

Supporting Information

Preeminent Designing of Complementary Ternary TRANSFER and COMPLEMENT alongside excitation Modulated Molecular logic systems

Monaj Karar,^{1±} Rikitha S Fernandes,^{2±} Snehasish Saha,³ Nilanjan Dey^{2*}

¹MLR Institute of Technology, Hyderabad, Telangana-500 043, India

²Department of Chemistry, Birla Institute of Technology and Science Pilani, Hyderabad, Telangana-
500078, India

³Electrical Engineering Dept., National Institute of Technology Durgapur, West Bengal-713209, India

ND: nilanjandey.iisc@gmail.com, nilanjan@hyderabad.bits-pilani.ac.in

[±]Both authors contributed equally

EXPERIMENTAL SECTION

General: All chemicals (solvents, reagents, and chemicals) were purchased from best-known local chemical suppliers and used without further purification. Solvents were distilled and dried prior to use. FTIR spectra were recorded on a Perkin-Elmer FT-IR Spectrum BX system and were reported in wave numbers (cm^{-1}). On the other hand, ^1H NMR and ^{13}C NMR spectra were recorded with a Bruker Avance Neo 400 spectrometer operating at 400 and 100 MHz for ^1H and ^{13}C NMR spectroscopy, respectively. Chemical shifts were reported in ppm downfield from the internal standard, tetramethylsilane (TMS). Mass spectra were recorded on Shimadzu LC-MS.

Spectroscopic studies. The UV-vis spectroscopic studies were recorded on a JASCO (model V-650) UV-Vis spectrophotometer. The slit-width for the experiment was kept at 5 nm. On the other hand, fluorescence experiments were performed in FluoroLog-TM (Horiba Scientific). The slit-width for the fluorescence experiment was kept at 5 nm (excitation) and 5 nm (emission) and the excitation wavelength was set at 390 and 465 nm.

The stock solution of compound **1** was made in dimethyl sulphoxide (DMSO) and the final concentration of DMSO in all the studies was less than 1%. Sensing was carried out by adding requisite amounts of mercury perchlorate trihydrate [$\text{Hg}(\text{ClO}_4)_2 \cdot 3\text{H}_2\text{O}$] and/or tetrabutylammonium cyanide to probe **1** (10×10^{-6} M). For studying in micelle medium, the aqueous solutions of Brij-58, SDS, and CTAB were at concentrations 1, 1.5, and 8 mM respectively used for the sensing studies. The pH of the medium was fixed to 7.4. In all cases, the concentrations of the surfactants were kept above the respective critical micellar concentrations to ensure the formation of micelles.

Design and synthesis of probe molecule: Compound **1** was synthesized following a literature-reported procedure with minor modifications.¹⁻⁴ Indole and 1-pyrene aldehyde were taken in 1:2 ratios in methanol (2 mL) and treated with iodine. After stirring for 15 min, DDQ (2,3-Dichloro-5,6-dicyano-1,4-benzoquinone) (1.0 mmol in 4 mL of methanol) was added slowly to this mixture, and the stirring was continued for the next 30 minutes at room temperature. Then the reaction mixture was acidified with diluted HCl (1:1 MeOH/ H_2O) to obtain the crude product as a red solid. Subsequently, the solid compound was washed with CH_3CN , dried, and then characterized.

ADDITIONAL SPECTROSCOPIC DATA

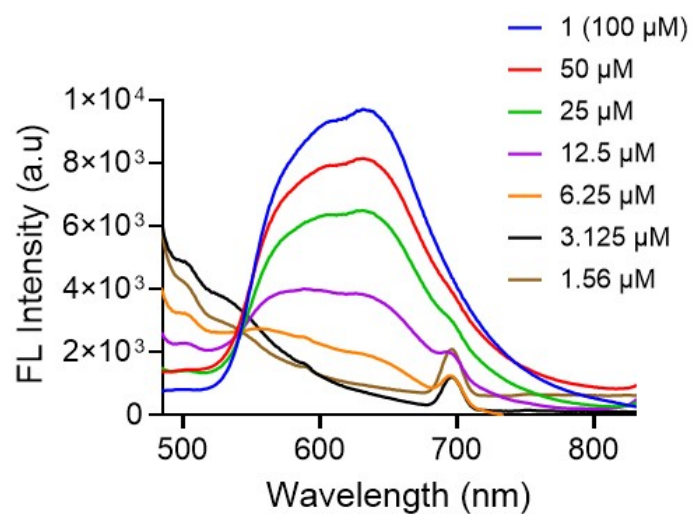


Figure. S1: Fluorescence spectra of probe 1 (100 μM , $\lambda_{\text{ex}}=465$ nm) upon dilution in aqueous medium.

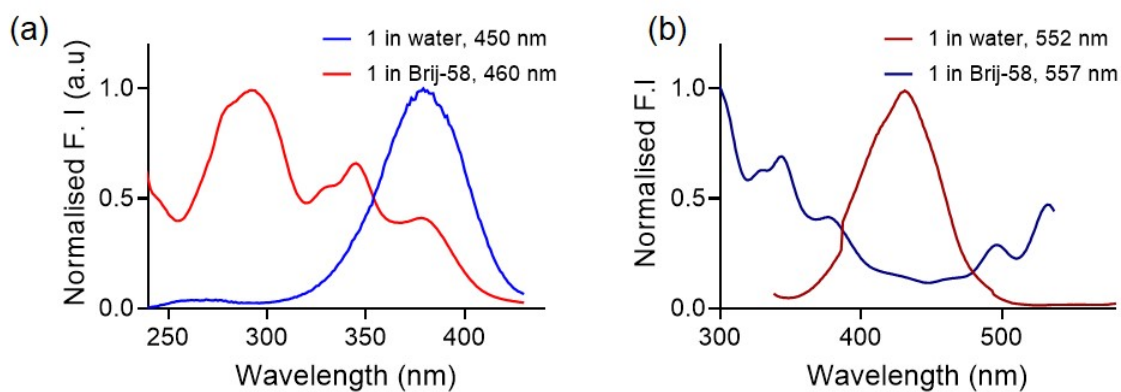


Figure. S2: (a) Excitation spectra of the probe 1 (10 μM) in water ($\lambda_{\text{em}}=450$ nm) and Brij-58 medium ($\lambda_{\text{em}}=460$ nm). (b) Excitation spectra of the probe 1 (10 μM) in water ($\lambda_{\text{em}}=552$ nm) and Brij-58 medium ($\lambda_{\text{em}}=557$ nm).

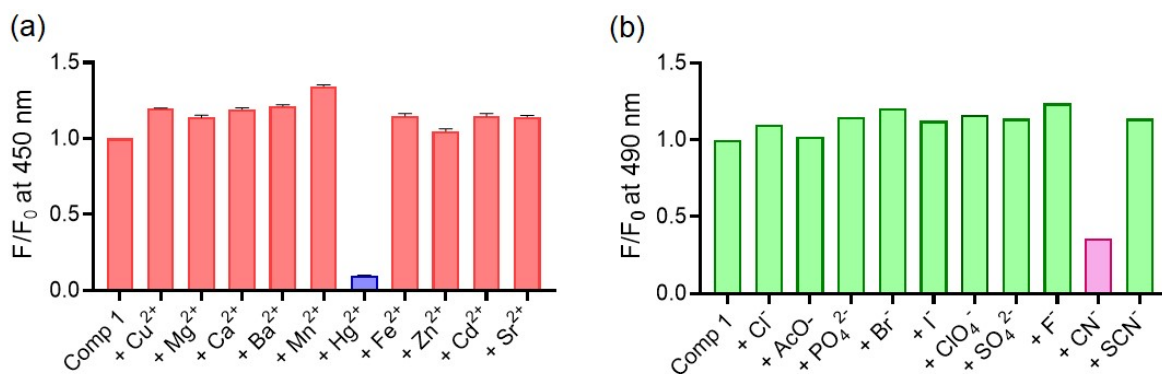


Figure. S3: (a) Change in fluorescence intensity (F/F_0) of the probe at 450 nm, upon addition of different metal ions (10 equiv.) in Brij-58 medium. (b) Change in fluorescence intensity of the probe at 450 nm, upon addition of different anions (10 equiv.) in Brij-58 medium.

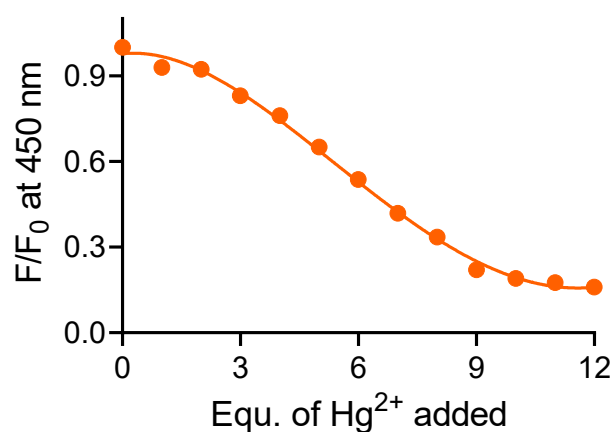


Figure. S4: Changes in fluorescence intensity of compound 1 ($10 \mu\text{M}$, $\lambda_{\text{ex}} = 390 \text{ nm}$) at 450 nm, upon addition of Hg^{2+} ions (0 - 12 equiv.) at pH 7.4 in Brij-58 micelle medium.

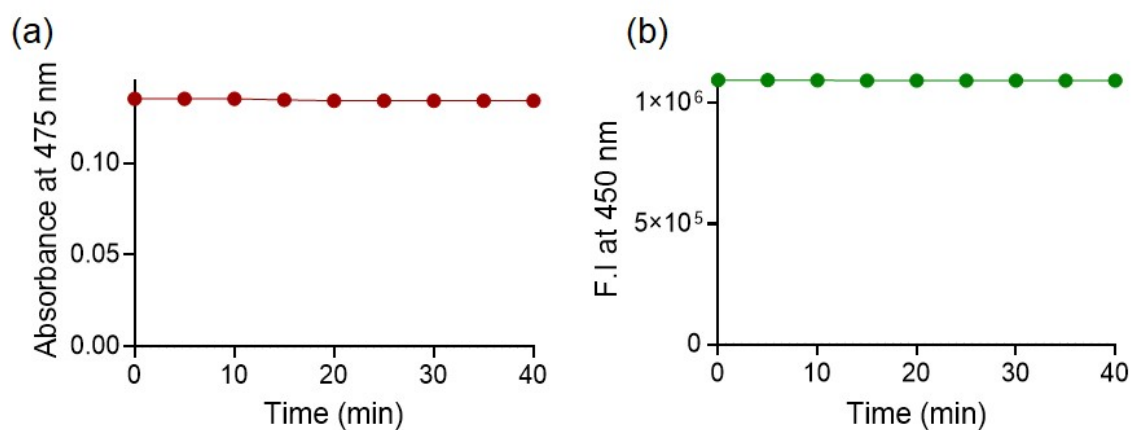


Figure. S5: (a) Absorbance of the probe (at 475 nm) in Brij-58 upon exposure to UV light for 40 minutes at 5-minute intervals. (b) Photostability (Fluorescence) of the probe at 450 nm ($\lambda_{\text{ex}}=390 \text{ nm}$) in Brij-58 upon exposure to UV light for 40 minutes at 5-minute intervals.

References

1. N. Dey and N. Kumari, *Results Chem.* 4, 100248 (2022).
2. R. S. Fernandes, J. Kumari, A. Gangopadhyay, D. Sriram, and N. Dey, *J. Mol. Liq.*, 125266 (2024).
3. R. S. Fernandes and N. Dey, *J. Mater. Chem. B*, (2024).
4. R. S. Fernandes and N. Dey, *Mater. Chem. Phys.*, 302, 127637 (2023).