Electronic Supplementary Information

Nanomolar Detection of Biothiols via Turn-ON Fluorescence Indicator Displacement

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Fig. S1. HR-TEM and elemental maps of the nanocomposite 3. Reproduced from Chem. Commun., 2019, 55, 5623-5626.

Fig. S2. UV-visible absorption spectrum of nanocomposite 1 (100 μg/mL) in water.
Fig. S3. Changes in the absorption spectrum of 1 (100 μg/mL) upon addition of (a) homocysteine (Hcy, 0 to 20 μM), (b) glutathione (GSH, 0 to 10 μM) and (c) sulfide anion (0 to 75 μM) in acetate buffer at pH 9.0.

Fig. S4. Changes in the emission spectrum of 1 (100 μg/mL) upon addition of (a) Hcy, 0 to 20 μM), (b) GSH (0 to 10 μM) and (c) sulfide anion (0 to 75 μM) in acetate buffer at pH 9.0. (d) Relative changes in the fluorescence at 505 nm of 1 (100 μg/mL) in the presence of Cys (10 μM), Hcy (20 μM), GSH (10 μM) and sulfide anion (75 μM). λ<sub>exc</sub>, 480 nm.
**Fig. S5.** Relative changes in the fluorescence at 505 nm of 1 (100 μg/mL) in the presence of Cys (10 μM), Hcy (20 μM), GSH (10 μM), sulfide anion (75 μM) and same concentration of all these analytes. λ_{ex} 480 nm.

**Fig. S6.** Linear response curves for the changes in the fluorescence of 1 at 505 nm depending on the concentration of Cys at (a) lower (50 nM to 3 μM) and (b) higher (4 to 30 μM) concentrations.
**Fig. S7.** Linear response curves for the changes in the fluorescence of 1 at 505 nm depending on the concentration of Hcy at (a) lower (50 nM to 10 μM) and (b) higher (5.5 to 30 μM) concentrations.

**Fig. S8.** Linear response curves for the changes in the fluorescence of 1 at 505 nm depending on the concentration of GSH at (a) lower (50 nM to 10 μM) and (b) higher (4 to 30 μM) concentrations.
**Fig. S9.** Fluorescence spectrum and (inset) a photograph of 1 (100 μg/mL) in the absence and presence of cysteine (120 pM) in acetate buffer (pH 9.0).

**Fig. S10.** Changes in the absorption spectrum of 1 (100 μg/mL) upon addition of (a) cysteine (Cys, 5 μM), (b) Hcy (20 μM) (c) GSH (10 μM) in phosphate buffered saline at pH 7.4.
**Fig. S11.** Changes in the emission spectrum of 1 (100 μg/mL) upon addition of (a) Cys (5 μM), (b) Hcy (20 μM) and (c) GSH (10 μM) in phosphate buffered saline at pH 7.4. λ<sub>exc</sub>, 480 nm.

**Fig. S12.** Changes in the emission spectrum of 1 (100 μg/mL) upon addition of Cys in (a) fetal bovine serum and in the presence of (b) human serum albumin (50 μM) and (c) bovine serum albumin (50 μM) in phosphate buffered saline at pH 7.4. Insets show the linear response curves for the changes in the fluorescence of 1 at 505 nm depending on the concentration of Cys. λ<sub>exc</sub>, 480 nm.
**Fig. S13.** Fluorescence decay profile of BDP in dichloromethane and 1 in the presence of Cys, Hcy and GSH. $\lambda_{exc}$, 402 nm, decay monitored at 505 nm.

**Fig. S14.** HR TEM images of (a) 1 and 1 in the presence of (b) Cys, (c) Hcy and (d) GSH.
Fig. S15. Particle size analysis of 1 in the presence of (a) Cys, (b) Hcy and (c) GSH by dynamic light scattering in water. The observed particle sizes were 53.6 ± 2.1, 54 ± 1.1, 58 ± 2.1 nm, respectively.

Fig. S16. ITC titration data of (a) 1 (300 μM) with Hcy (2000 μM) (n = 0.55, $K_d$ = 41.1 μM) and (b) 1 (100 μM) with GSH (2000 μM) (n = 2.61, $K_d$ = 4.5 μM). Each titration comprises of thirteen injections at an expense of 2 μL of Hcy per injection and thirty nine injections at an expense of 2 μL of GSH. Experiments were carried out at 25 °C.
Fig. S17. (Top panel) Bright field and (bottom panel) fluorescence microscopic images of MDA-MB 231 cancer cell lines after incubating with different concentrations of the nanocomposite 1 for 24 hours. Fluorescence images were recorded in the wavelength region of 490-520 nm.

Fig. S18. Naked eye detection of (a, c) Hcy and (b, d) GSH using a test paper strip of 1 viewed under (a, b) ambient and (c, d) UV light. The legends indicate the concentration of Hcy and GSH.