Supporting Information For:

A comparative study of recognizing G-quadruplex by dimeric cyanine dyes with different size of aromatic substituents

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1. **Synthesis.**

**B-P4**: 1.14-[bis-[2-3′[3″-(3″′-sulfurpropyl)-benzothiazolium-2″-ylidene][prop-2′-en-1′-yl]-3H-benzothiazolium]-3, 6, 9, 12-tetraoxo-tetradecane (B-P4): yield 36%. $^1$H NMR: (500 MHz, DMSO-d$_6$) δ 165.7, 146.7, 142.1, 141.7, 131.7, 128.3, 127.9, 125.5, 125.3, 124.6, 123.3, 123.2, 117.9, 114.4, 99.6, 70.9, 70.3, 68.3, 65.5, 50.6, 48.4, 46.21. HR-MS (MALDI): Calcd for 1085.2056(M+Na)$^+$, Found 1085.2060 (C$_{68}$H$_{52}$N$_{10}$O$_{10}$S$_5$Na$^+$).

**TC-P4**: 1.14-[bis-[2-3′[3″-(3″′-sulfurpropyl)-β-naphthothiazolium-2″-ylidene][prop-2′-en-1′-yl]-3 H-benzothiazolium]-3, 6, 9, 12-tetraoxo-tetradecane. yield 38.9 %. $^1$H NMR (DMSO-d$_6$): δ 8.55 (d, $J = 8.2$ Hz, 1H), 7.89 (d, $J = 8.3$ Hz, 1H), 7.81 (s, 1H), 7.74 (d, $J = 8.4$ Hz, 2H), 7.66 (s, 1H), 7.53 (s, 1H), 7.48 (t, $J = 12.5$ Hz, 2H), 7.32 (s, 1H), 7.09 (s, 1H), 6.68 (d, $J = 13.2$ Hz, 1H), 6.39 (d, $J = 12.7$ Hz, 1H), 4.73 (s, 2H), 4.32 (s, 2H), 3.79 (s, 2H), 3.55 (s, 2H), 3.55 (s, 2H), 3.45 (s, 2H), 3.41 (s, 2H), 2.80 (s, 2H), 2.29 (s, 2H). $^{13}$C NMR (500 MHz, DMSO-d$_6$, 80°C): δ 146.1, 130.2, 128.8, 128.1, 127.6, 127.2, 125.1, 123.1, 122.3, 119.8, 114.1, 100.3, 98.9, 71.0, 70.4, 70.3, 68.0, 50.2, 48.5, 47.1. HR-MS (MALDI): Calcd for 1185.2369 (M+Na)$^+$, Found 1185.2361(C$_68$H$_{52}$N$_{10}$O$_{10}$S$_5$Na$^+$).

**AB-P4**: 1.14-[bis-[2-3′[3″-(3″′-sulfurpropyl)-β-naphthothiazolium-2″-ylidene][prop-2′-en-1′-yl]-3 H-α-naphthiazole]-3,6,9,12-tetraoxo-tetradecane: yield 16%. $^1$H NMR (500 MHz, CD$_3$OD) δ 7.06 (s, 1H), 6.25 (s, 1H), 6.18 (s, 1H), 5.85 (s, 1H), 5.51 (d, $J = 12.8$ Hz, 1H), 5.30 (d, $J = 11.5$ Hz, 1H), 3.07 (s, 2H), 2.06 (s, 2H). $^{13}$C NMR (500 MHz, CD$_3$OD): δ 163.5, 163.4, 144.0, 138.5, 134.5, 132.6, 129.0, 128.8, 128.1, 127.3, 127.2, 126.0, 125.1, 122.1, 121.5, 120.2, 119.5, 117.7, 111.3, 98.4, 97.3, 70.5, 69.2, 67.7. HR-MS (MALDI): Calcd for 1285.2612 (M+Na)$^+$, Found 1285.2683 (C$_{68}$H$_{52}$N$_{10}$O$_{10}$S$_5$Na$^+$).

2. **The affection of solution polarity to B-P4, TC-P4 and AB-P4.**

Fluorescence spectra were carried out on a Hitachi F-4500 spectrophotometer in a 10 mm quartz cell at room temperature. The excitation wavelength for B-P4 was 510 nm, TC-P4 at 537 nm and AB-P4 at 550 nm. The excitation and emission slits were 10 nm, the voltage were 400 V for B-P4, TC-P4 and AB-P4 with a scan speed of 1200 nm•min$^{-1}$.

Figure S1. The absorption spectra of 10 μM B-P4 (a), TC-P4 (b) and AB-P4 (c) in the presence of dichloromethane (CH$_2$Cl$_2$), dimethyl formamide (DMF), H$_2$O, methanol (MeOH), acetonitrile (CH$_3$CN). The fluorescence intensity of 10 μM B-P4 (a), TC-P4 (b) and AB-P4 (c) in the presence of CH$_2$Cl$_2$, DMF, H$_2$O, MeOH, CH$_3$CN.
The comparison of fluorescence intensity of 10 μM B-P4, TC-P4 and AB-P4 in the presence of H2O.

3. The structure identification of 9 sequences by CD spectroscopy.
   All the CD spectra were recorded on a JASCO J-815 spectrophotometer in a 10 mm path-length quartz cell from 200 nm to 320 nm at room temperature.

4. The fluorescence titration of dyes with different DNA motifs.

5. The absorption titration of AB-P4 with bcl-2 2345.
Figure S5. The absorption titration of AB-P4 (5 µM) in the various concentration of bcl-2 2345, 0 µM, 2.5 µM, 5 µM, 7.5 µM, 10 µM, 20 µM, 30 µM and 40 µM.

6. The ¹H-NMR titration of dyes with different DNA motifs.

Figure S6. The NMR-based folding topologies of the c-myc (a) and bcl-2 2345(b). Variation trajectories for chemical shifts (Δδ) of protons of imino region (c) on c-myc when c-myc is titrated with AB-P4 in the in 0.6 mL PBS (10 mM K$_2$PO$_4$/KH$_2$PO$_4$, 70 mM KCl, 1 mM EDTA, pH 7.4, H$_2$O/D$_2$O(9/1, v/v)), or on bcl-2 2345 when bcl-2 2345 is titrated with TC-P4(d) or AB-P4 (e). Δδ values are calculated by chemical shifts of each c-myc/AB-P4 ratio minus those of c-myc, bcl-2 2345/TC-P4 or bcl-2 2345/AB-P4 ratio minus those of bcl-2 2345. Solid red lines indicate those protons shifting dramatically.