Supporting Information

Nucleic Acid Induced Tetraphenylethene Probe Noncovalent Self-Assembly and the Superquenching of Aggregation-Induced Emission

Jian Chen,[a] *Yan Wang,*[ab] *Wenying Li,*[ab] *Huipeng Zhou,*[a] *Yongxin Li,*[a] *and Cong Yu**[ab]

[a] State Key Laboratory of Electroanalytical Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, P. R. China

E-mail: congyu@ciac.ac.cn; Fax: (+86) 431-8526-2710

[b] University of the Chinese Academy of Sciences, Beijing 100049, P. R. China

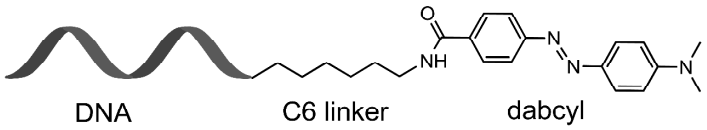
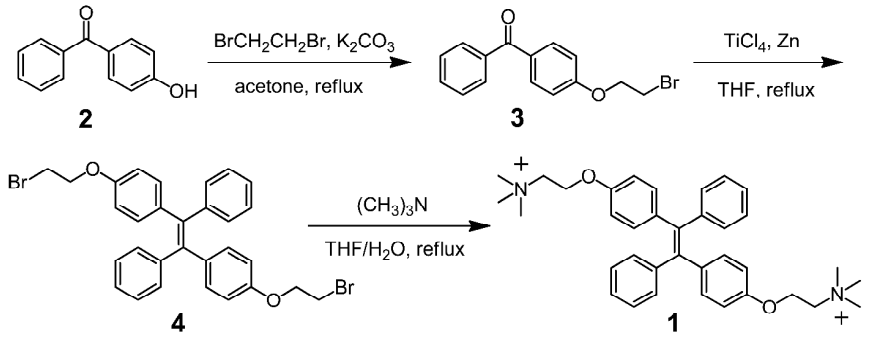


Figure S1. Structure of the quencher (dabcyl) labeled single stranded DNA used in the current investigation.

Scheme S1. Synthetic route for compound **1**.



Synthesis of compound 3: 1,2-dibromoethane (5.64 g, 30.0 mmol) was added to a mixture of compound **2** (1.98 g, 10.0 mmol) and K_2CO_3 (3.45 g, 25.0 mmol) in acetone (50 mL). The mixture was refluxed under stirring for 24 hours. After filtration and solvent evaporation, the crude product was purified by a silica gel column using a mixture of CH_2Cl_2/petroleum ether (1:1) as eluent. After dying under vacuum, compound **3** (2.26 g, 74%) was obtained as a white powder. ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.83 (d, 2H), 7.76 (d, 2H), 7.56 (t, 1H), 7.46 (t, 2H), 6.98 (d, 2H),

4.38 (t, 2H), 3.68 (t, 2H).

Synthesis of compound 4: $TiCl_4$ (3.79 g, 20.0 mmol) was added to a mixture of compound **3** (3.05 g, 10.0 mmol) and Zn dust (2.61 g, 40.0 mmol) in anhydrous THF (50 mL). After refluxing for 24 hours, the reaction mixture was cooled to room temperature and filtered. The solvent was evaporated under vacuum, and the crude product was purified by a silica gel column using a mixture of CH_2Cl_2/petroleum ether (1:3) as eluent. After dying under vacuum, compound **4** (2.65 g, 46%) was obtained as a white powder. ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) = 6.93–7.13 (m, 14H), 6.61–6.68 (m, 4H), 4.21 (s, 4H), 3.57–3.63 (m, 4H).

Synthesis of compound 1: Compound **4** (5.78 g, 10.0 mmol) was dissolved in THF (100 mL) in a 250 mL round bottom flask. An excess amount of trimethylamine (5 mL, 30% aqueous solution) was added, and the solution was refluxed for 3 days. During this period, water (total of 15 mL) was added at several intervals. The organic solvent was evaporated under reduced pressure, and the aqueous solution was washed with $CHCl_3$ (20 mL) three times. After solvent evaporation and drying under vacuum, compound **1** (6.46 g, 93%) was obtained as a white solid. ^{1}H-NMR (400 MHz, D_2O): δ (ppm) = 7.07–7.12 (m, 6H), 7.01–7.06 (m, 4H), 6.91–6.96 (m, 4H), 6.56–6.66 (m, 4H), 4.23 (s, 4H), 3.64 (s, 4H), 3.08 (s, 18H).

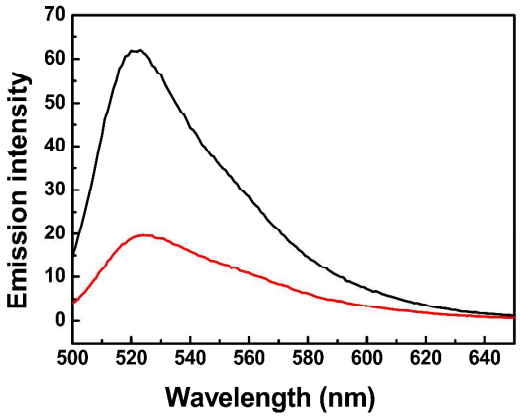


Figure S2. Emission spectra of SYBR Green I (1×) in the presence of 500 nM dsDNA3 (black line), and dsDNA3 reacted with Dam MTase and DpnI (red line). The spectra were taken at 25 ºC.

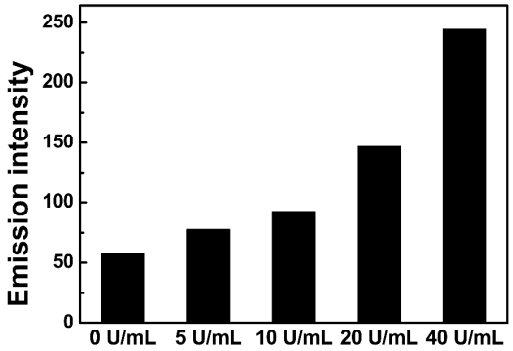


Figure S3. Changes in emission intensity of compound **1** at 470 nm against Dam MTase of various concentrations in 1% calf serum samples.

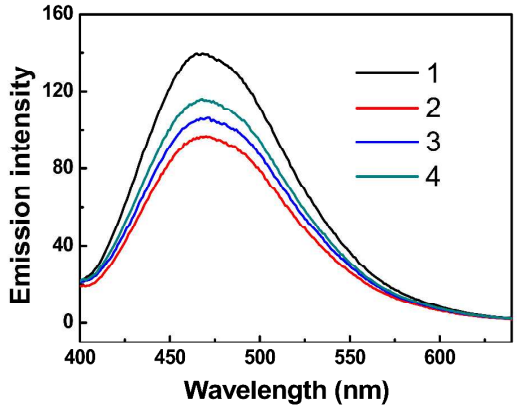


Figure S4. Changes in emission spectra of compound **1** upon the addition of different drugs. (1) No drug, (2) 5-fluorouracil, (3) benzylpenicillin and (4) gentamycin. Drug concentration: 1 μM each.

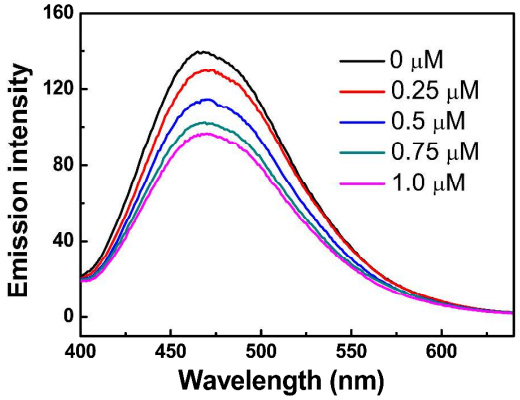


Figure S5. Changes in emission spectra of compound **1** upon the addition of increasing concentrations of 5-fluorouracil.

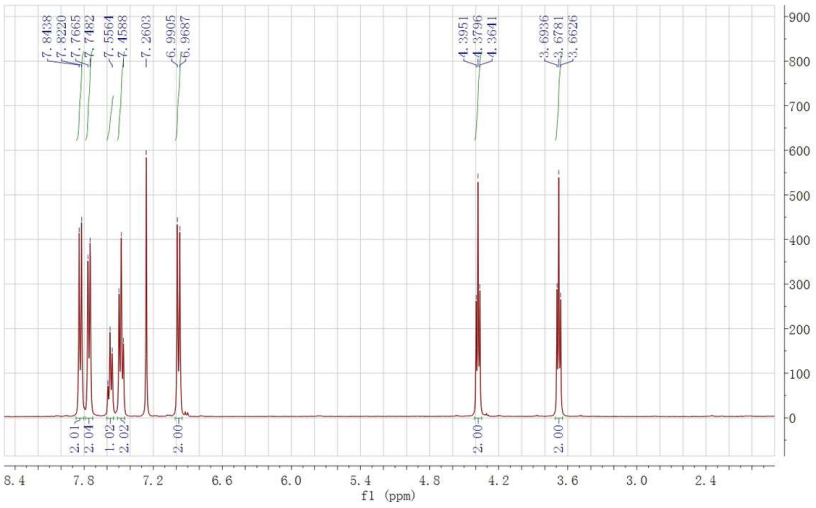


Figure S6. [1]H-NMR spectrum of compound **3**.

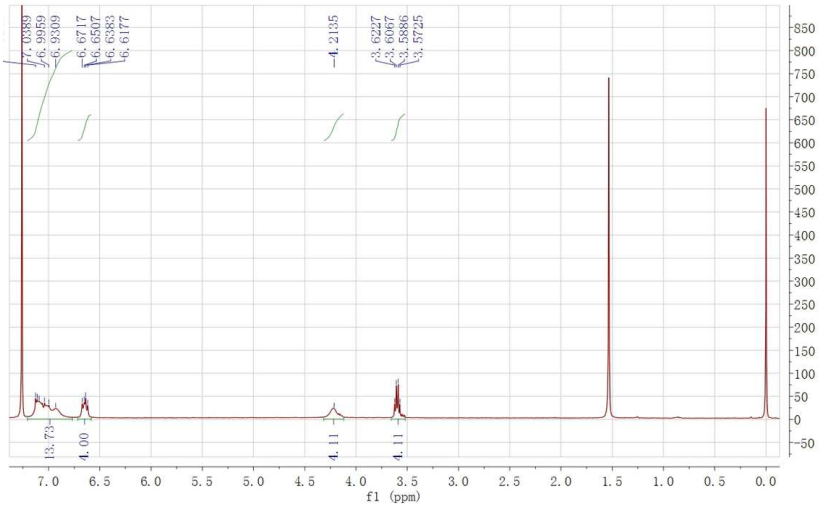


Figure S7. [1]H-NMR spectrum of compound **4**.

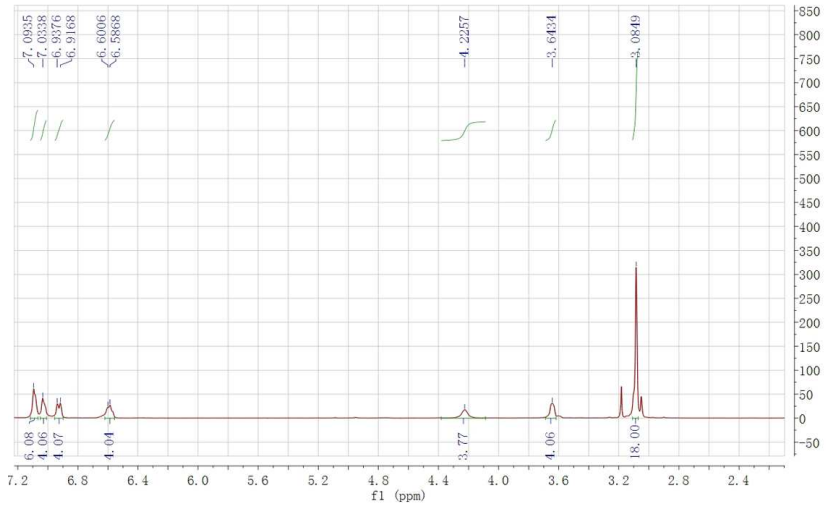


Figure S8. ^{1}H-NMR spectrum of compound **1**.