

Supporting Information

New Fast, Highly Selective Probe with Both Aggregation-Induced Emission Enhancement and Intramolecular Charge-Transfer Characteristics for Homocysteine Detection

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Synthesis of compound DBTC

Compound 2-(4-bromo- phenyl)-2*H*-[1,2,3]triazole-4-carboxaldehyde (**1**) (252 mg, 1 mmol), 10 mL of 5 M K₂CO₃ aqueous solution and a catalytic amount Pd(PPh₃)₄ (30 mg, 0.026 mmol) in 15 mL THF were refluxed for 0.5 h and then injected 10 mL THF containing 4-(diphenylamino) phenyl) boronic acid (**2**) (206.4 mg, 1.2 mmol). After heated to 90 °C and refluxed for 8 h under nitrogen atmosphere, the mixture was poured into water and extracted with CH₂Cl₂. The organic portion was combined and removed by rotary evaporation. The residue was purified by column chromatography on silica using petroleum ether/ethyl acetate (10:1, v/v) as eluent to yield 269 mg of a yellow crystal (65% yield). m.p. = 155 °C. ¹H NMR (400 MHz, CDCl₃) δ 10.23 (s, 1H), 8.28 (s, 1H), 8.18 (d, *J* = 8.9 Hz, 2H), 7.72 (d, *J* = 8.9 Hz, 2H), 7.51 (d, *J* = 8.7 Hz, 2H), 7.29 (dd, *J* = 8.5, 7.3 Hz, 4H), 7.18 - 7.13 (m, 6H), 7.06 (t, *J* = 7.3 Hz, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 184.21, 147.84, 147.50, 141.35, 137.91, 135.53, 133.10, 129.39, 127.72, 127.48, 124.70, 123.56, 123.29, 119.88). TOF MS ES⁻ *m/z* (M-H⁻): = calcd, 415.1553; found, 415.1548.

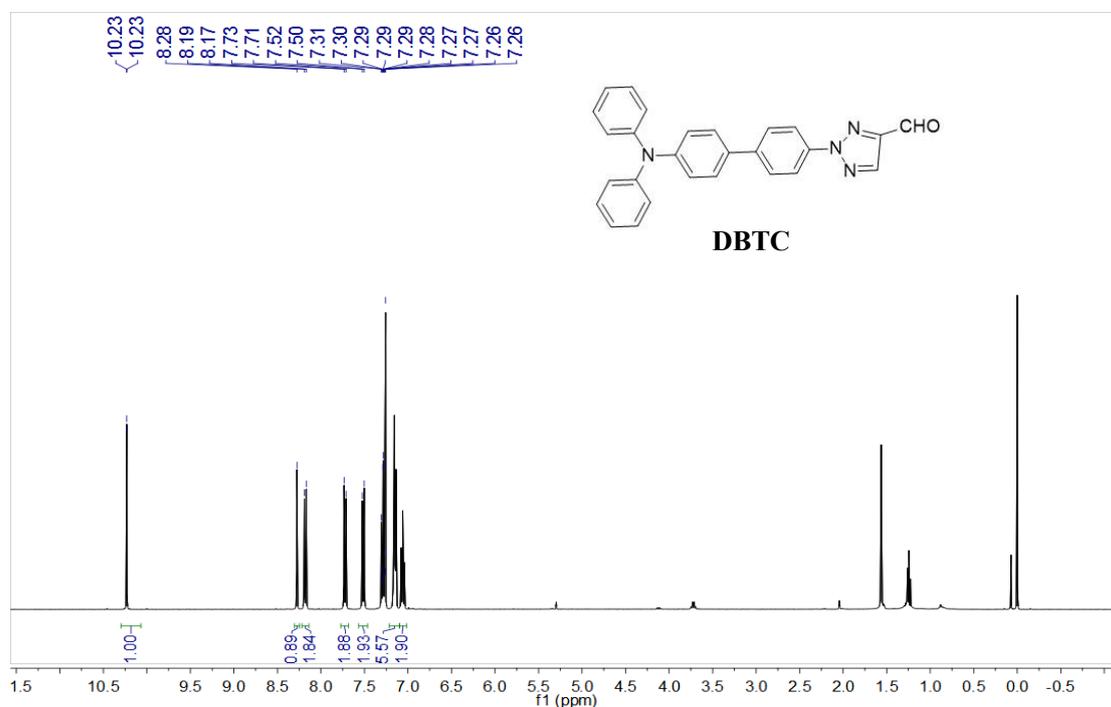


Figure S1. ¹H NMR (400 MHz, CDCl₃) spectrum of DBTC.

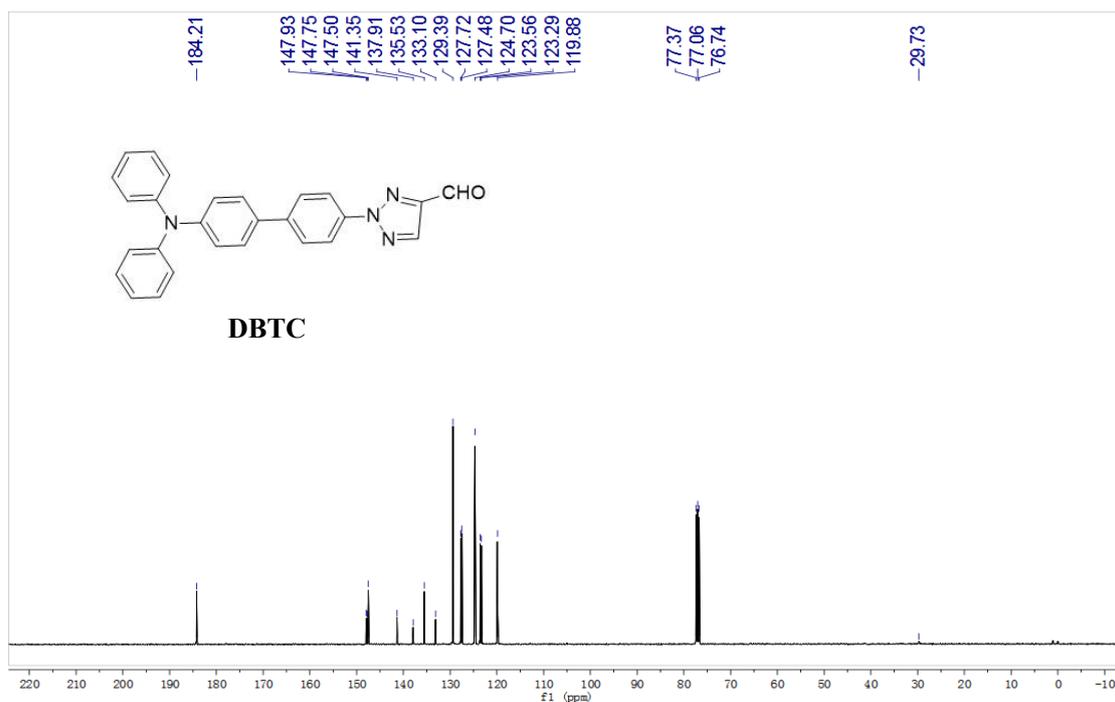


Figure S2.13C NMR (101 MHz, CDCl₃) spectrum of DBTC.

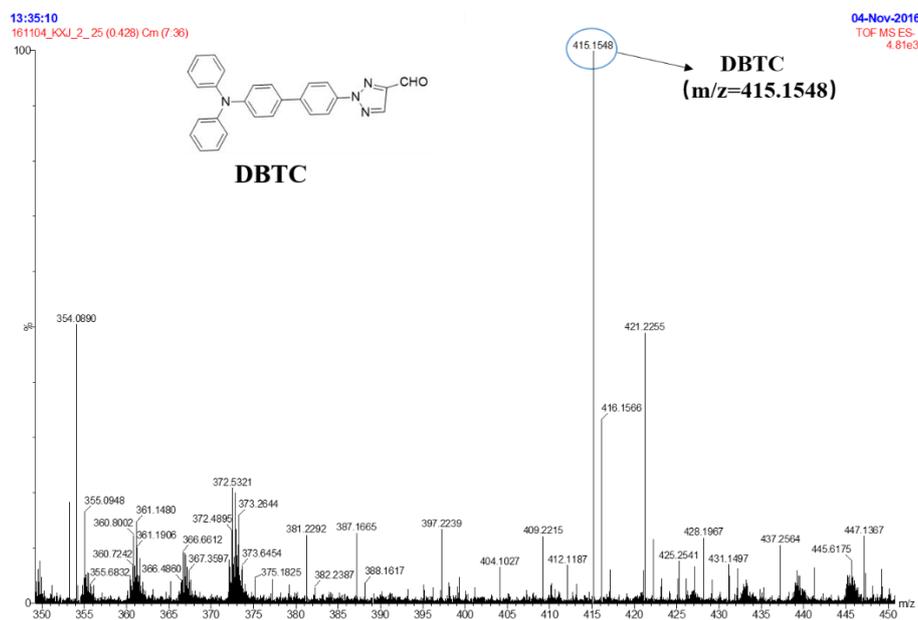


Figure S3. The mass spectrum of DBTC.

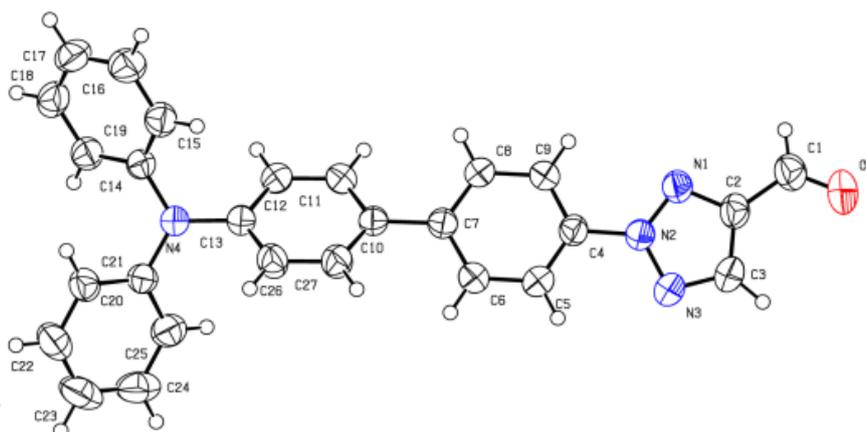


Figure S4. Single crystal structure of DBTC

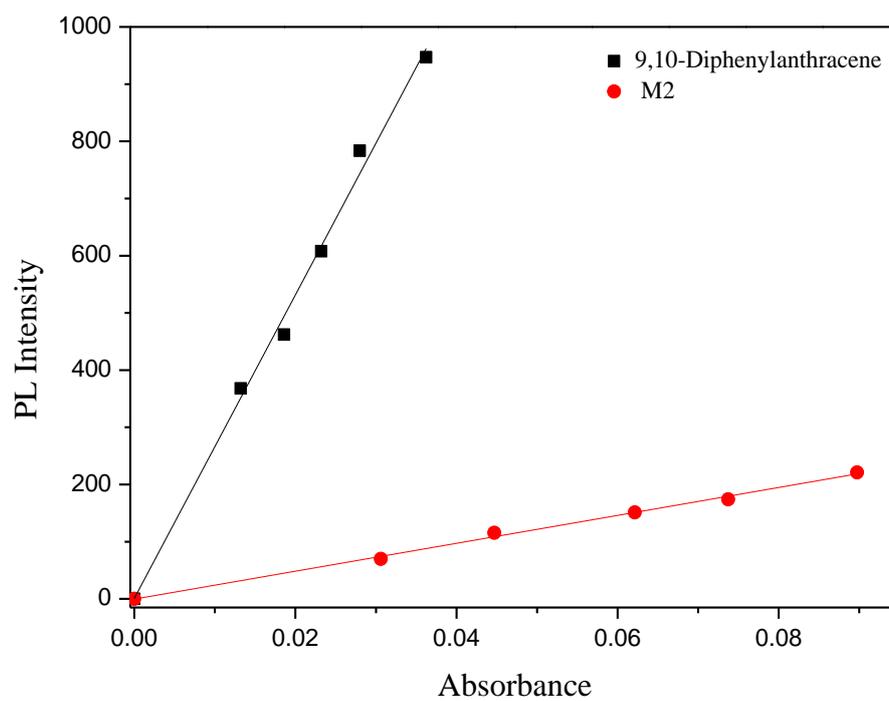


Figure S5. Linear plots for standard sample (*9, 10*-Diphenylanthracene in cyclohexane) and DBTC in $\text{CH}_3\text{CN}:\text{H}_2\text{O}=1:99$ ($\lambda_{\text{ex}}=362$ nm).

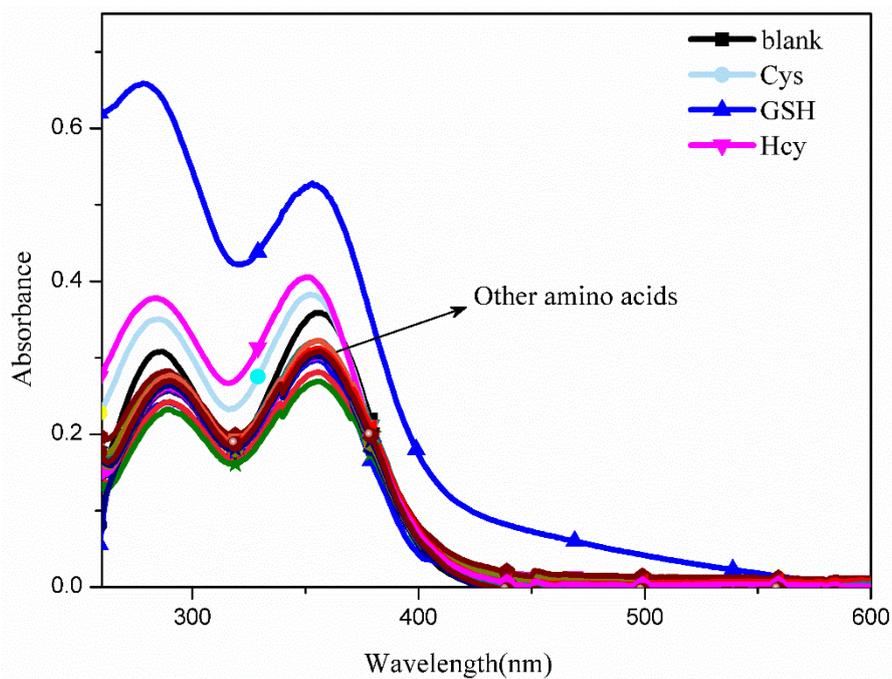
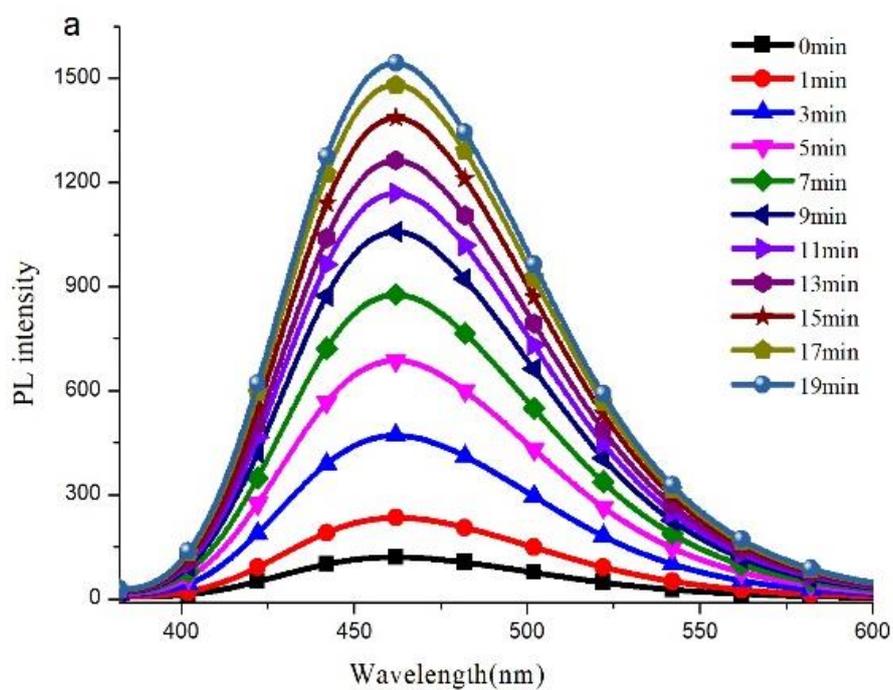


Figure S6. UV-Vis absorption spectra of probe DBTC (1.0×10^{-5} M) in CH₃CN/H₂O solution upon addition of various amino acids (Hcy, Cys, GSH, Ala, Arg, Asp, Gln, Glu, Gly, His, Lie, Lue, Lys, Met, Phe, Pro, Ser, Thr, Try, Tyr, Val) (25 equiv.)



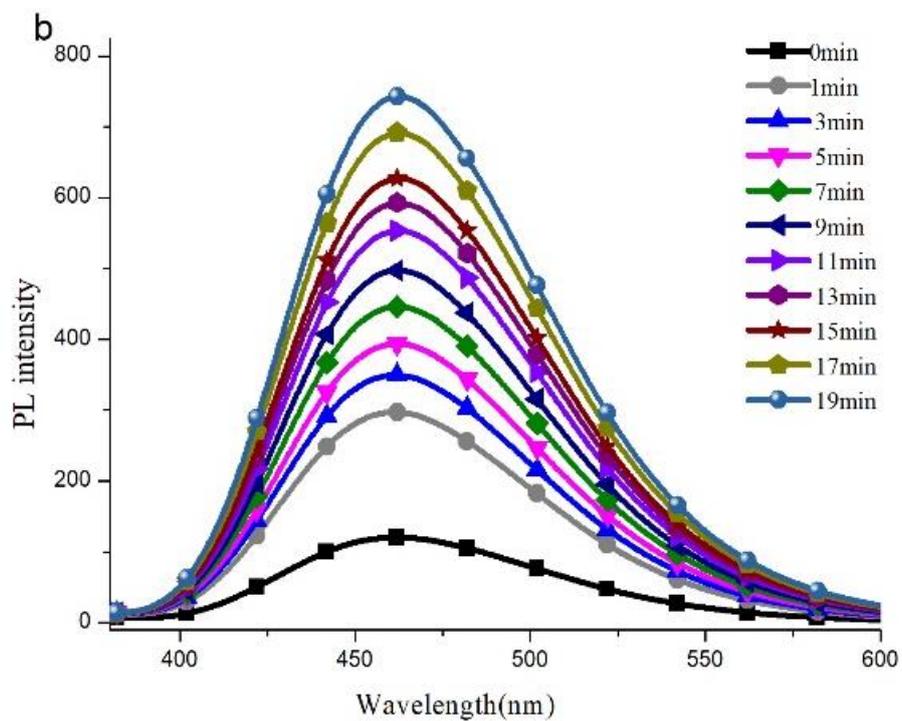


Figure S7. Response time of DBTC to (a) Hcy and (b) Cys.

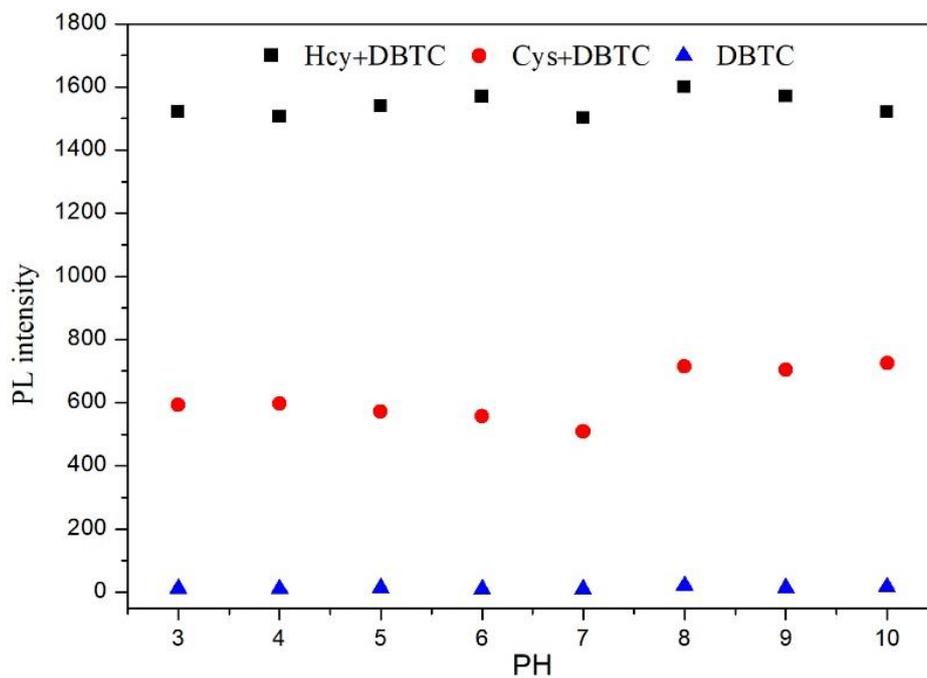


Figure S8. pH dependence of probe DBTC, measured at 362nm, with and without Hcy/Cys (10equiv) in different pH (range from 3.0 to 10.0)

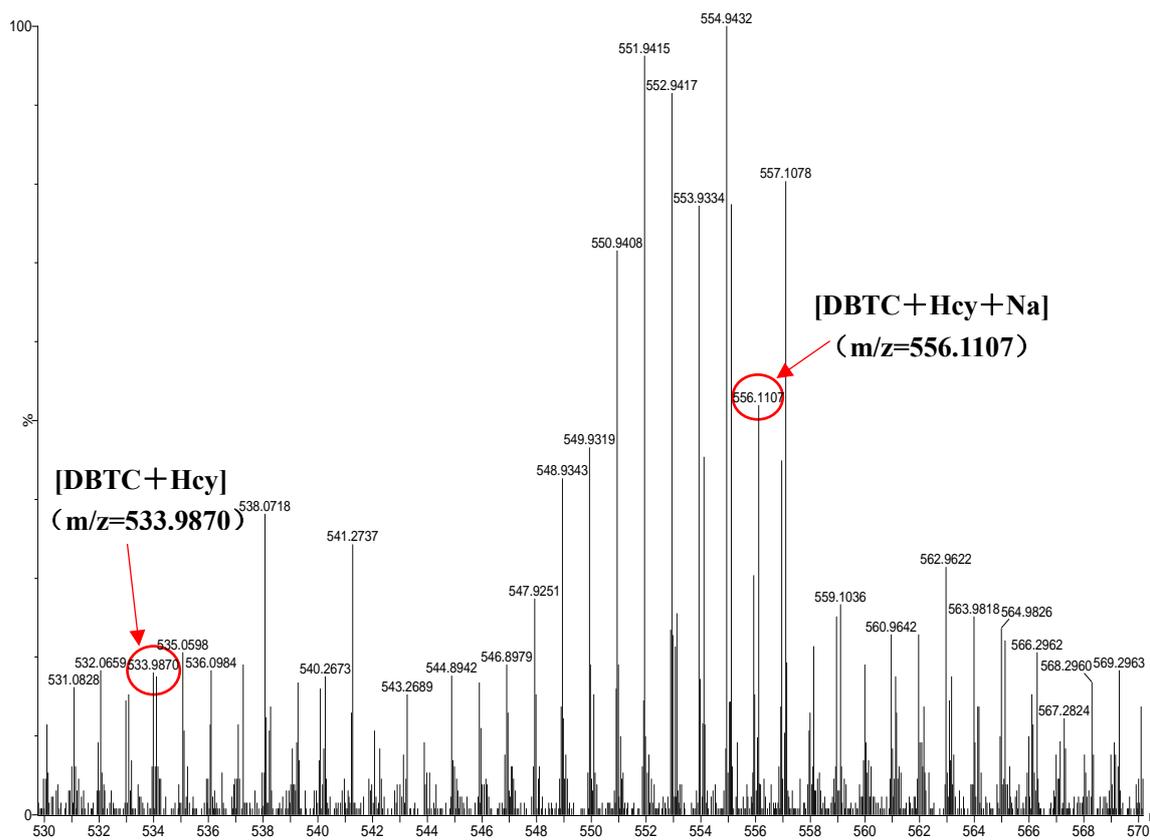


Figure S9. HR-MS spectra of [DBTC+Hcy],[DBTC+Hcy+Na]⁺,m/z=533.9870,556.1107.

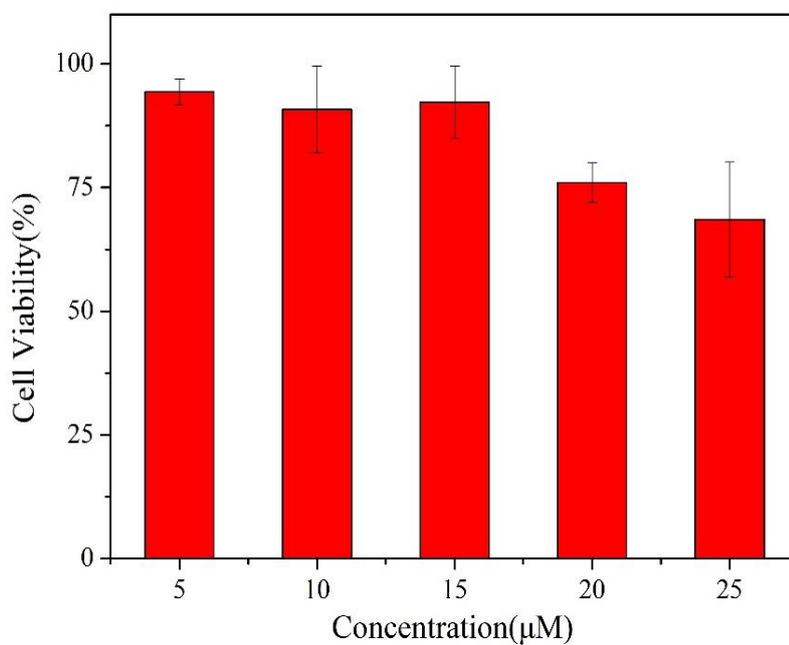


Figure S10. Cytotoxicity assay of Probe DBTC for HeLa cells at different concentrations.