Multi-approach cysteine detection based on supramolecular transformation induced by G-quadruplexes

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Synthesis and Characterization of MTC

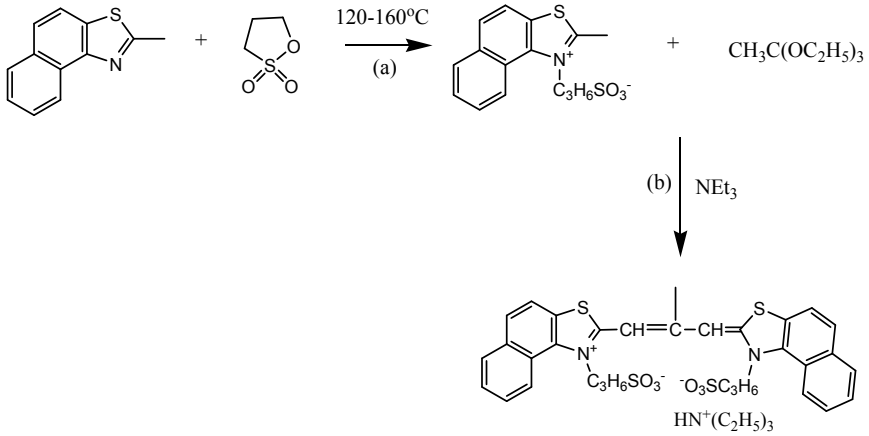

Figure S1. Synthesis of MTC. Reagents and conditions: (a) melting synthesis, 120~160°C, 10h; (b) phenol, 120°C, 1.5h.

Table S1. Elemental analysis of MTC $C_{38}H_{45}N_3O_6S_4 \cdot 3H_2O$

Element	N	C	H	S
Calculated Value (%)	5.11	55.52	6.25	15.60
Measured Value (%)	5.37	55.17	6.04	16.01

Data of infrared spectra ν_{max}: 3434 (OH), 2971, 2936 (CH_2), 2736, 2676, 2490 (HN^+), 1583, 1503, 1476, 1448, 1387, 1320, 1269, 1219, 1199, 1167, 1140, 1034 (S=O), 985, 907, 859, 832, 815, 758, 742 cm^{-1}.

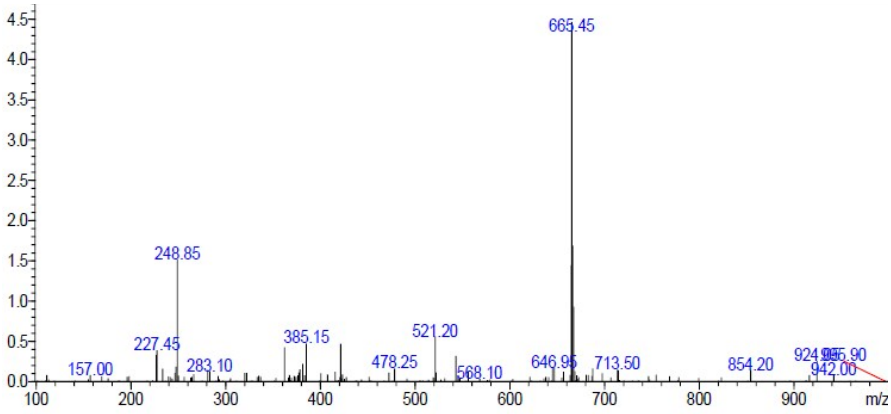

Figure S2. MS-ESI spectrum of MTC.

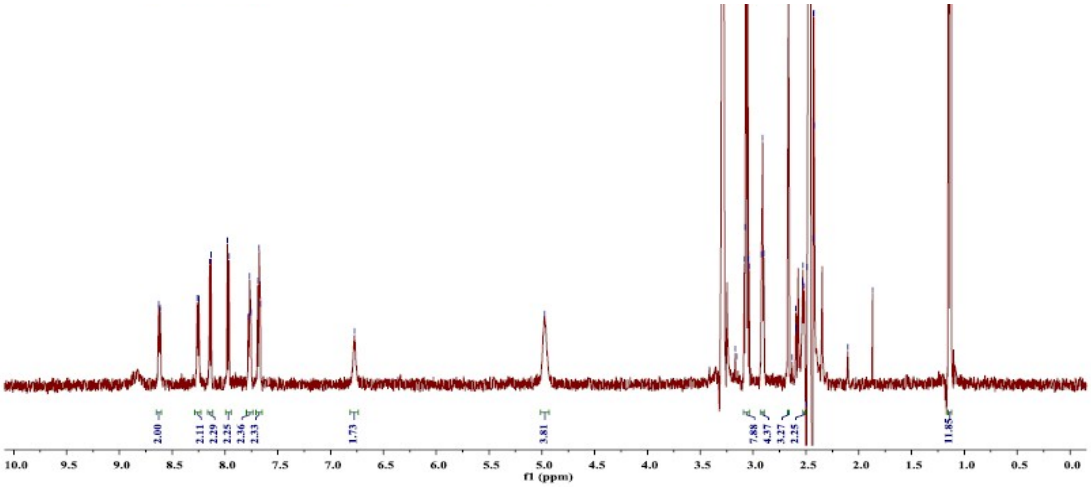

Figure S3. ^{1}H-NMR spectrum of cyanine dye MTC in DMSO-d_6. δ^{1}H: 8.63−8.61 (d, 2H), 8.26−8.25 (d, 2H), 8.15−8.13 (d, 2H), 7.98−7.96 (d, 2H), 7.77 (t, 2H), 7.68 (t, 2H), 6.78 (s, 2H), 4.97 (s, 2H), 3.06 (m, 8H), 2.91 (t, 4H), 2.67 (s, 3H, CH_3), 2.51 (s, 2H), 1.14 (s, 12H) ppm.

4. ^{13}C-NMR spectrum

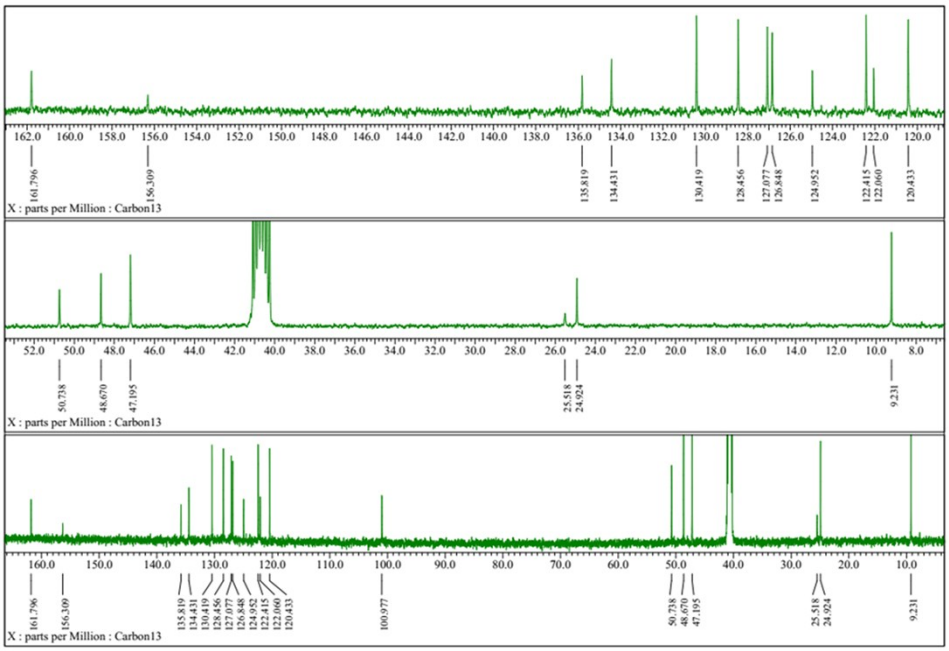

Figure S4. ^{13}C-NMR spectrum of MTC in DMSO-d_6. δ 161.80, 156.31, 135. 82, 134.43, 130.42, 128.46, 127.08, 126.85, 124.95, 122.41, 122.06, 120.43, 100.98, 50.74, 48.67, 47.20, 25.52, 24.92, 9.23

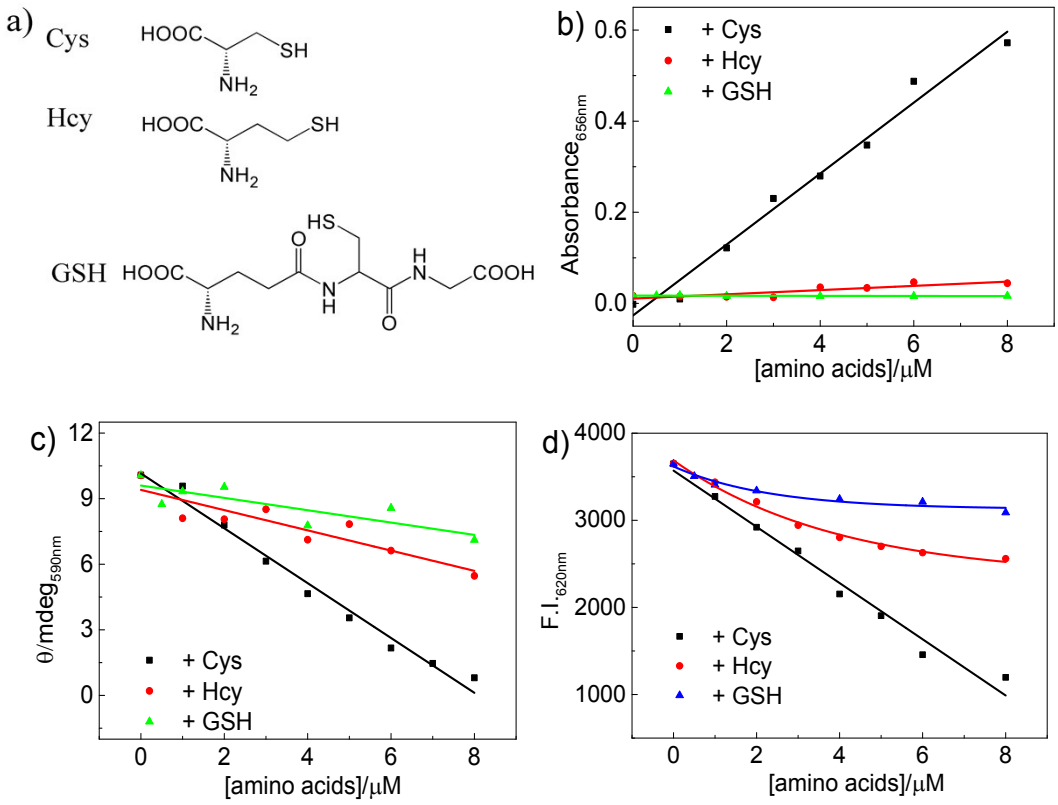

Figure S5. (a) Molecular structure of Cys, Hcy and GSH. (b–c) Plots of the absorbance at 656 nm, CD at 590 nm, and fluorescence at 620 nm of the probe system consisting of MTC (4 μM), ONS (2 μM) and Ag^+ (15 μM) as a function of different sulfur-containing amino acid concentration in phosphate buffer solution (pH 7.2, 1 mM EDTA). λex= 570 nm

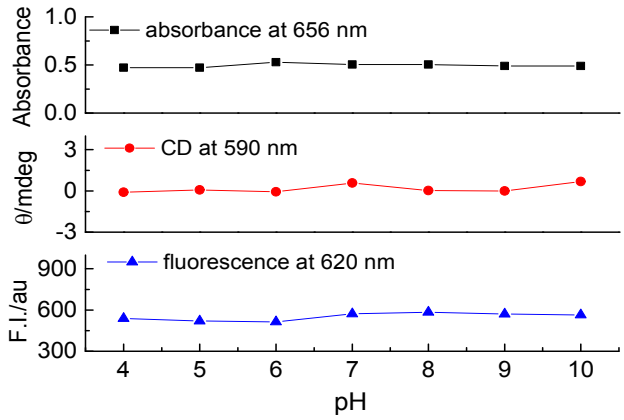

Figure S6. Plots of the absorbance at 656 nm, CD intensity at 590 nm and fluorescence at 620 nm of MTC (4 μM) as a function of pH in the presence of ONS (2 μM), Ag^+ (15 μM) and Cys (15 μM) in phosphate buffer solution (pH 7.2, 1 mM EDTA).