Supporting information for:

Targeting of parallel c-myc G-quadruplex by dimeric cyanine dye supramolecular assembly: dependence on the linker length

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1. The spectra characteristics of TC and TC-P3-7.

Table S1. Absorption and emission maxima (λ_{max}), Stokes's shifts ($\Delta\nu_{st}$) and quantum yields (Φ) of dyes TC and TC-P3-7.

Complex	λ_{max}(Abs) (nm)	λ_{max}(Em) (nm)	Stoke shift $\Delta\nu_{st}$ (nm)	Φ
TC	586	607	21	0.17[a]
TC-P3	586	609	23	0.21 [a]
TC-P4	587	610	23	0.11 [a]
TC-P5	586	611	23	0.21 [a]
TC-P6	587	611	24	0.13 [a]
TC-P7	590	625	35	0.13 [a]

[a] The fluorescence quantum yield (Φ) were measured in DMSO solution using crystal violet in methanol as the reference.

2. Absorption and fluorescence spectra of TC-P4

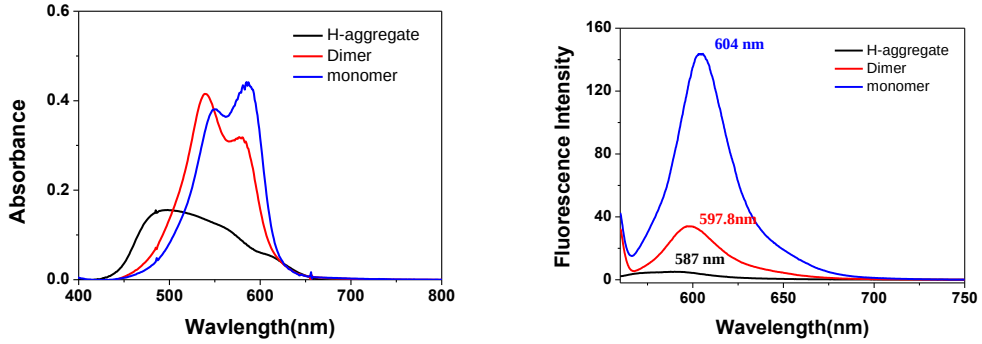


Figure S1. The absorbance (left) and fluorescence emission (right) of TC-P4 in MeOH (red), CH_2Cl_2 (blue) and water (black).

As shown in Figure S1, TC-P4 shows different assembly in different solvents. TC-P4 shows strong enhancement fluorescence intensity around 604 nm assigned to monomer in CH_2Cl_2, moderate enhancement fluorescence intensity around 597.8 nm assigned to dimer in MeOH, and strongly quenched around 587 nm assigned to H-aggregates in PBS. It is well documented that the fluorescence of H-aggregates is strong quenched in aqueous solution[1].

3. The stability of TC-P3-7

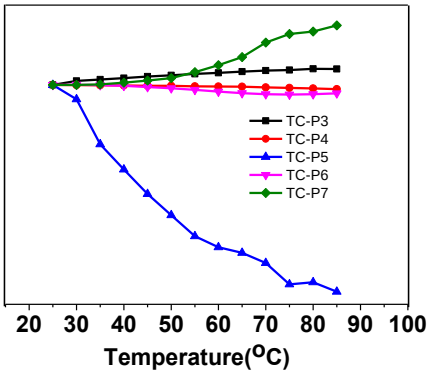


Figure S2. The stability of dyes TC-P3-7 was carried out in PBS. The absorbance spectra of these dyes were normalized at 470 nm.

4. The sequence and origin of 4 oligonucleotides in the study

Table S2. Sequence and origin of 4 oligomers

	Sequence (from 5′ to 3′)	**Motifs**	**Origin**
c-myc 22	TGAGGGTGGGTAGGGTGGGTAA	Parallel G-quadruplex	Oncogenic promoter
c-myc	TGAGGGTGGGGAGGGTGGGGAA	Parallel G-quadruplex	Oncogenic promoter
CT		Linear double-stranded	Calf thymus
S17	CCAGTTCGTAGTAACCC	Single-Stranded	

5. The Structure identification of 4 sequences by CD spectroscopy.

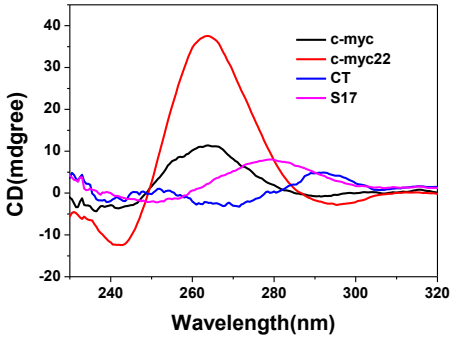
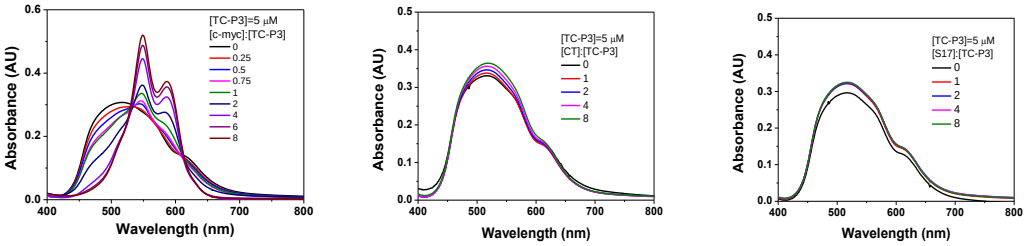


Figure S3. The CD spectra for 4 oligomers in 10 mM PBS (K^+).

6. UV titration spectra of c-myc with TC-P3, TC-P5, TC-P6 and TC-P7.



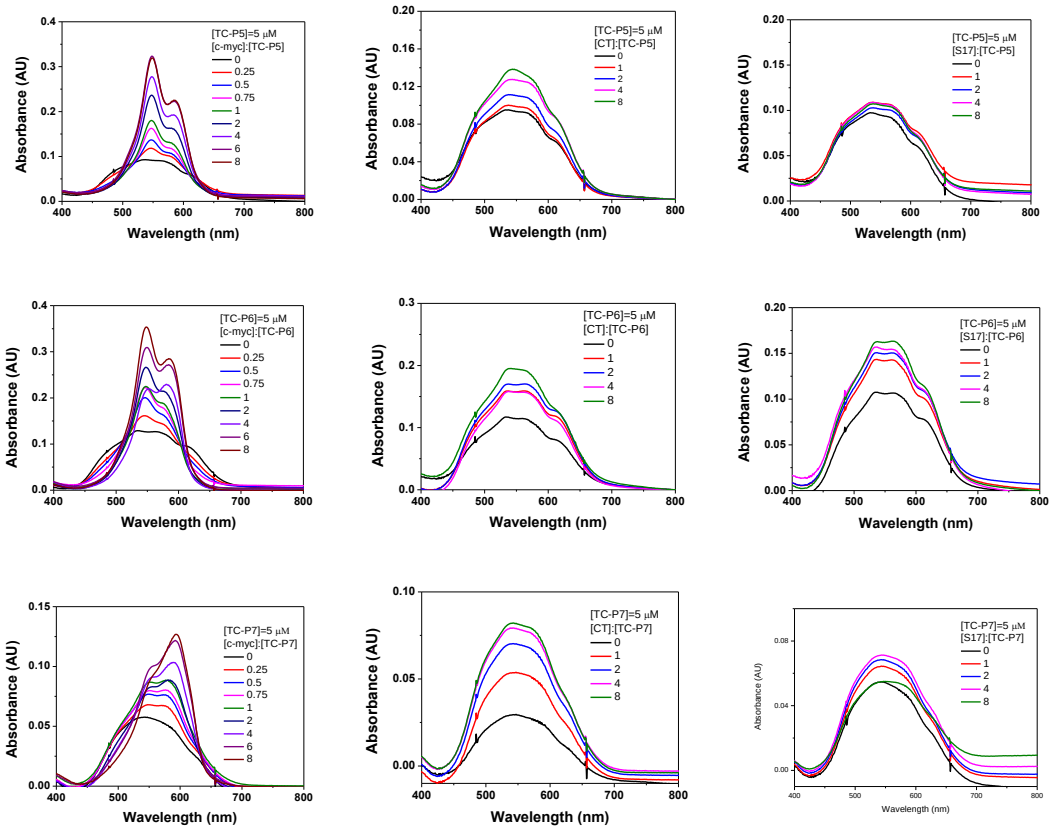
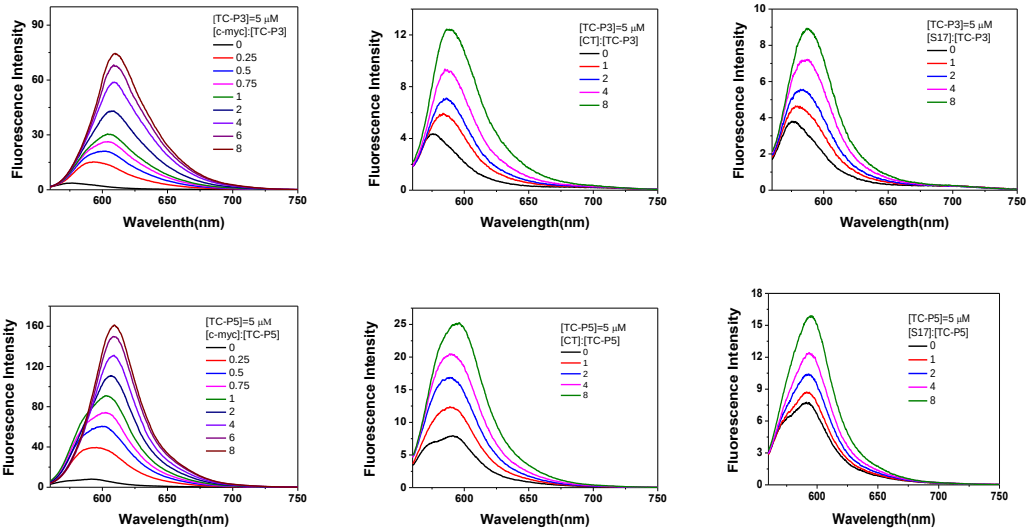


Figure S4. The UV titration spectra of 5 μM TC-P3 and TC-P5-7 in 10 mM PBS with parallel G-quadruplex c-myc, duplex CT and single-stranded S17.

7. The FL titration spectra of c-myc with TC-P3, TC-P5, TC-P6 and TC-P7.



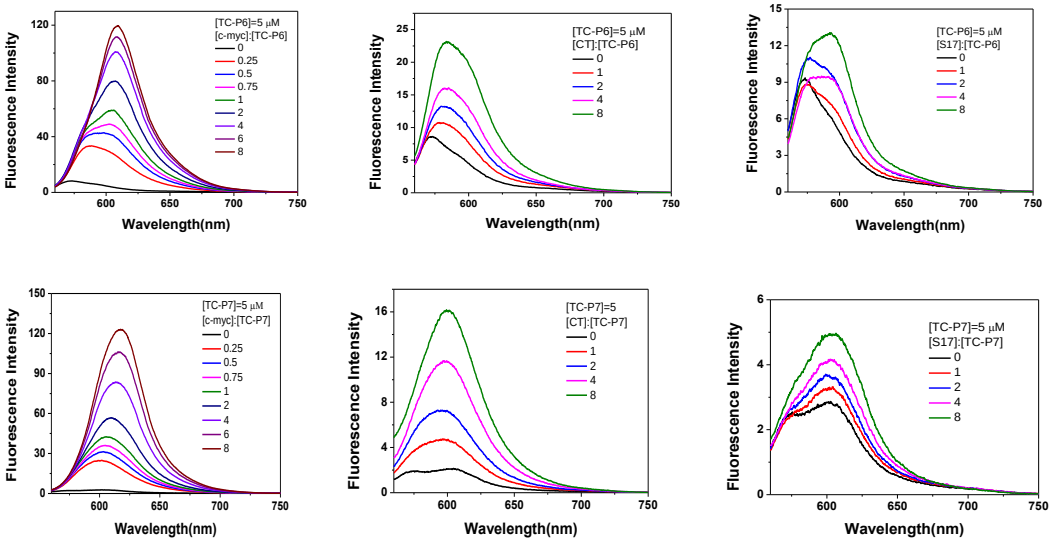


Figure S5. The FL titration spectra of 5 μM TC-P3 and TC-P5-7 in 10 mM PBS with parallel G-quadruplex c-myc, duplex CT and single-stranded S17.

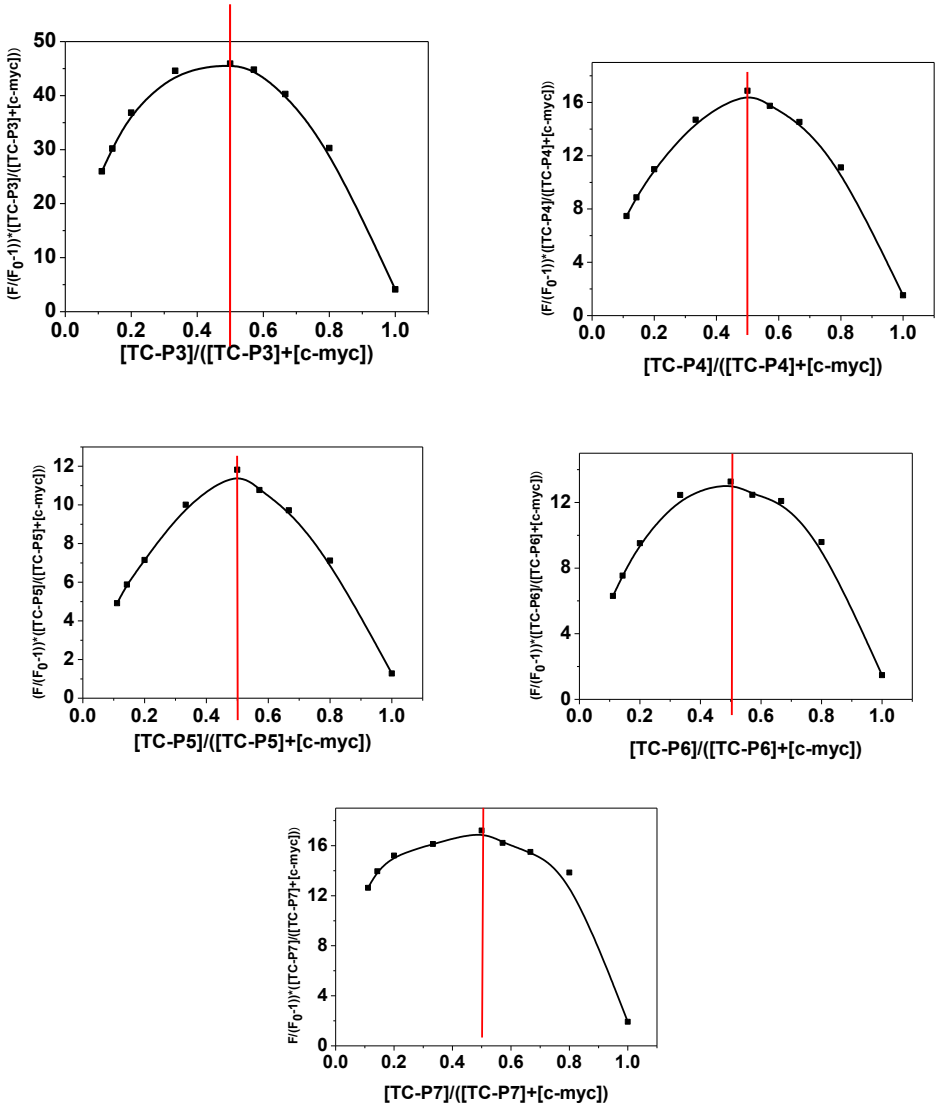


Figure S6. Job plot analysis[2]. TC-P3 and TC-P5-7 were mixed with c-myc at different ratio in 10 mM PBS.

8. Inhibition activity of TC-P3 and TC-P5-7 on the peroxidase activity of G4/hemin complexes.

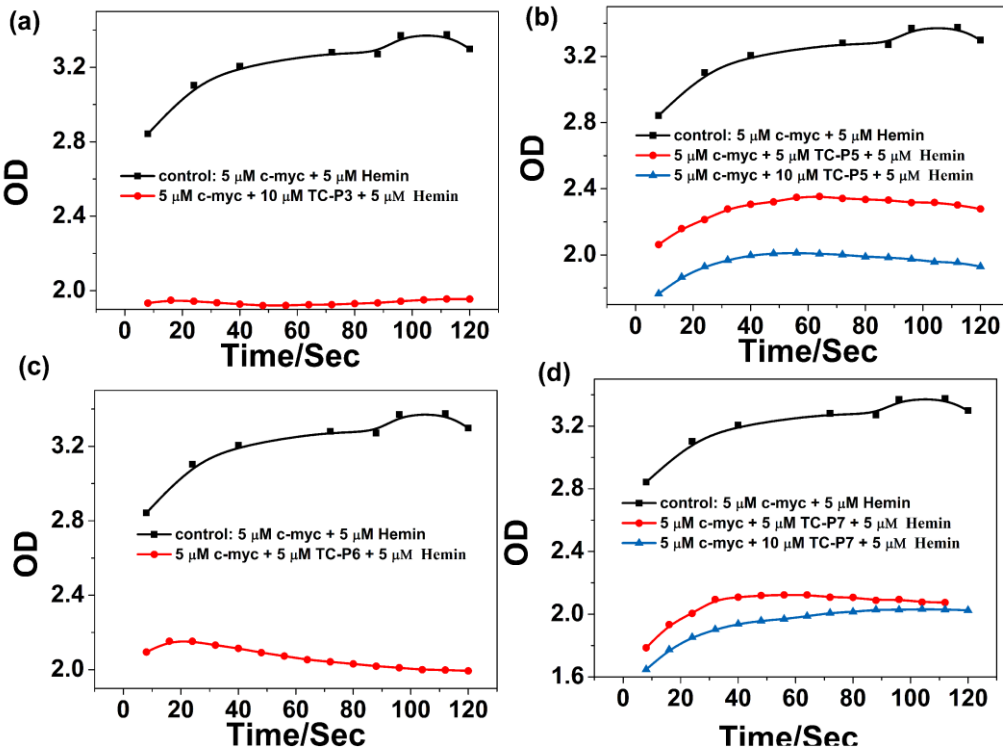


Figure S7. Inhibition of activity of **TC-P3** (a) and **TC-P5-6** (b-d) on the peroxidase activity of G4/Hemin complexes. The curves represent the changes of the product concentration (absorbance at 415 nm) of peroxidase reaction with 2 min. The G4/hemin peroxidase reaction in the absence of dyes was used as a control.

9. Molecular docking experiment

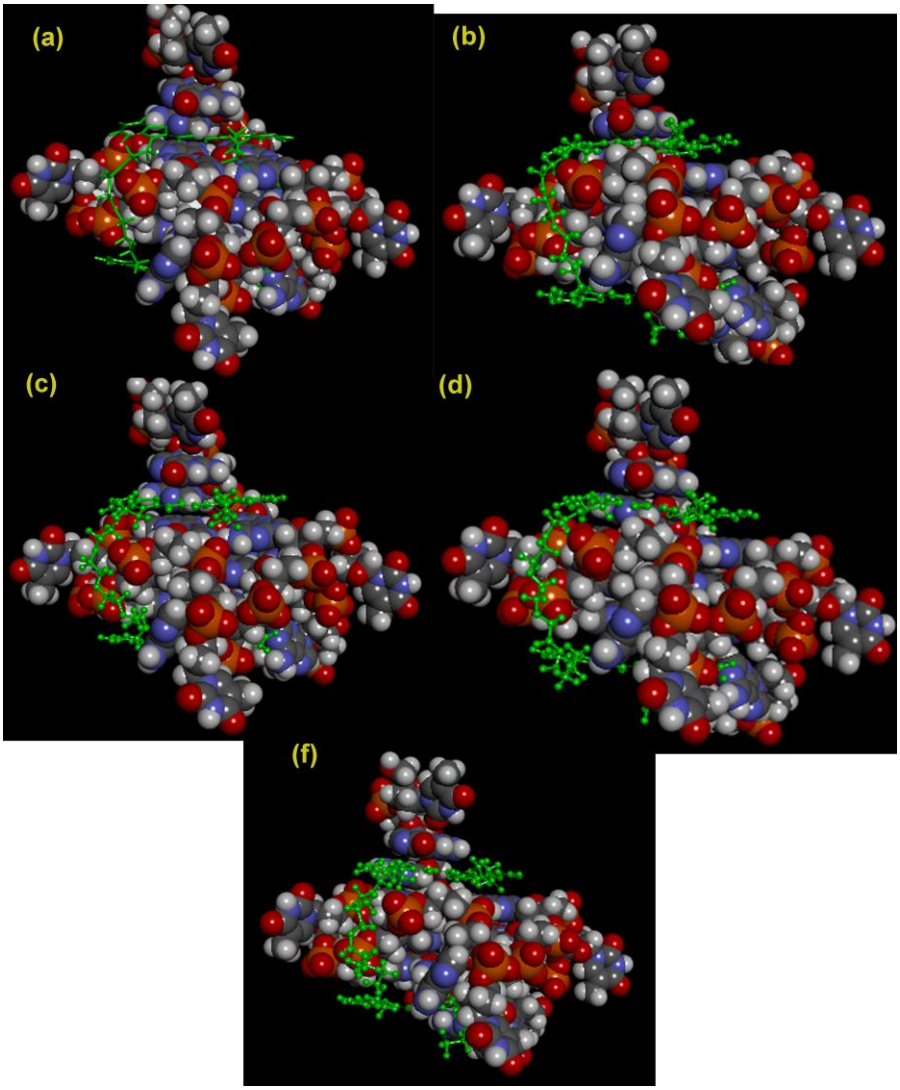


Figure S8. Molecular models showing interaction of TC-P3-7 (a-f) with G-quadruplex (PDB: 2L7V). TC-P3-7 could stack on both ends of G-quadruplex.

10. The flow cytometric analysis.

Table S3. Flow cytometric analysis of CRL 2614 and Hela cells by TC-P3

Cell	Cell No.		TC-P3 Uptake(/10^5 cell)		
	control	stained	control	stained	Δ/ uptake No.
CRL2614	30059	100000	585	79716	79131
Hela	100000	100000	99	11475	11376

Table S4. Flow cytometric analysis of CRL 2614 and Hela cells by TC-P4

Cell	Cell No.		TC-P4 Uptake(/10^5 cell)		
	control	stained	control	stained	Δ/ uptake

					No.
CRL2614	100000	100000	102	51601	51499
Hela	100000	100000	265	91235	90970

Table S5. Flow cytometric analysis of CRL 2614 and Hela cells by TC-P5

Cell	Cell No.		TC-P5 Uptake(/10^5 cell)		
	control	stained	control	stained	Δ/ uptake No.
CRL2614	100000	100000	109	3665	3556
Hela	100000	100000	94	51012	50918

Table S6. Flow cytometric analysis of CRL 2614 and Hela cells by TC-P6

Cell	Cell No.		TC-P6 Uptake(/10^5 cell)		
	control	stained	control	stained	Δ/ uptake No.
CRL2614	100000	100000	109	867	758
Hela	100000	100000	94	47654	47560

Table S7. Flow cytometric analysis of CRL 2614 and Hela cells by TC-P7

Cell	Cell No.		TC-P7 Uptake(/10^5 cell)		
	control	stained	control	stained	Δ/ uptake No.
CRL2614	100000	100000	109	2103	1994
Hela	100000	100000	94	13341	13247

Reference

1. U. Rösch, S. Yao, R. Wortmann and F. Würthner, *Angewandte Chemie*, 2006, **118**, 7184-7188.
2. P. Job, *Annali di Chimica Applicata*, 1928, **9**, 113-203.