Supporting Information File for

Reversible Color Changing Response of Pyrenylated Charge-Transfer Probes towards Hg^{2+}: Linker-Driven Modulation of Sensitivity and Selectivity

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Experimental Section

Materials and methods: All chemicals (starting materials, reagents and chemicals) were bought from 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, ^{1}H-NMR and ^{13}C-NMR spectra were recorded with a Bruker Advance DRX 400 spectrometer operating at 400 and 100 MHz for ^{1}H and ^{13}C NMR spectroscopy, respectively. Chemical shifts were reported in ppm downfield from the internal standard, tetramethylsilane (TMS). Mass spectra were recorded on Micromass Q-TOF Micro TM spectrometer.

Spectroscopic studies: The UV−vis spectroscopic studies were recorded on a Shimadzu model 2100 spectrometer. The slit-width for the experiment was kept at 5 nm. Sensing was carried out by adding requisite amounts of metal ions (from 10 mM DMSO stock solutions) to acetonitrile solution of compounds **1** and **2** (1×10^{-5} M). ^{1}H NMR spectra of compounds **1** and **2** were recorded in DMSO-d_6 medium. The detection limits for Hg^{2+} ions in both cases were calculated using the blank variability method. The stoichiometry of complexations with Hg^{2+} ion was determined using Job plot (continuous variation method). The total molar concentration of the two binding species (here, probes **1** or **2** and Hg^{2+} were kept constant (1 x 10^{-4} M) and the mole fraction was varied. Binding constants were calculated on the basis of Benesi-Hildebrand equation for 1:1 stoichiometry. The changes in absorbance were recorded at 427 nm band.

Design of Paper Strips: To prepare the compound-coated paper strips, 40 μL of CH_2Cl_2 solution of **1** (0.02 mM) was drop-cast onto the filter paper strips (rectangular in shape, 1 x 1.5 cm) using a micropipette in two fractions (2 x 20 μL). The concentration of **1** in the solution as well as immersion time were varied systematically to obtained optimum response with Hg^{2+} ions. The solution was completely absorbed in filter paper within 5-10 min and then the filter papers were kept overnight to air dry. The stability of paper strips was verified over a couple days under ambient condition. Finally, the paper strips were ready for sensing studies.

Design of Probe Molecules

Synthesis and Characterization of 1:

1-((Pyren-6-yl)methylene)hydrazine was synthesized based on a procedure reported in the literature.[1] In the next step, 1.0 mmol of this precursor was stirred at room temperature with 1.1 mmol of 4-pyridine aldehyde for overnight in EtOH medium. The yellow-colored product (**1**) was filtered and washed thoroughly with EtOH. Yield 72 %; yellow solid, HRMS *m*/*z* calcd for $C_{23}H_{15}N_3$ $(M + H)^+$ 134.1344, found 134.1349.

Synthesis and Characterization of 2:

The precursor molecule diethyl (pyren-1-ylmethyl)phosphonate was synthesized based on a procedure reported in the literature.[2] To a solution of diethyl (pyren-1-ylmethyl)phosphonate (0.58 g, 1.64 mmol) in dry THF, sodium hydride (1.2 equiv.) was added at 0 °C and the mixture was stirred for 30 min under N_2 atmosphere. A solution of 4-pyridine aldehyde (0.16 g, 1.5 mmol) in THF (3 mL) was added dropwise over a period of 10 min. The reaction mixture was then stirred at rt for 10 h. After complete conversion of reaction, cold water (2 mL) was added into the reaction mixture under stirring. The crude material was obtained after extraction with EtOAc (3 x 5 mL) followed by evaporation of the solvent. The final compound **2** was obtained after purification on silica gel column chromatography (2% MeOH/$CHCl_3$). Yield 0.43 g, 86%; ; HRMS m/z calcd. C23H15N (M+H)+ 306.1282, found 306.1284.

Sensor	Medium of Detection	Mode of Response	Limit of Detection	Application(s)	Reference
pyridine-attached phenanthridine	$CH_3CN–H_2O$ mixture	Ratiometric response (UV-visible)	49.87 nM	Paper strips/ water analysis	New J. Chem., 2021,45, 17667-17673
Antipyrine based salen derivative	CH_3CN	Ratiometric response (UV-visible)	88 nM	Paper strips/ water analysis	Inorg. Chem. Commun. 2024, 163, 112315
Imidazo[1,2-a]pyridine	H_2O–EtOH (8 : 2)	Bathochromic shift (UV-visible)	1.0 ppb	Cell imaging	RSC Adv., 2019,9, 29856-29863
1,4-bis[2-(4-pyridyl)ethenyl]benzene	10 mM HEPES, pH = 7.4, buffer	Turn-on fluorescence response	407 nM	Cell imaging	RSC Adv., 2014,4, 47000-47004
Anthracene based probe	THF/PBS buffer (1:1 medium)	Turn-on fluorescence response	59 nM	Cell imaging	ACS Omega 2018, 3, 10, 12341–12348
2-(2-(8-hydroxyquinolin) -yl)benzimidazole	Tris–HCl buffer (1% DMSO)	Turn-off fluorescence response	254 nM	Not mentioned	RSC Adv., 2014,4, 16612-16617
Fluorescein-thiourea	PBS buffer (pH 7.00)	Turn-off fluorescence response	0.24 nM	Water analysis	J. Photochem. Photobiol. A, 2022, 422, 113569

Table S1. Table shows recently reported sensory probes for Hg^{2+} ion.

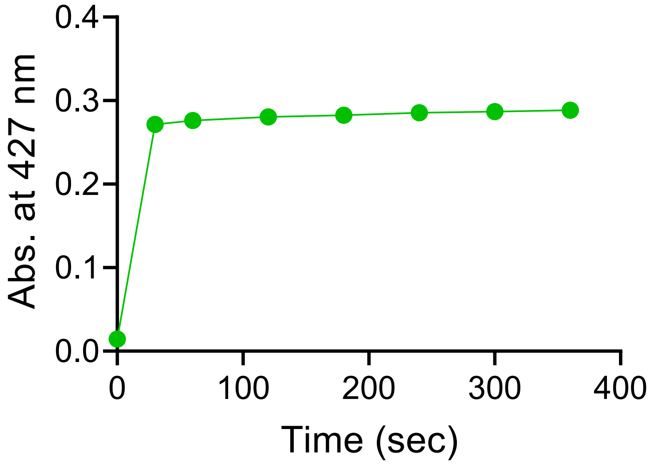

Figure S1. Time-dependent changes in absorbance of **1** (10 μM) in the presence of Hg^{2+} (20 μM) in CH_3CN medium.