Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Colorimetric Detection and Ratiometric Quantification of Mercury (II) Using Azophenol Dye: 'Dip & Read' Based Handheld Prototype Device Development

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SUPPLYMENTRY INFORMATION

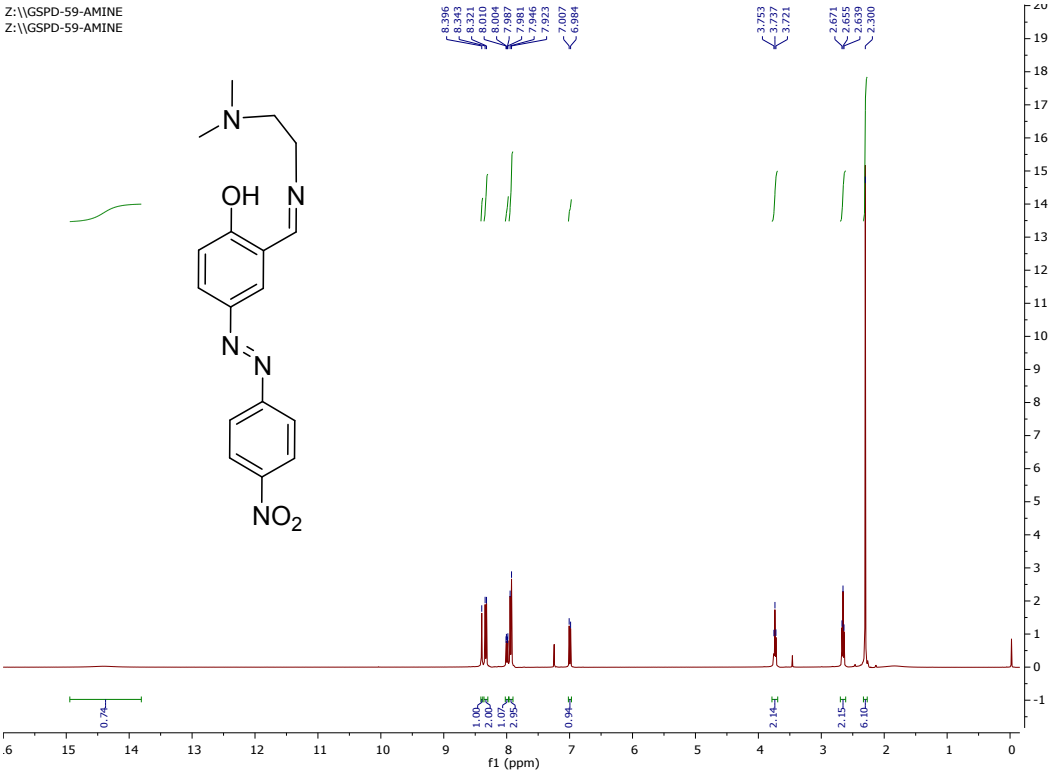

Figure S_1: ^{1}H NMR spectrum of compound **3**

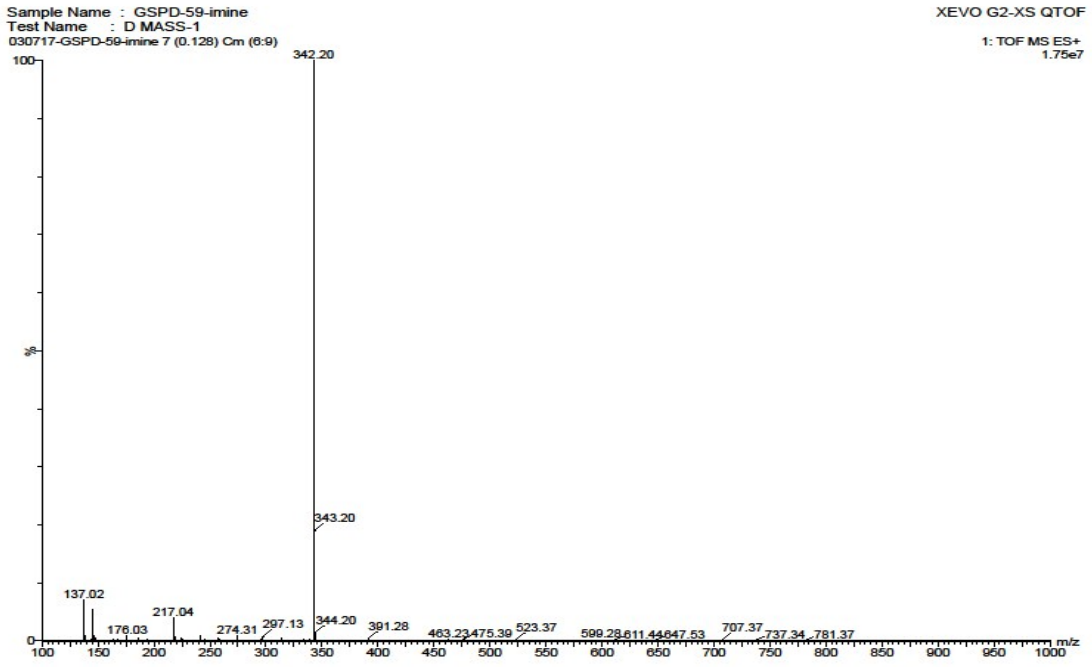

Figure S_2: Mass Analysis spectrum for compound **3**

2-((2-(dimethylamino)ethyl)amino)methyl)-4-((4-nitrophenyl)diazenyl)phenol (**2**)

R_f 0.33 ($CHCl_3$/hexane 8:2); Dark red powder, Yield = 75%).

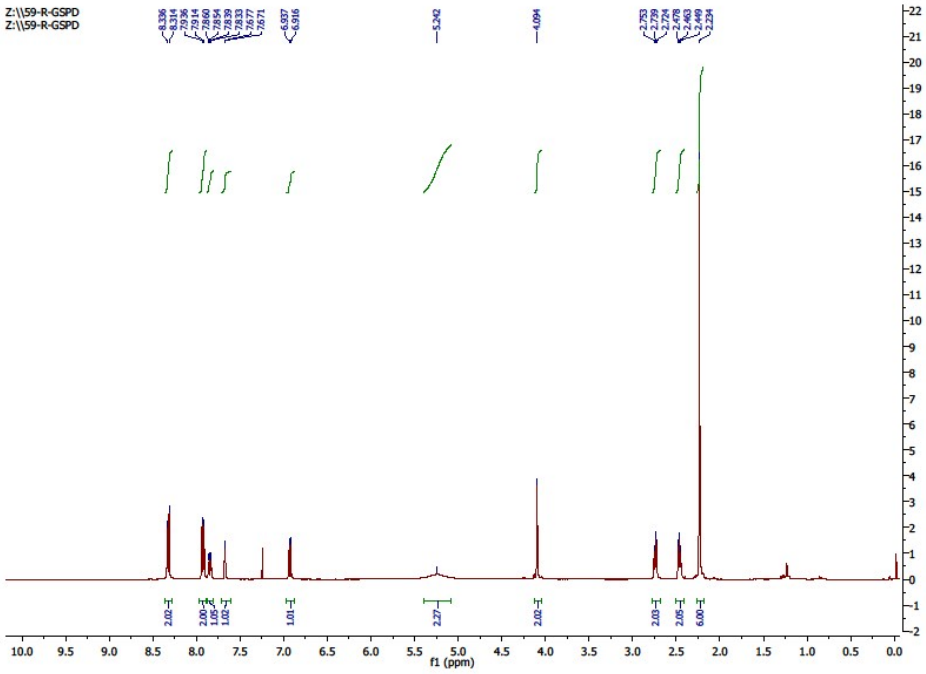

Figure S_3: ^{1}H NMR spectrum of compound **2**

^{1}H NMR ($CDCl_3$, 400 MHz):

δ 8.32 (m, 2H, Ar-H), 7.92 (m, 2H, Ar-H), 7.83 (m, 1H, Ar-H), 7.67 (s, 1H, Ar-H), 6.92 (m, 1H, Ar-H), 5.34 (br s, 2H, OH and NH), 4.09 (s, 2H), 2.73 (t, 2H, J = 6.0 Hz), 2.46 (t, 2H, J = 6.0 Hz), 2.23 (s, 6H, $CH_3 \times 2$).

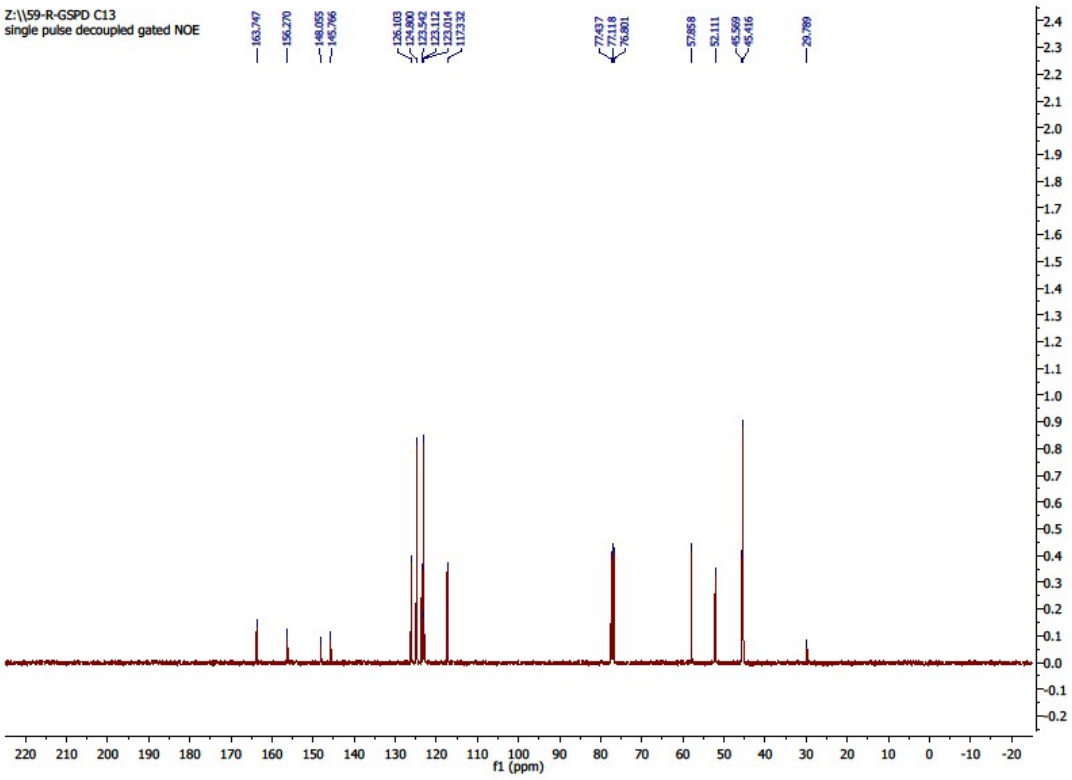

Figure S$_4$. ^{13}C NMR spectrum of compound **2**

^{13}C NMR ($CDCl_3$, 100 MHz):

δ 163.74, 156.27, 148.05, 145.76, 126.10, 124.80, 123.54, 123.11, 123.01, 117.33, 57.85, 52.11, 45.56, 29.78

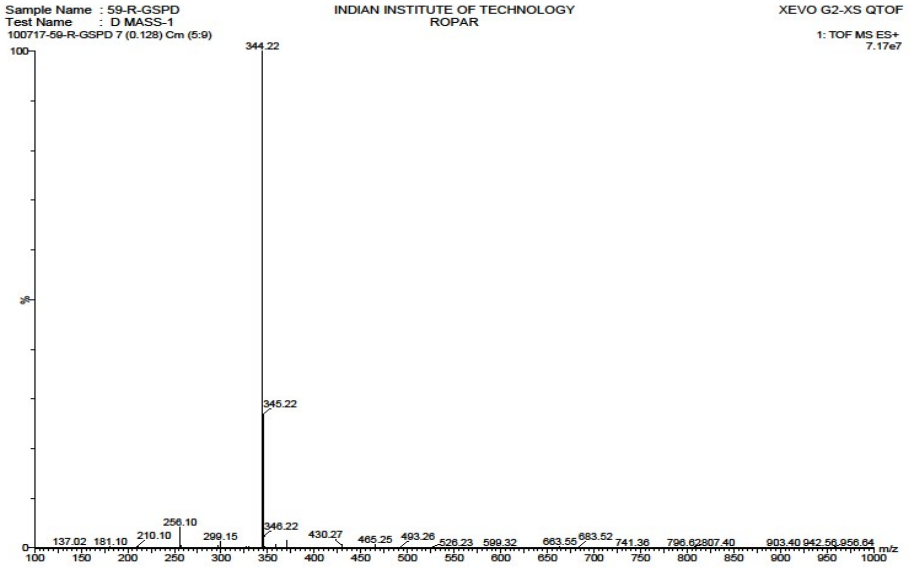

Figure S_5. Mass spectrum for compound **2**

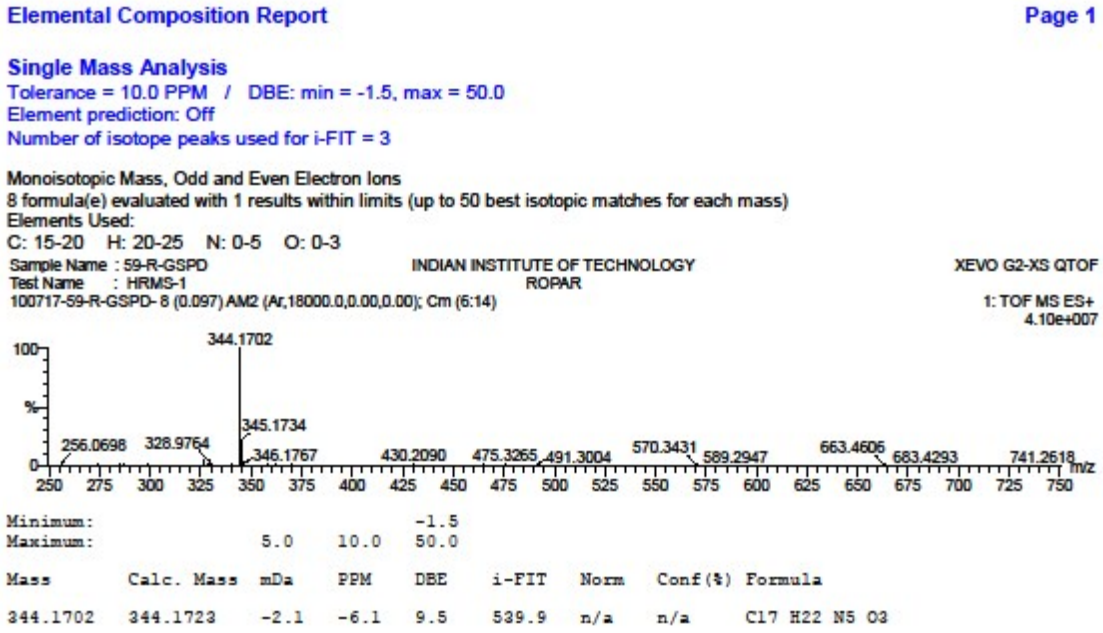

Figure S_6. HRMS spectrum for compound **2**

HRMS (ESI, m/z):

calculated for $C_{17}H_{22}N_5O_3$ $[M + H]^+$, 344.1723, found 344.1702.

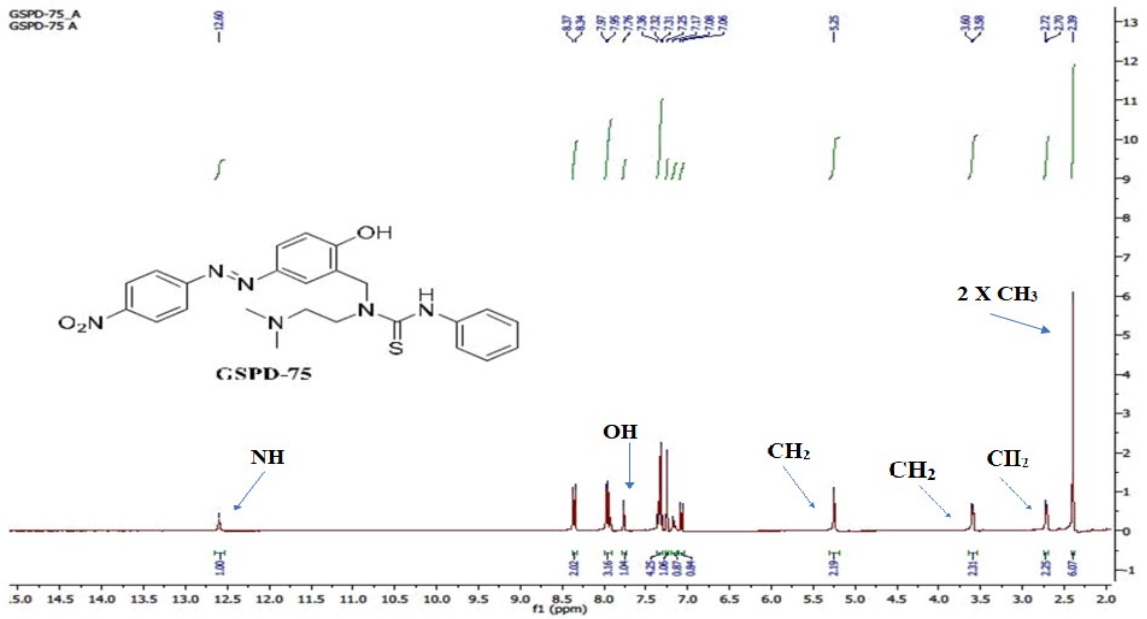

Figure S_7: ^{1}H NMR Spectrum of Probe **1**

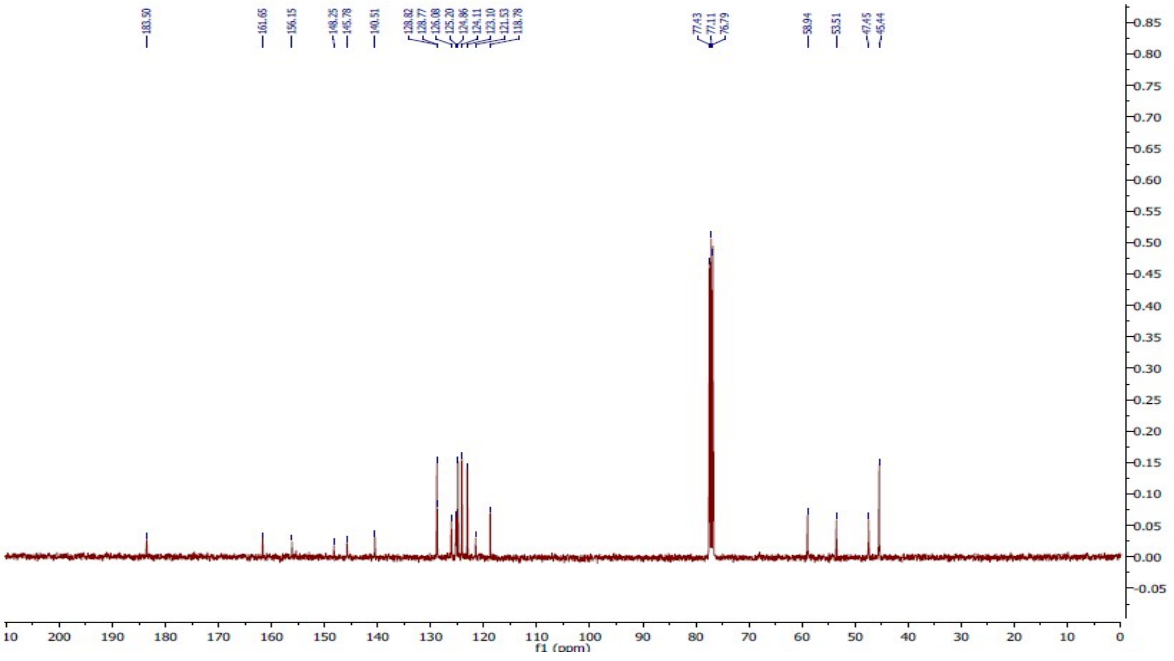

Figure S_8: ^{13}C NMR Spectrum of Probe **1**

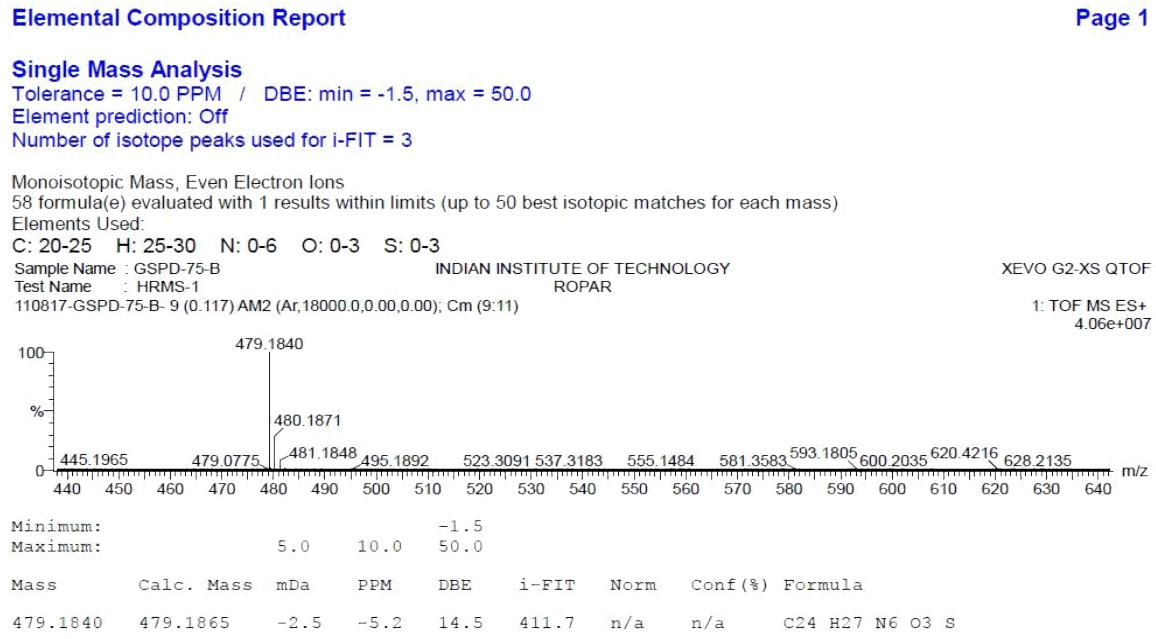

Figure S_9: HRMS Spectrum of Probe **1**

Crystal structure description:

Experimental details: The X-ray diffraction data for NS327 were collected on a Bruker D8 Venture PHOTON 100 CMOS CCD diffractometer at 293 K using mirrors monochromatized Mo-Kα radiation (λ = 0.71073 Å). The crystals were positioned at 50 mm from the CCD and the diffraction spots were measured using a counting time of 10 s. Data reduction and multi-scan absorption were carried out using the APEX II program suite (Bruker, 2007). Crystal of NS327 was solved with olex2.solve52 structure solution program using Charge Flipping and refined with the olex2.refine refinement package using Gauss−Newton minimization.[1]

Table S_1: Bond Lengths for probe **1.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C7	C6	1.387(4)	C15	C16	1.378(6)
C7	C8	1.387(4)	C15	C14	1.406(5)
C6	C11	1.386(4)	C3	C4	1.526(3)
C6	N3	1.416(3)	C3	N1	1.463(4)
C12	C13	1.506(4)	C4	N2	1.472(3)
C12	N2	1.470(3)	C22	C21	1.353(6)
C8	C9	1.374(5)	C22	C23	1.370(5)
C5	N2	1.358(3)	C22	N6	1.464(5)

C5	S1	1.694(3)	C21	C20	1.282(7)
C5	N3	1.342(3)	C23	C24	1.391(5)
C11	C10	1.377(4)	N6	O3	1.192(5)
C10	C9	1.378(5)	N6	O2	1.201(5)
C13	C18	1.391(4)	N1	C2	1.461(4)
C13	C14	1.391(4)	N1	C1	1.464(3)
C18	C17	1.377(4)	C24	C19	1.455(7)
C17	C16	1.362(6)	N5	C19	1.479(6)
C17	N4	1.575(5)	N5	N4	1.189(5)
O1	C14	1.353(4)	C19	C20	1.372(7)

Table S_2: Bond Angles for probe **1**

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C8	C7	C6	119.7(3)	N1	C3	C4	111.5(2)
C7	C6	N3	117.0(2)	N2	C4	C3	115.2(2)
C11	C6	C7	119.8(2)	C21	C22	C23	125.0(4)
C11	C6	N3	122.9(2)	C21	C22	N6	116.1(4)
N2	C12	C13	113.4(2)	C23	C22	N6	118.9(4)
C9	C8	C7	120.1(3)	C20	C21	C22	120.2(5)
N2	C5	S1	122.1(2)	C22	C23	C24	116.6(4)
N3	C5	N2	114.4(2)	O3	N6	C22	118.6(4)
N3	C5	S1	123.53(18)	O3	N6	O2	122.8(5)
C10	C11	C6	119.9(3)	O2	N6	C22	118.6(5)
C11	C10	C9	120.4(3)	C3	N1	C1	111.7(2)
C18	C13	C12	119.4(3)	C2	N1	C3	111.6(2)
C14	C13	C12	122.8(3)	C2	N1	C1	109.6(2)
C14	C13	C18	117.9(3)	C12	N2	C4	114.9(2)
C17	C18	C13	122.7(3)	C5	N2	C12	122.2(2)
C8	C9	C10	120.1(3)	C5	N2	C4	122.9(2)
C18	C17	N4	110.5(3)	C5	N3	C6	128.6(2)
C16	C17	C18	118.8(4)	C23	C24	C19	116.8(4)
C16	C17	N4	130.7(3)	N4	N5	C19	106.4(4)
C16	C15	C14	120.3(4)	C24	C19	N5	122.3(5)
C17	C16	C15	120.9(3)	C20	C19	C24	120.6(4)
C13	C14	C15	119.4(3)	C20	C19	N5	117.1(5)
O1	C14	C13	123.6(3)	N5	N4	C17	106.7(4)
O1	C14	C15	117.0(3)	C21	C20	C19	120.7(5)

Table S_3: Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for probe **1**

Atom	***x***	***y***	***z***	**U(eq)**
H7	-514	3980	5958	64
H12A	1220	2884	2212	58
H12B	-459	2763	2069	58
H8	491	4210	7333	86
H11	3258	1524	5404	61
H10	4225	1734	6785	78
H18	-1133	800	1450	71
H9	2847	3074	7746	89
H1	3122	1207	2724	112
H15	3569	-1750	1721	103
H16	1741	-2605	986	108
H3A	-2568	3000	3343	61
H3B	-3268	1573	3758	61
H4A	-704	511	4222	54
H4B	-1172	548	3216	54
H21	-3108	-5000	-1274	112
H23	-5905	-1864	-366	95
H2A	-3809	1168	5305	100
H2B	-2808	1718	5989	100
H2C	-2125	530	5412	100
H1A	-3286	4696	4249	106
H1B	-3450	4234	5298	106
H1C	-4510	3717	4632	106
H3	-361	2393	4808	53
H24	-3918	-1209	419	113
H20	-1231	-4520	-505	120

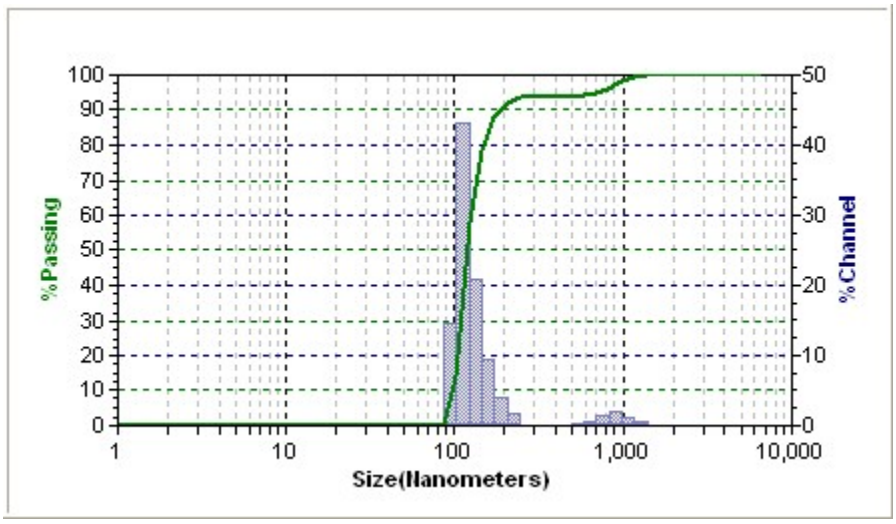

Figure S_{10}: DLS histogram of probe **1** (ONP) showing a particle distribution under 117 for DMF/Water solvent system

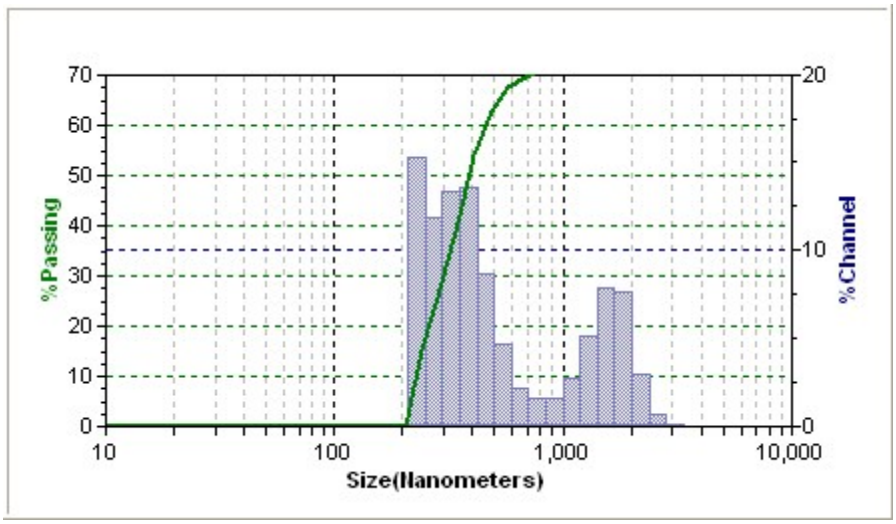

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Figure S_{11}: DLS histogram of probe **1** (ONP) showing a particle distribution under 386 for ACN/Water solvent system

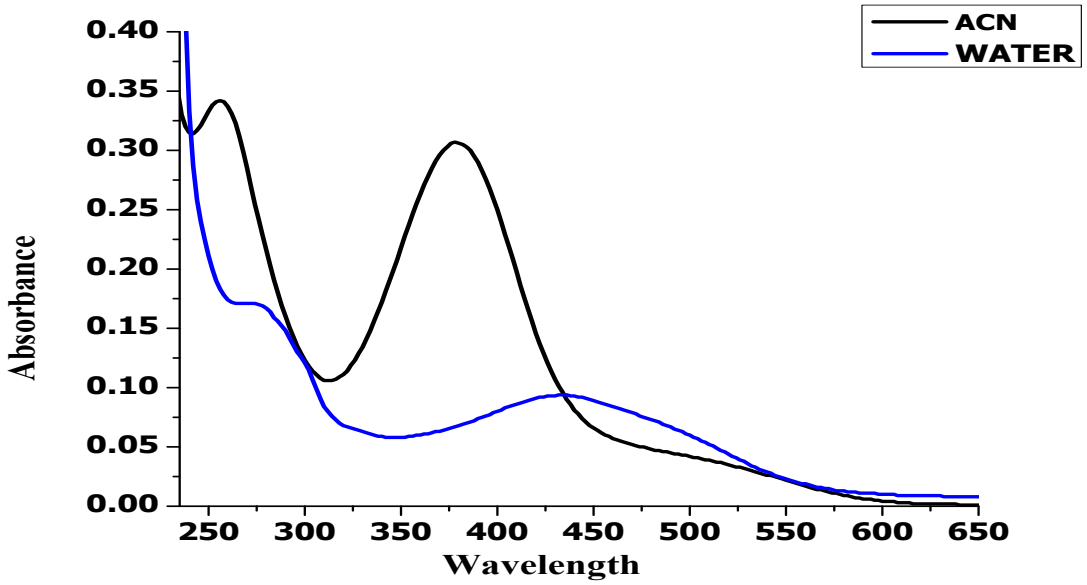


Figure S_{12}: Comparison of absorbance spectra of probe 1 in different solvent systems such as Water and ACN

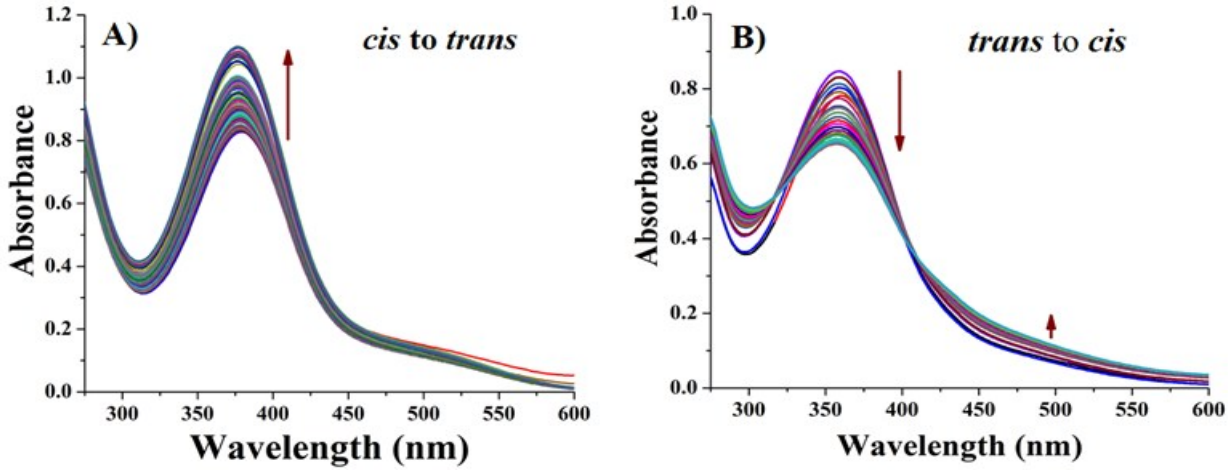


Figure S_{13}: a) The thermal back relaxation data of probe **1**; **b**) Absorbance as a function of wavelength before and after UV illumination

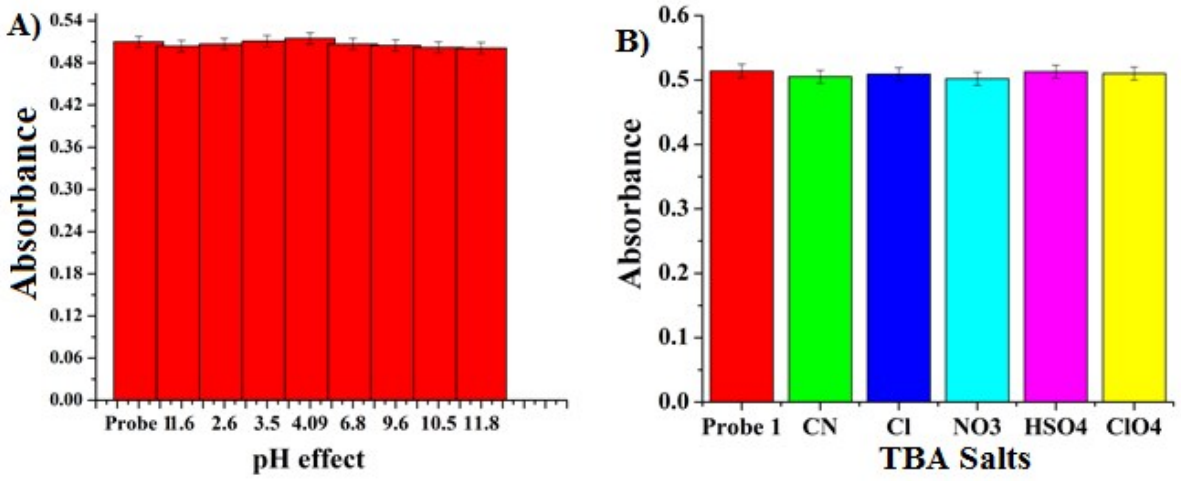


Figure S_{14}: **A**) Effect of varied pH on the absorbance of Probe **1**; **B**) Salt effect on absorbance of Probe **1**

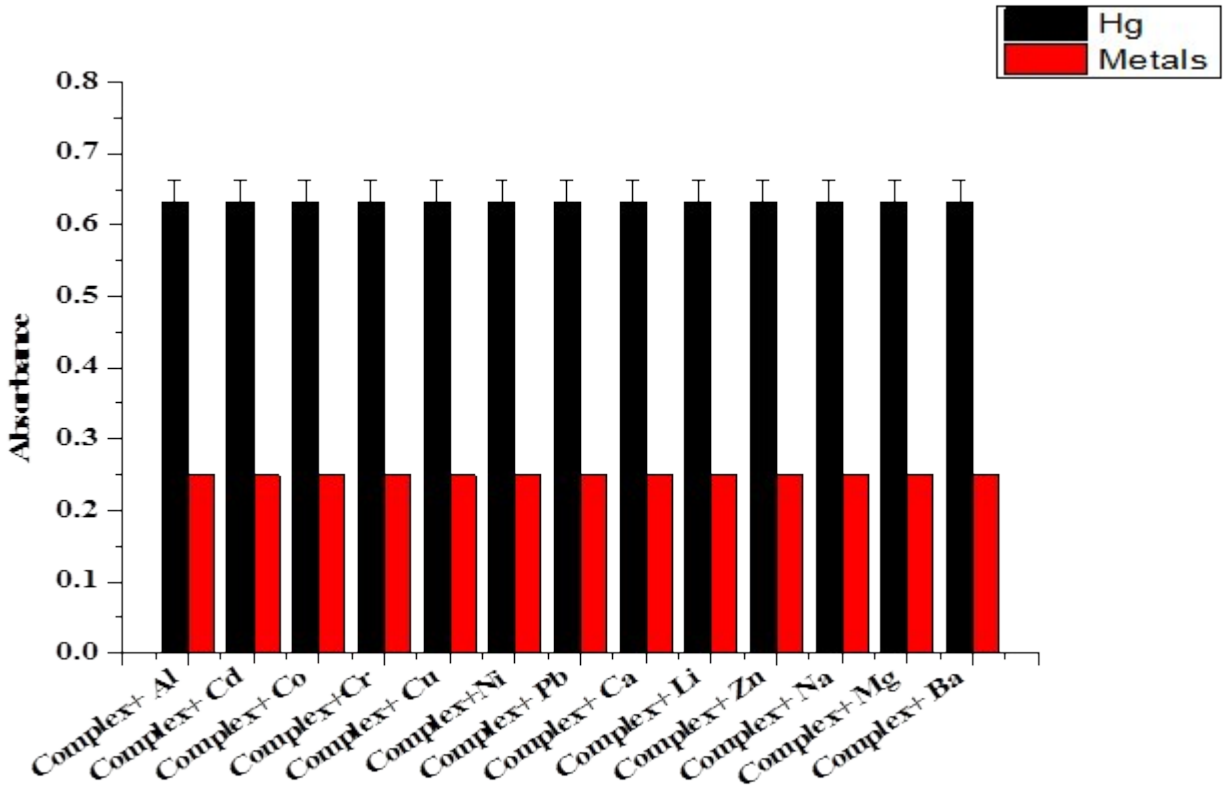


Figure S_{15}: Interference study with Different metal ions

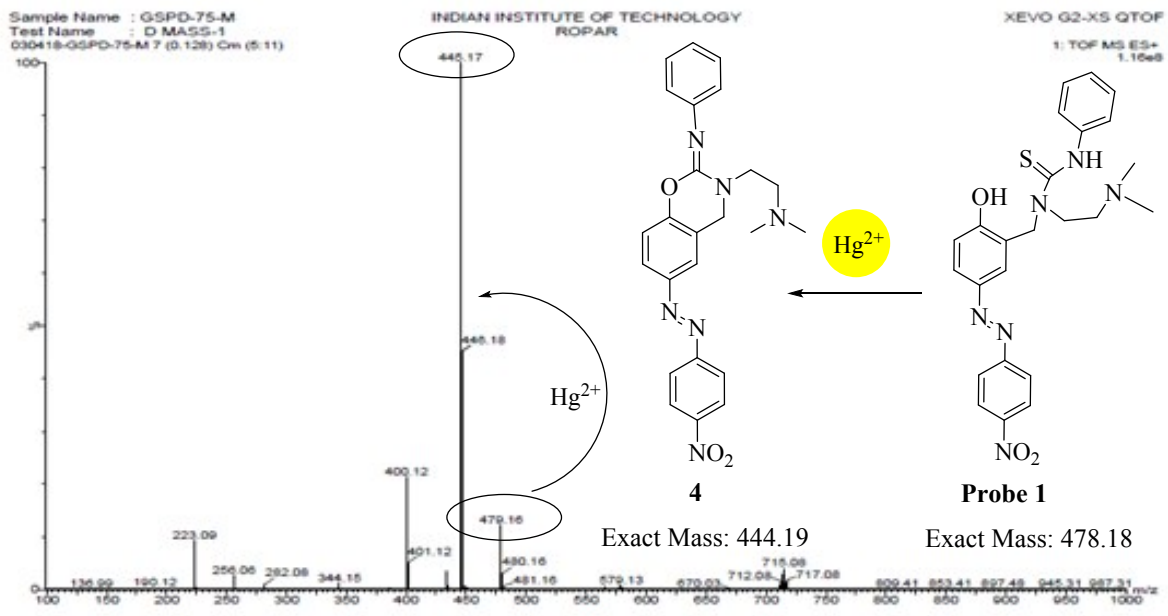


Figure S_{16}: Mass analysis data of compound **4**

Table S_4: HOMO and LUMO energies and HOMO-LUMO separation (ΔE) for probe **1** and Dye **4** by DFT calculations.

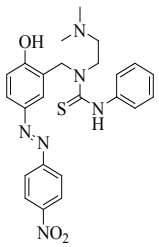
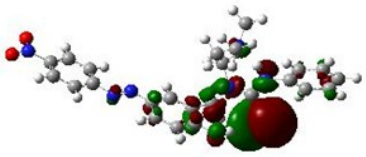
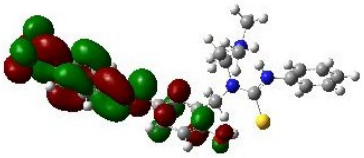
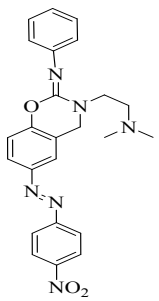
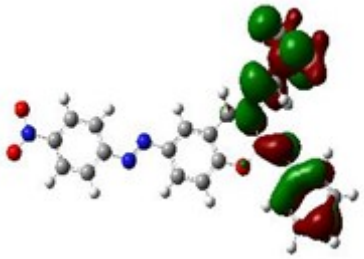
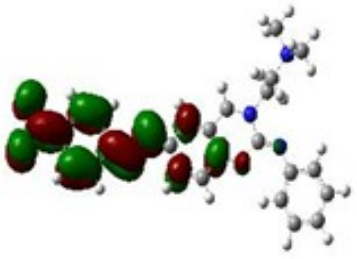
Compound	Molecular orbital of HOMO-LUMO of Intermediates		HOMO-LUMO gap energies
 Probe **1**	 HOMO (-3.452 eV)	 LUMO (-5.852 eV)	2.399 eV
 Dye **4**	 HOMO (-5.613eV)	 LUMO (-3.646eV)	1.966eV

Table S_5: Determination of Hg^{2+} ions in real water samples

Sample	Spiked Sample with Hg^{2+} (μM)	% Recovery
Satluj River Water	2	101
	4	99
	6	98
	8	99.5
	10	102
	12	98
	14	99
	16	97
	18	96
	20	99
	22	101
	24	102
	26	99
	28	98.5
	30	97
	32	99
	34	101
	36	103
	38	99.5
	40	98
Pond Water	2	99
	4	97
	6	99
	8	100.5
	10	99.5
	12	97
	14	99.5
	16	98
	18	97
	20	98.6
	22	102
	24	98
	26	97
	28	97
	30	99
	32	103
	34	99
	36	98
	38	96
	40	99
Tap Water	2	103
	4	99
	6	97
	8	96
	10	101
	12	99
	14	103
	16	98
	18	96
	20	101
	22	102
	24	99
	26	97
	28	99
	30	98
	32	103
	34	97
	36	101
	38	98
	40	99

Hardware Design:

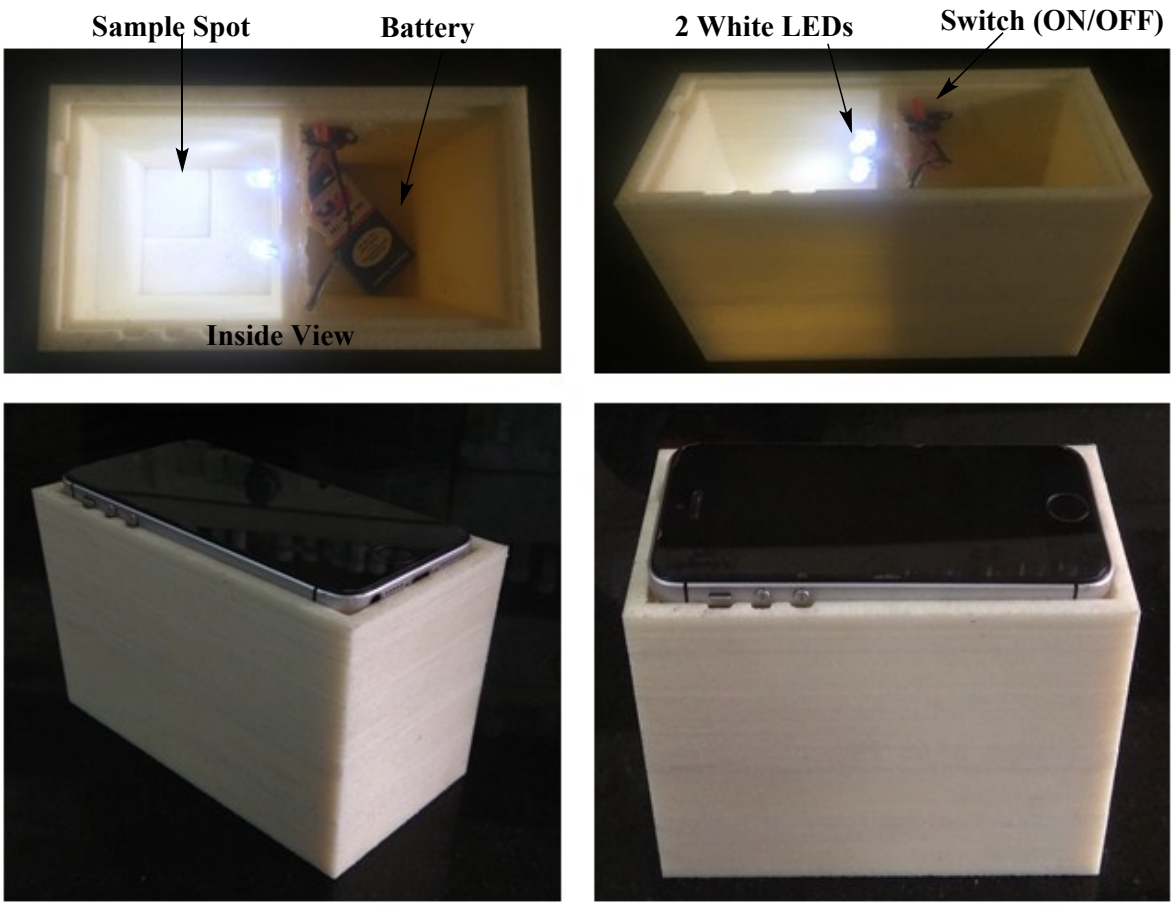


Figure S_{17}: Hardware Design