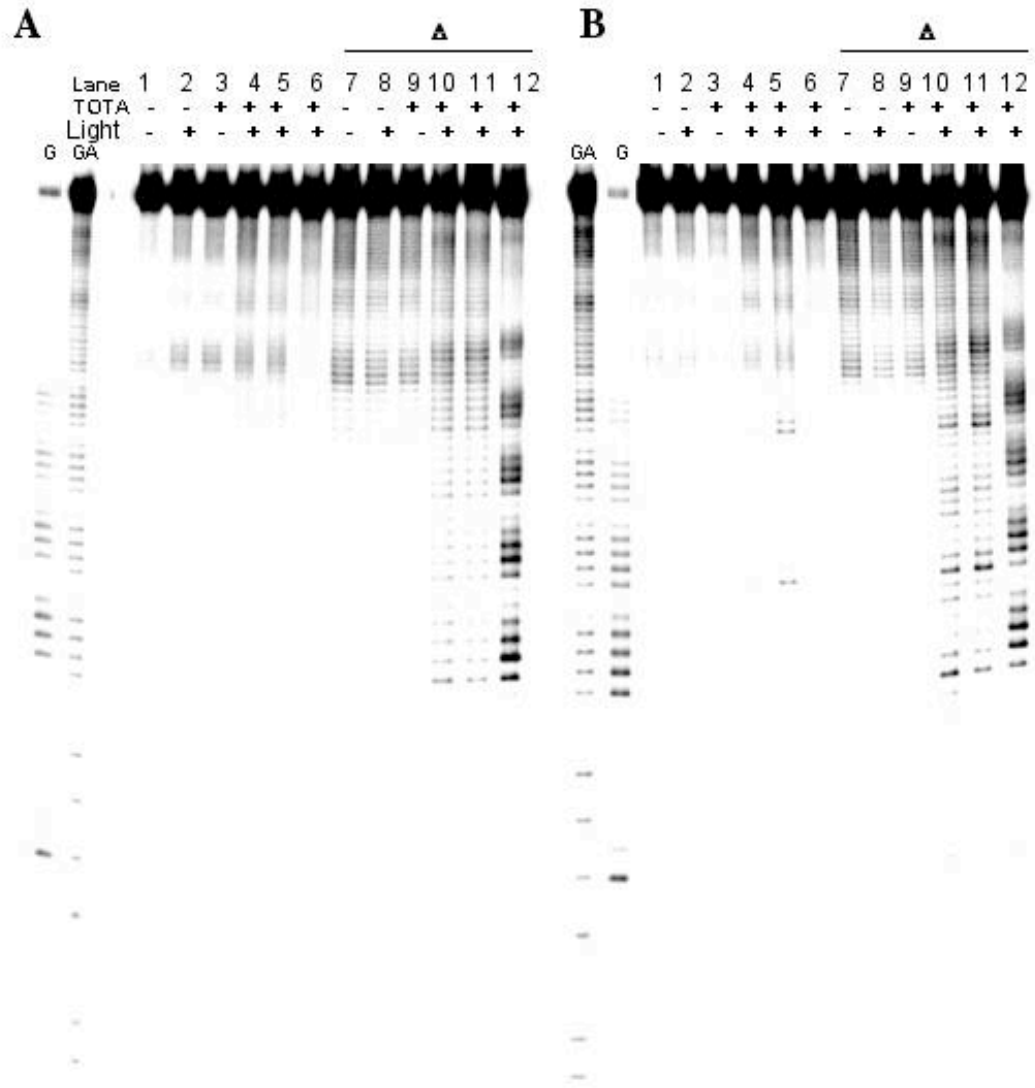


Figure 4S.

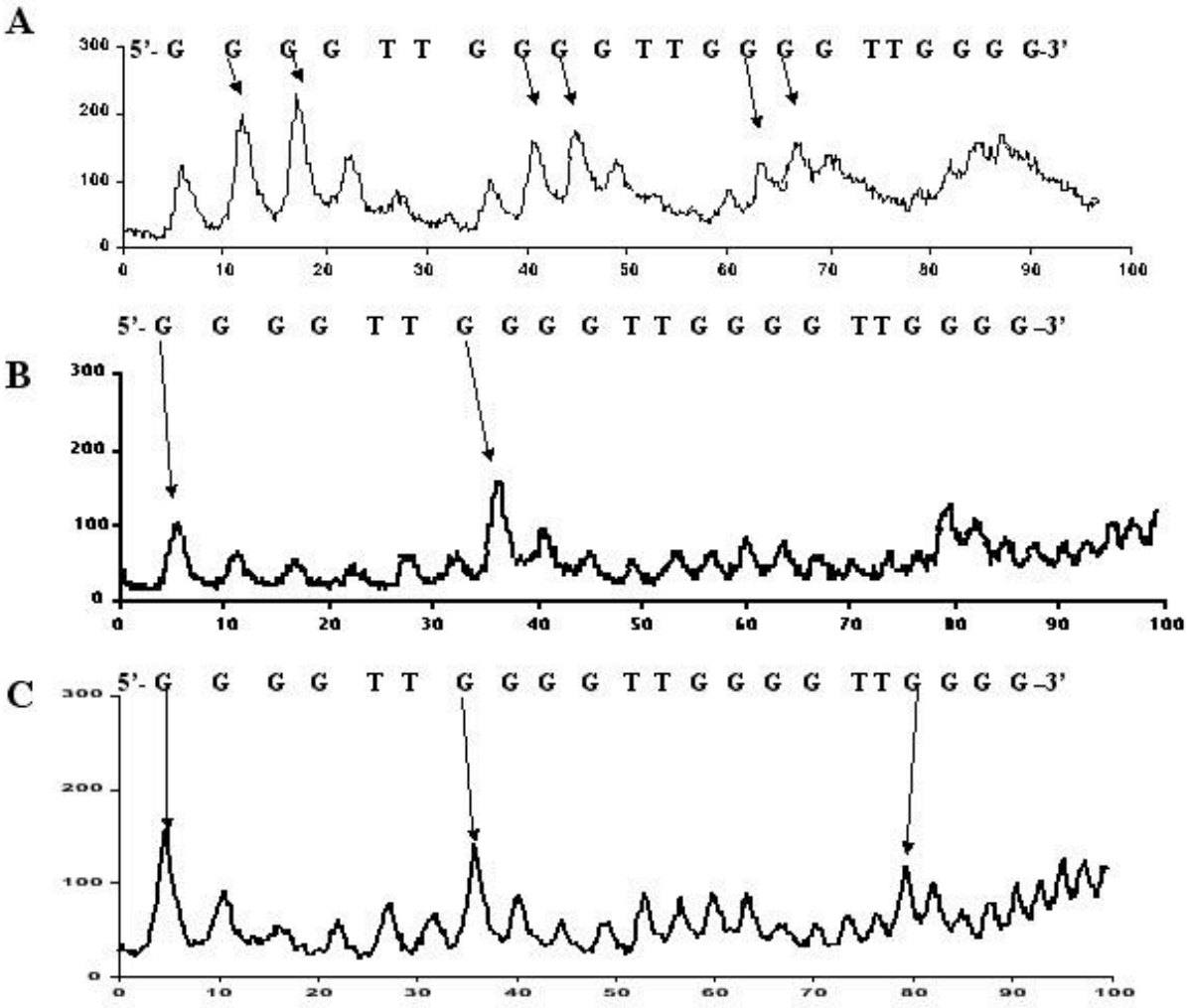
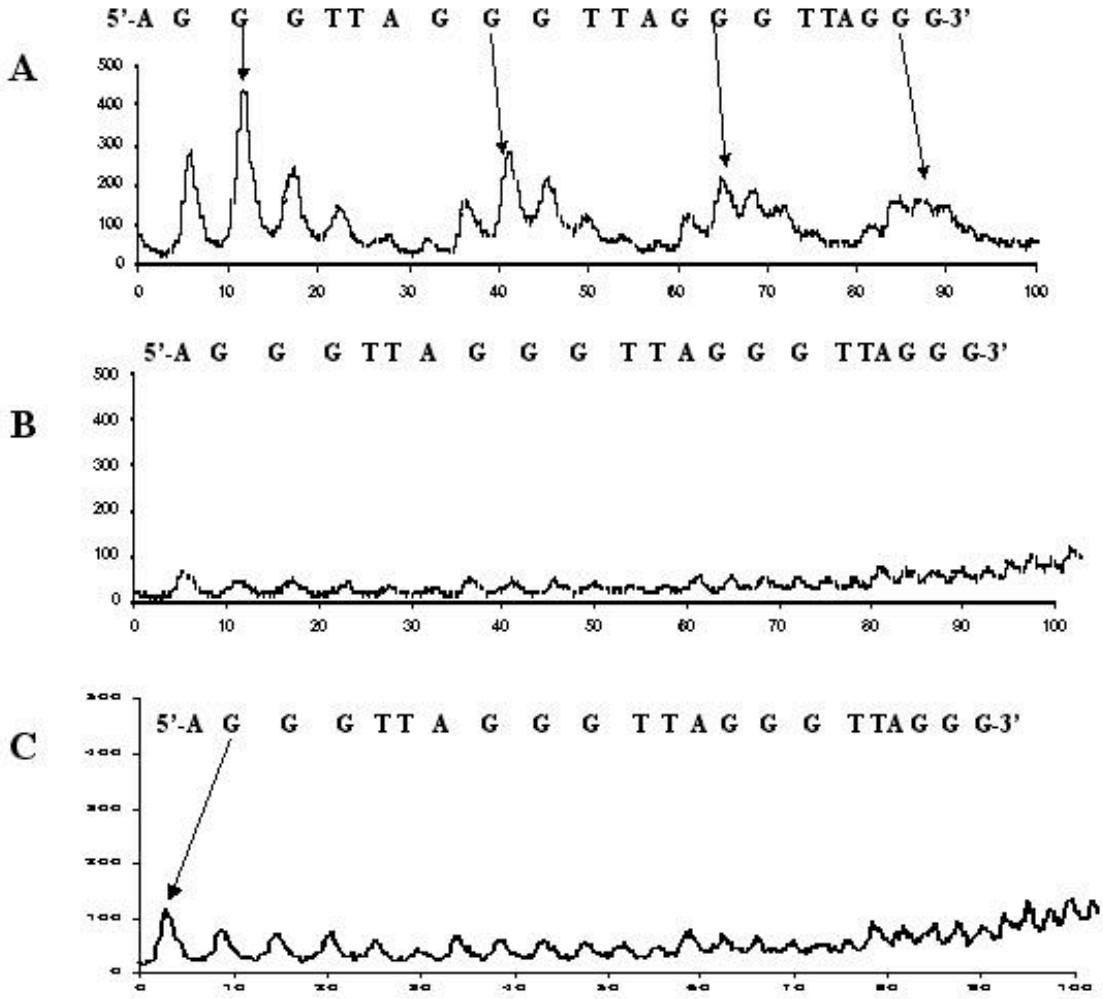

A
5'- G G G G T T G G G G T T G G G G TT G G G G-3'
B
5'- G G G G T T G G G G T T G G G G TT G G G G-3'
C
5'- G G G G T T G G G G T T G G G G TT G G G G-3'

Figure 5S.


A
5'-A G G G TT A G G G TTAG G G TTAG G G-3'
B
5'-A G G G TT A G G G TTAG G G TTAG G G-3'
C
5'-A G G G TT A G G G TTAG G G TTAG G G-3'