Supporting Information

A novel signal-amplified strategy based on assembly reactivation for highly selective and sensitive detection of chair-like antiparallel G-quadruplex

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Contents:

S(a) – Identification of cyanine dye DMSB

The structure and purification of cyanine dye DMSB were identified by MS-ESI, NMR and absorption spectroscopy.

a) MS-ESI: From the mass spectrum, the measured molecular weight of DMSB is 475.1, which is consistent with the calculated value, 475.5.

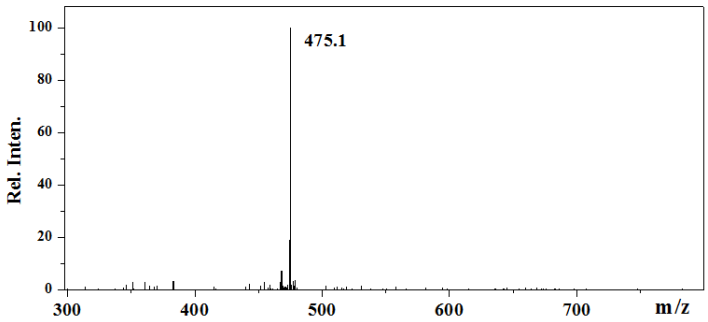

Figure S1. The MS-ESI spectrum of cyanine dye DMSB

b) NMR spectrum

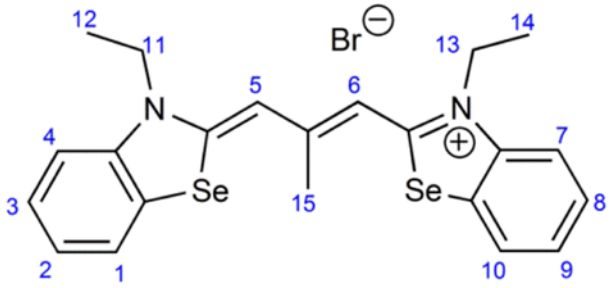

Figure S2. The numbering scheme of molecular structure of DMSB

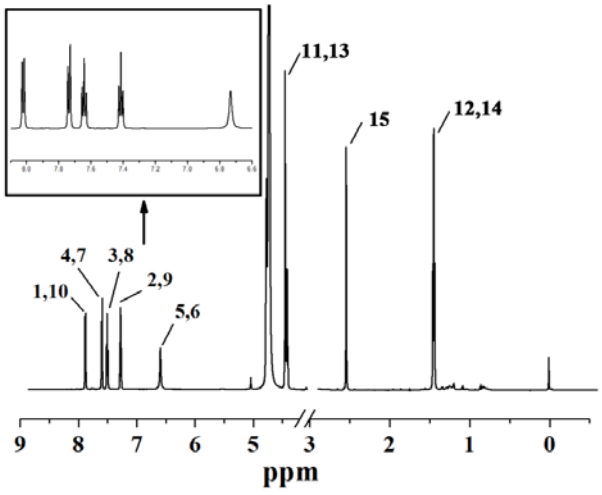

Figure S3. The ^{1}H-NMR spectrum of 1 mM cyanine dye DMSB in CD_3OD

The full assignments of cyanine dye DMSB proton resonance signals in ^{1}H-NMR were performed according to the work of (*Z. V. Voitenko, et al., Tetrahedron, 2003*) and (*William E. Evenson et al., J. Org. Chem., 2012*). There are totally 15 different proton spin systems on DMSB. Because DMSB is a symmetric molecule, 14 out of the 15 spin systems exhibit 7 resonance signals. So there are 8 resonance signals could be observed from the ^{1}H-NMR spectrum, including two primary carbon proton signals, one secondary carbon proton signal, one tertiary carbon proton signal and four aromatic proton signals. The specific assignment is tabulated in Table S1.

Table S1. The full assignments of the proton resonance signals of DMSB

Proton number	Proton kind	^{1}H peak	Proton number	Proton kind	^{1}H peak
1	Aromatic	7.93-7.91, d	9	Aromatic	7.31, t
2	Aromatic	7.31, t	10	Aromatic	7.93-7.91, d
3	Aromatic	7.54, t	11	Secondary	4.48-4.44, q
4	Aromatic	7.63-7.64, d	12	Primary	1.45, t
5	Tertiary	6.63, s	13	Secondary	4.48-4.44, q
6	Tertiary	6.63, s	14	Primary	1.45, t
7	Aromatic	7.63-7.64, d	15	Primary	2.55, s
8	Aromatic	7.54, t			

c) UV-vis spectrum research and absorption coefficient calculation

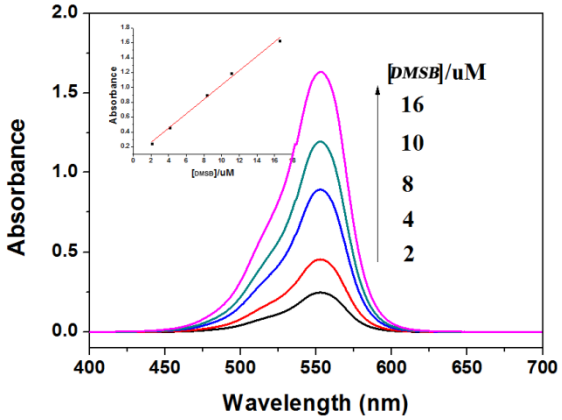

Figure S4. The absorption spectra of DMSB monomer in methanol. Inset gives the curve of the absorbance at 554 nm against the concentration of DMSB. Based on lambert-beer's law, the molar absorption coefficient of DMSB monomer is: $\varepsilon^{M}_{1cm,554nm} = 1.083 \times 10^5 M^{-1} \cdot cm^{-1}$.

S(b) – The spectral features of DMSB in different solvents

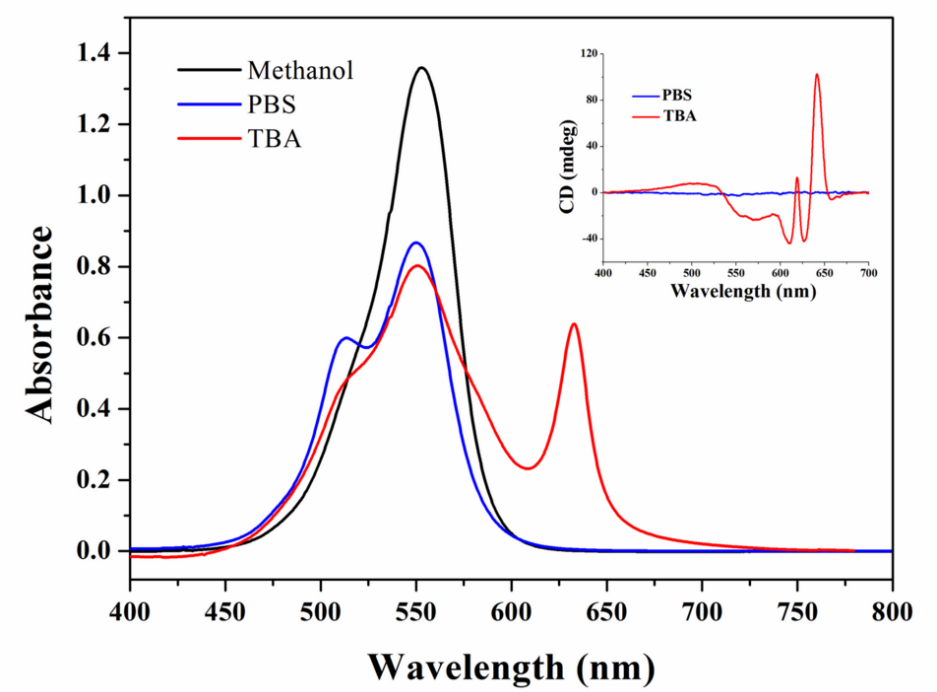

Figure S5. The absorption spectra of 12 μM DMSB in methanol (black), phosphate buffer solution (PBS, 20 mM K_2HPO_4/KH_2PO_4, 100 mM KCl, pH = 7.4) (blue) and PBS in the presence of 0.6 μM ***TBA*** (red). Inset gives the circular dichroism spectra of DMSB in PBS with (red) and without (blue) ***TBA*** added.

S(c) – The structure identification of 11 sequences by CD spectroscopy

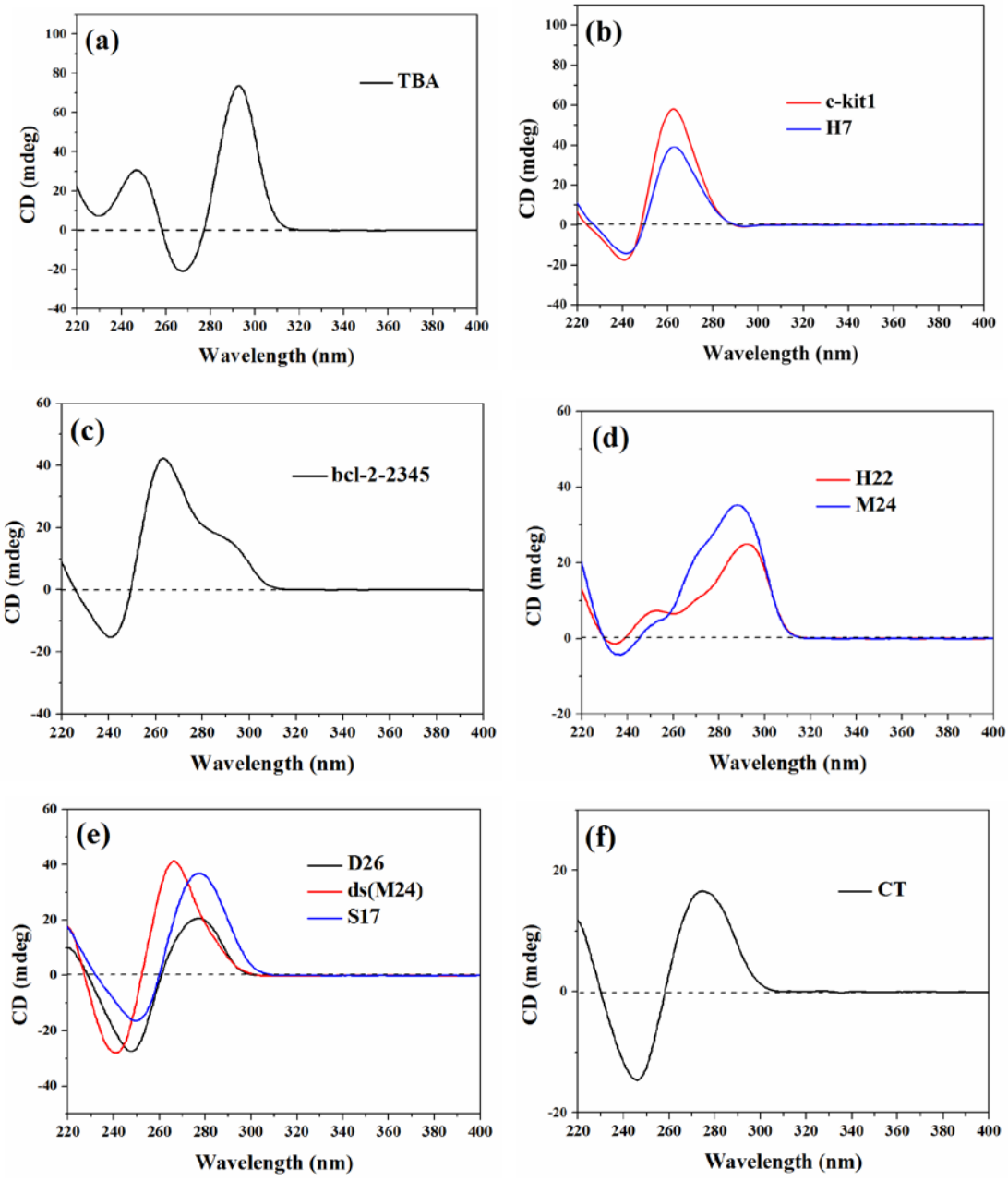

Figure S6. The circular dichroism spectra for the 11 oligomers in PBS: (a) ***TBA***, intramolecular anti-parallel G-quadruplexes; (b) ***c-kit1*** and ***H7***, parallel-stranded G-quadruplexes; (c) ***bcl-2-2345***, (3+1) hybrid G-quadruplex; (d) ***H22*** and ***M24***, mixed-type G-quadruplexes forms in experimental condition; (e) ***D26***, and ***ds(M24)***, double-stranded and ***S17***, a random single-stranded oligomer; (f) ***CT***, genomic DNA.

S(d) – ^{1}H-NMR spectra of TBA titrated with DMSB

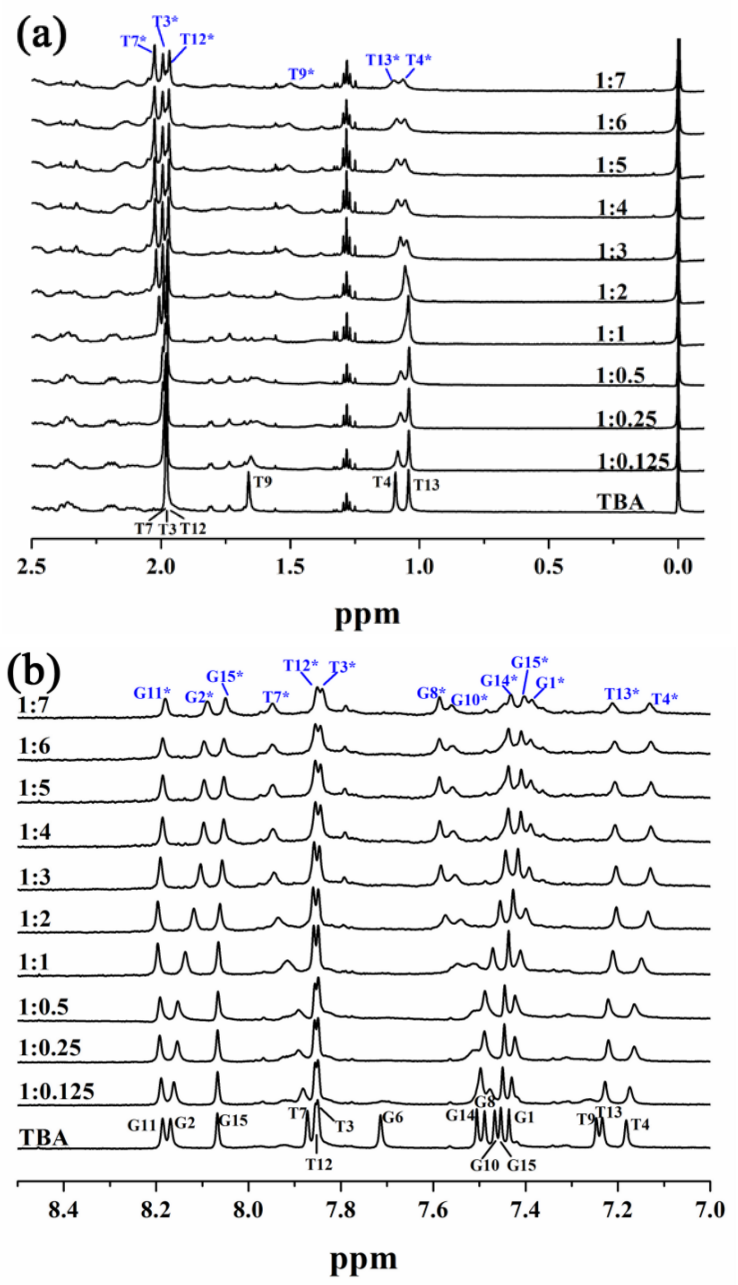

Figure S7. The unambiguous assigned aliphatic region (a) and the aromatic region (b) of ^{1}H-NMR spectra for 0.5 mM ***TBA*** titrated with DMSB in 120 mM PBS (K^{+}) at 303 K. The [***TBA***] : [DMSB] molar ratios are shown along the side of each spectrum. The spectrum for ***TBA*** without DMSB added is shown at the bottom of both Figures.

S(e) – TBA sequence mutation experiments

Table S2. Sequences of the six mutated TBA

Name	Sequence
TBA	5′-GGTTGGTGTGGTTGG-3′
T3-mutated TBA	5′-GG**A**TGGTGTGGTTGG-3′
T4-mutated TBA	5′-GGT**A**GGTGTGGTTGG-3′
T7-mutated TBA	5′-GGTTGG**A**GTGGTTGG-3′
T9-mutated TBA	5′-GGTTGGTG**A**GGTTGG-3′
T12-mutated TBA	5′-GGTTGGTGTGG**A**TGG-3′
T13-mutated TBA	5′-GGTTGGTGTGGT**A**GG-3′

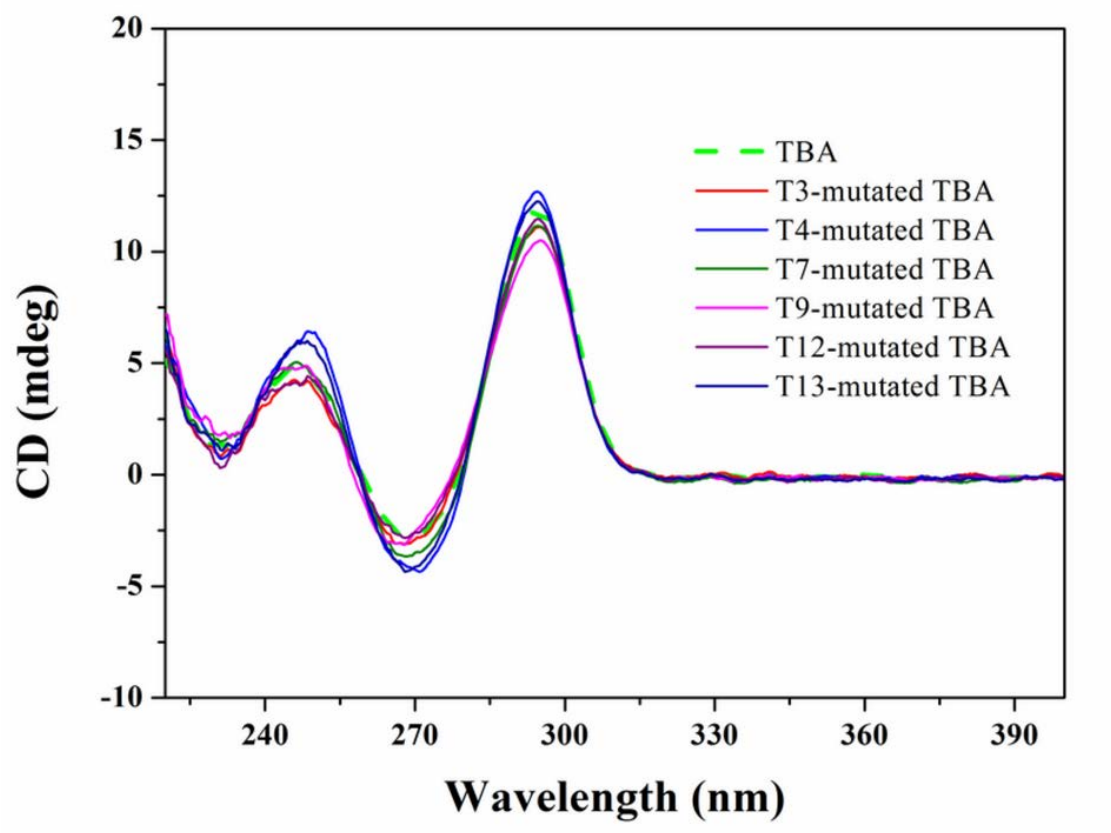

Figure S8. The circular dichroism spectra of the six mutated ***TBA*** (3 μM). All the six mutated sequences could form antiparallel G-quadruplexes as ***TBA*** (green dash), which indicates that T → A mutations do not change the structure of ***TBA***.

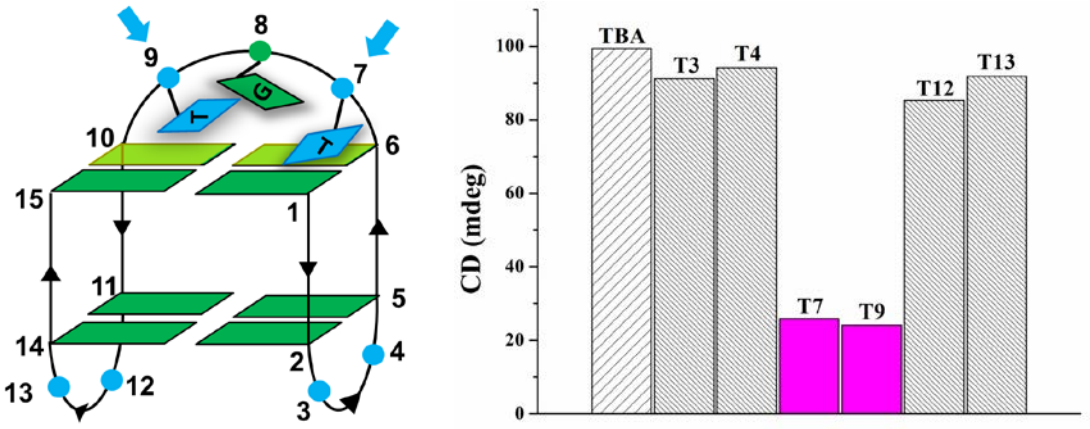

Figure S9. The schematic presentation of the sites of mutated thymines (left, light blue) and the intensity of circular dichroism signal of DMSB J-aggregates induced by the six mutated TBA in PBS measured at 4 °C (right). The concentration of ***TBA*** and mutated ***TBA*** sequences are 0.6 μM while the concentration of DMSB is 12μM.

S(f) – Comparison of induced circular dichroism of DMSB monomer

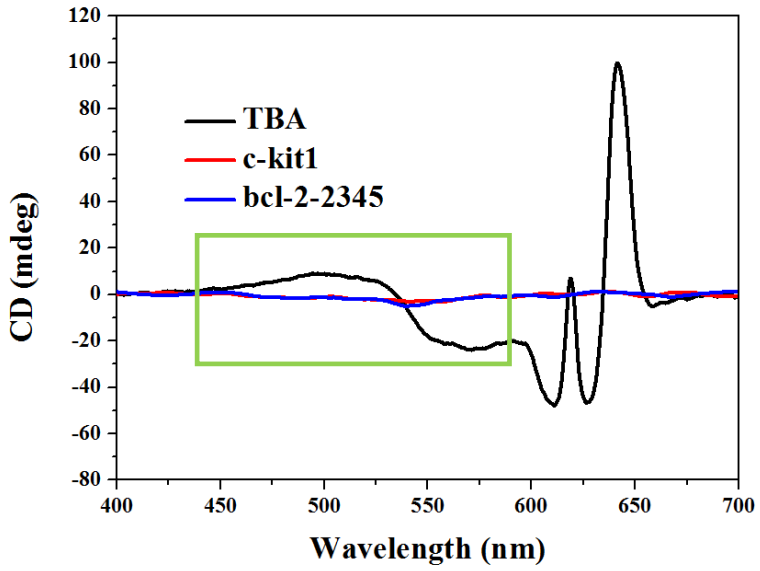

Figure S10. Circular dichroism spectra of 12 μM DMSB in the presence of 1 μM ***TBA*** (black), 1 μM ***c-kit1*** (red) and 1 μM ***bcl-2-2345*** (blue), respectively. The region in light green box presents a bisignated CD signal of DMSB monomer in the presence of ***TBA***.