Supporting Information

Exploration of selective recognition of iodide with dipodal sensor: 2,2'-[ethane-1,2-diylbis(iminoethane-1,1-diyl)]diphenol

Kundan Tayade[a,b], Judith Gallucci[c], Hemant Sharma[d], Sanjay Attarde[b], Rahul Patil[a], Narinder Singh[d]*, Anil Kuwar[a]*

[a]School of Chemical Sciences, North Maharashtra University, Jalgaon 425 001 (MS) India.
[b]School of Environmental and Earth Sciences, North Maharashtra University, Jalgaon 425 001 (MS) India.
[c]Department of Chemistry and Biochemistry, Ohio State University, Columbus, OH 43210 USA
[d]Department of Chemistry, Indian Institute of Technology, Ropar, Rupanagar (Punjab) India

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*** Corresponding authors**. Tel.: +91-257-2257432; fax: +91-257-2257403

E-mail addresses: kuwaras@gmail.com
nsingh@iitrpr.ac.in

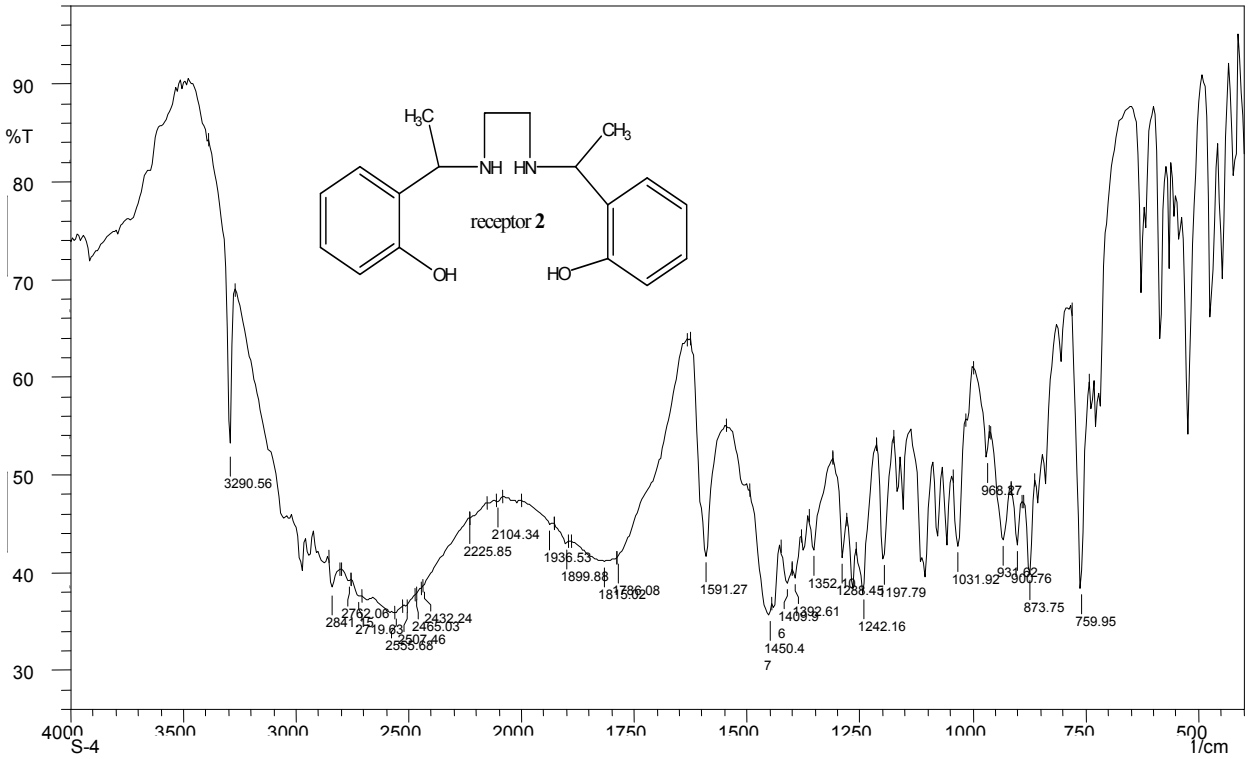

Figure S1. IR spectra of receptor **2**

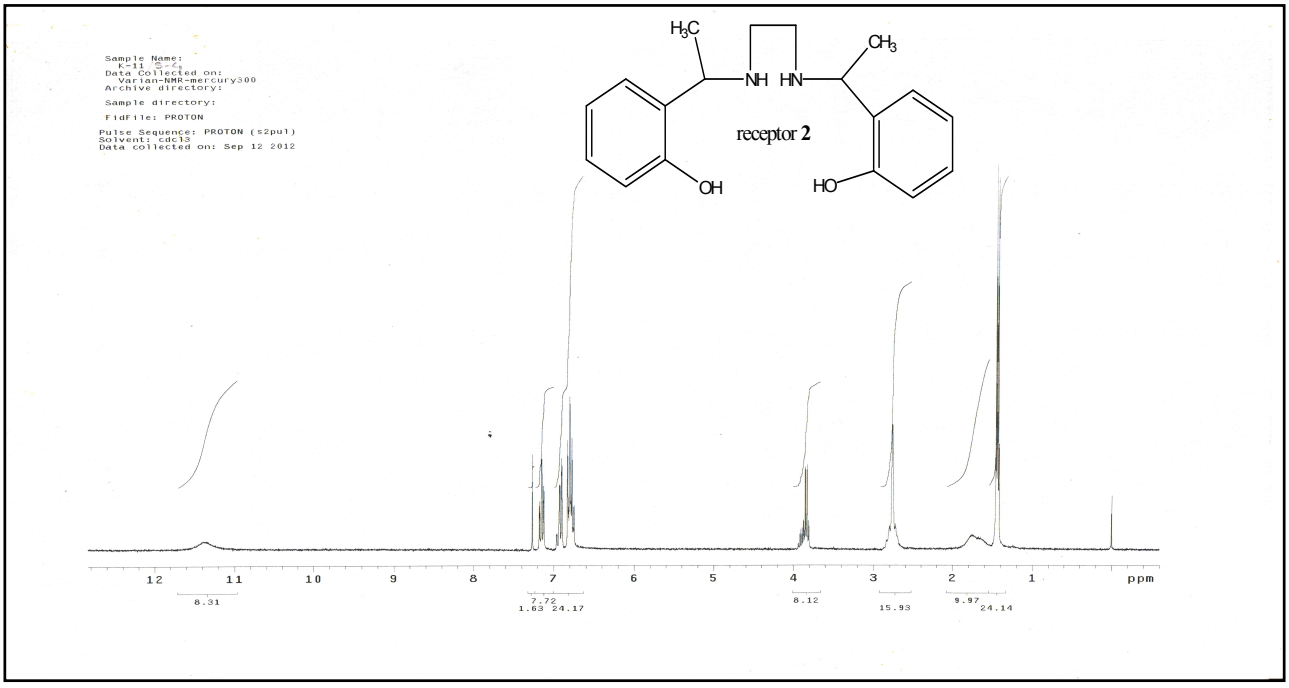

Figure S2. ^{1}H-NMR spectra of receptor **2**

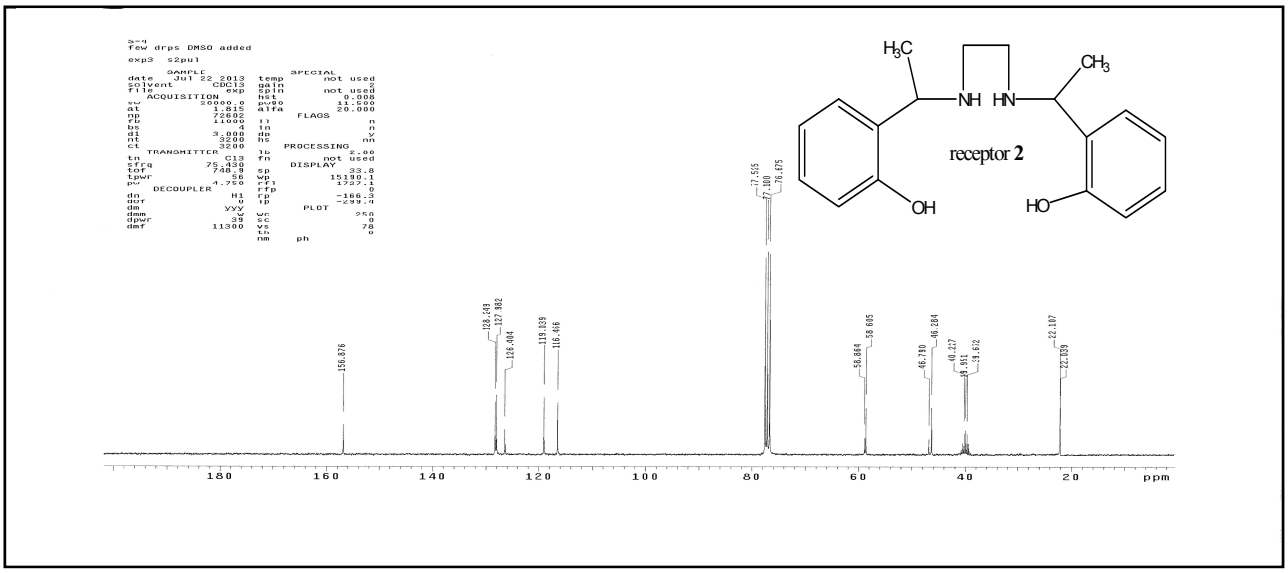

Figure S3. ^{13}C-NMR spectra of receptor **2**

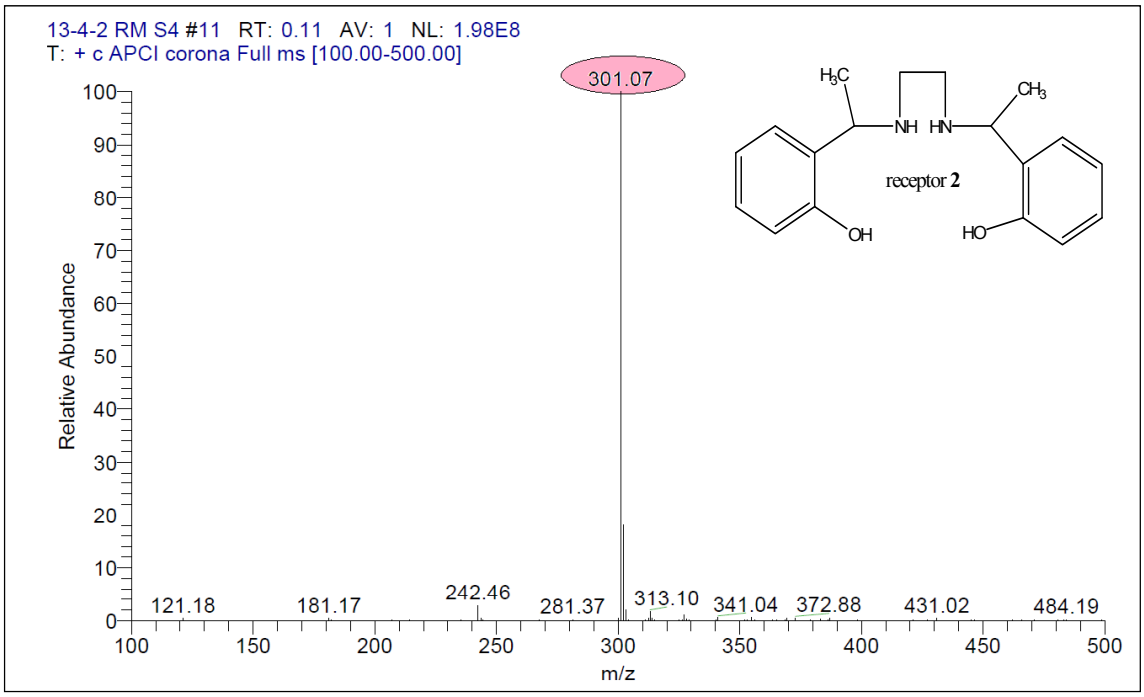

Figure S4. LC-MS spectra of receptor **2** (**M+H$^+$**)

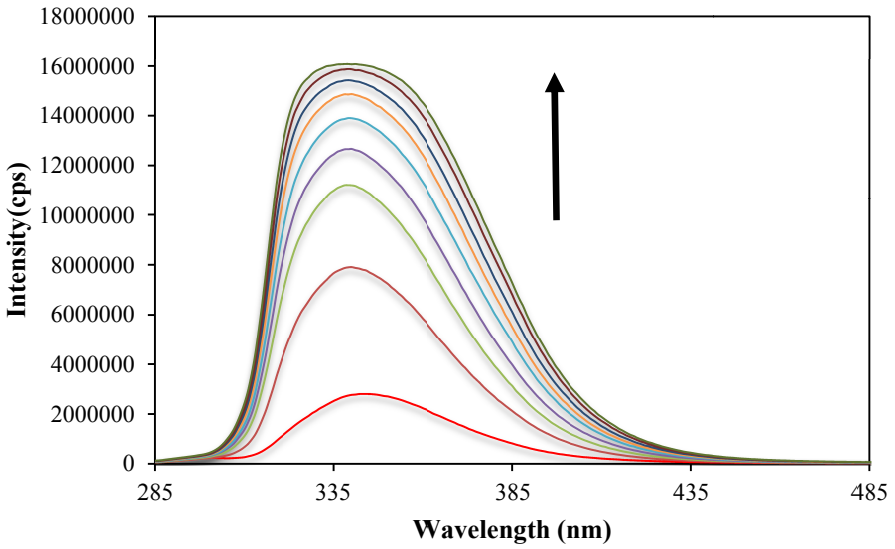

Fig. S5. Fluorescent titrations of receptor **2**(0.1mM) with tetrabutylammonium iodide in CH_3CN.

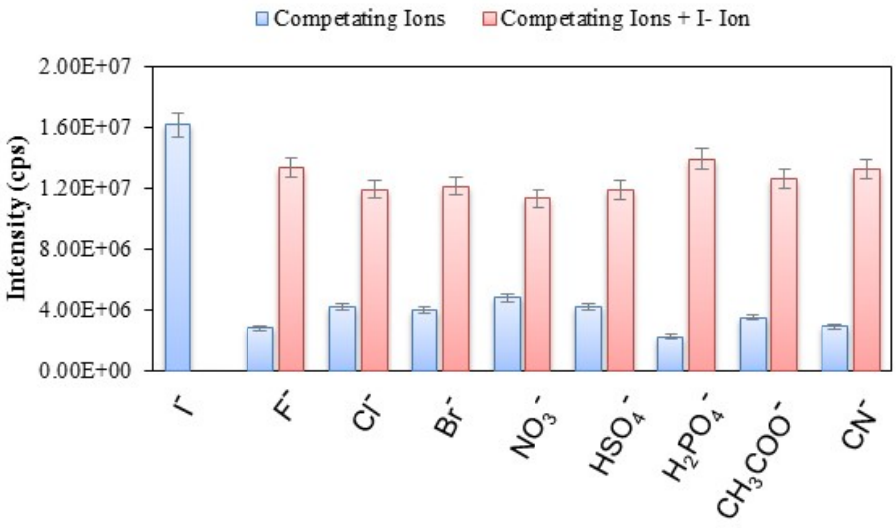

Figure S6. A sensing of I^- by receptor **2** (0.1 mM) in the presence of other competing anions.

To determination of binding constant

Linear fitting of the titration profiles using Benesi-Hildebrand methodology (Eq.1), Scatchard methodology (Eq.2) and Connor's fitting method (Eq.3,) based on a 1:1 binding mode results in a good linearity. The binding constant was calculated to be $8.6 \pm 0.01 \times 10^4\ M^{-1}$. We calculated the association constant (K_a) by using the following equation.

$$\frac{1}{(F-F_0)} = \frac{1}{(F_\infty - F_0)K_a[G]} + \frac{1}{(F_\infty - F_0)} \qquad \text{(Eq.1)}$$

$$\frac{(F-F_0)}{[G]} = (F_\infty - F_0)K_a - (F - F_0)K_a \qquad \text{(Eq.2)}$$

Connor's fitting method was carried out by the following equation as,

$$[H] + [G] \underset{}{\overset{K_a}{\rightleftharpoons}} [HG]$$

$$F = k_s[H] + k_p[HG]$$

$$F_0 = k_s\,[H]_t$$

$$[H]_t = [H] + [HG]$$

$$K_a = \frac{[HG]}{[H][G]}$$

$$\frac{F}{F_0} = \frac{(1+\frac{k_p}{k_s})}{(1+K_a[G])} \Longrightarrow \frac{(1-\frac{F}{F_0})}{[F]} = K_a(\frac{F}{F_0}) - \alpha K \qquad (\text{as } \frac{k_p}{k_s} = \alpha) \qquad \text{(Eq.3)}$$

Where, F_0 represents the fluorescence intensity in the absence of guest ion (I^- ion), F represents the fluorescence intensity in presence of guest ion, F_∞ represents fluorescence intensity after titration and $[G]$ represents the concentration of guest.

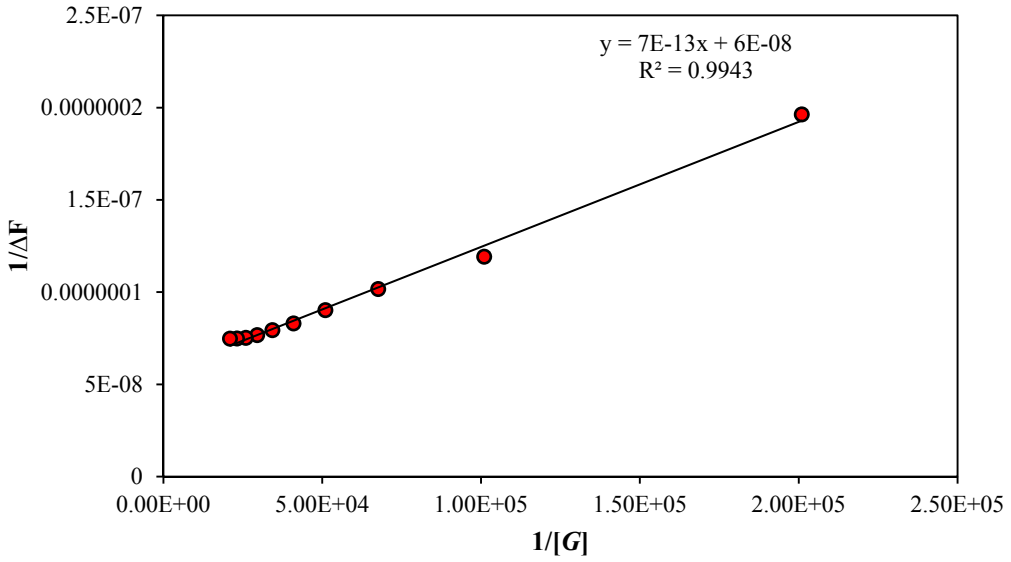

Figure S7. A Benesi-Hildebrand methodology for receptor **2,** ($1/\Delta F$) vs $1/[G]$, K_a = $8.57 \times 10^4\ M^{-1}$.

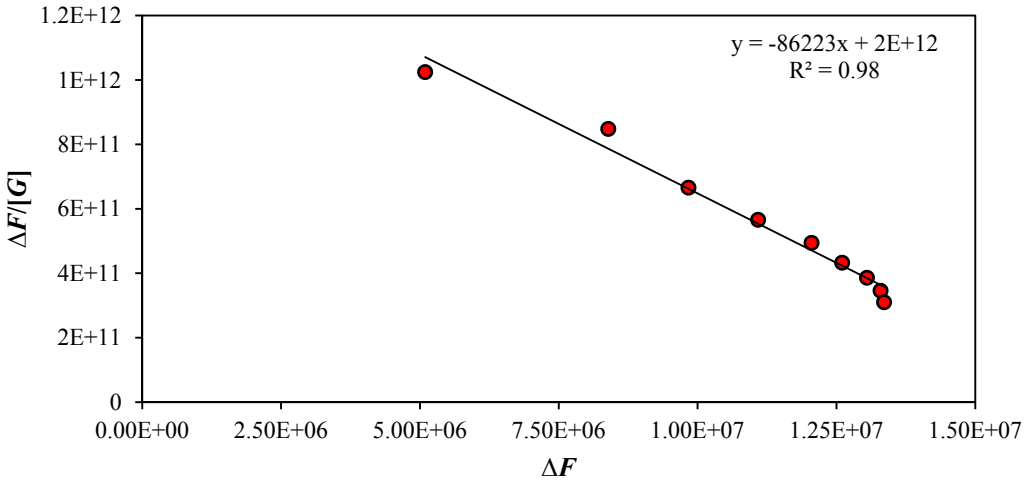

Figure S8. A Scatchard methodology for receptor **2**, $\Delta F/[G]$ vs ΔF, $K_a = 8.62 \times 10^4\ M^{-1}$.

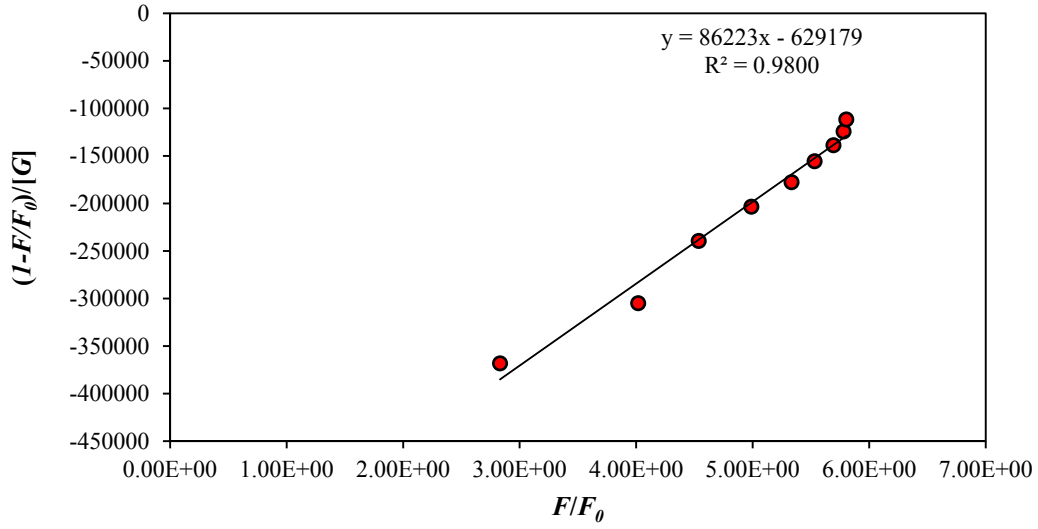

Figure S9. Connor's fitting method for receptor **2,** *(1-F/F₀)/[G]* vs *F/F₀*, $K_a = 8.62 \times 10^4\ M^{-1}$.

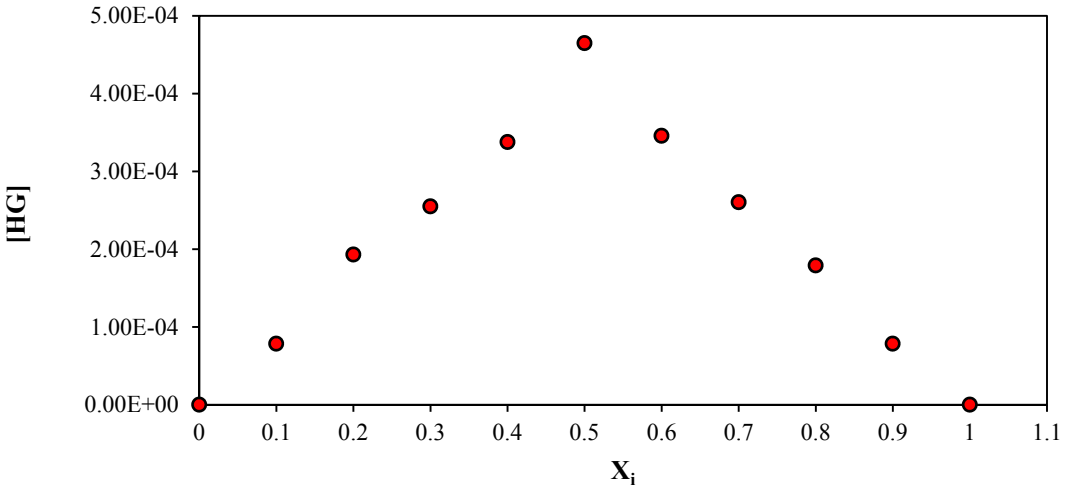

Figure S10. 1:1 Stoichiometry of the host guest relationship realized from the Job's plot for receptor **2**.

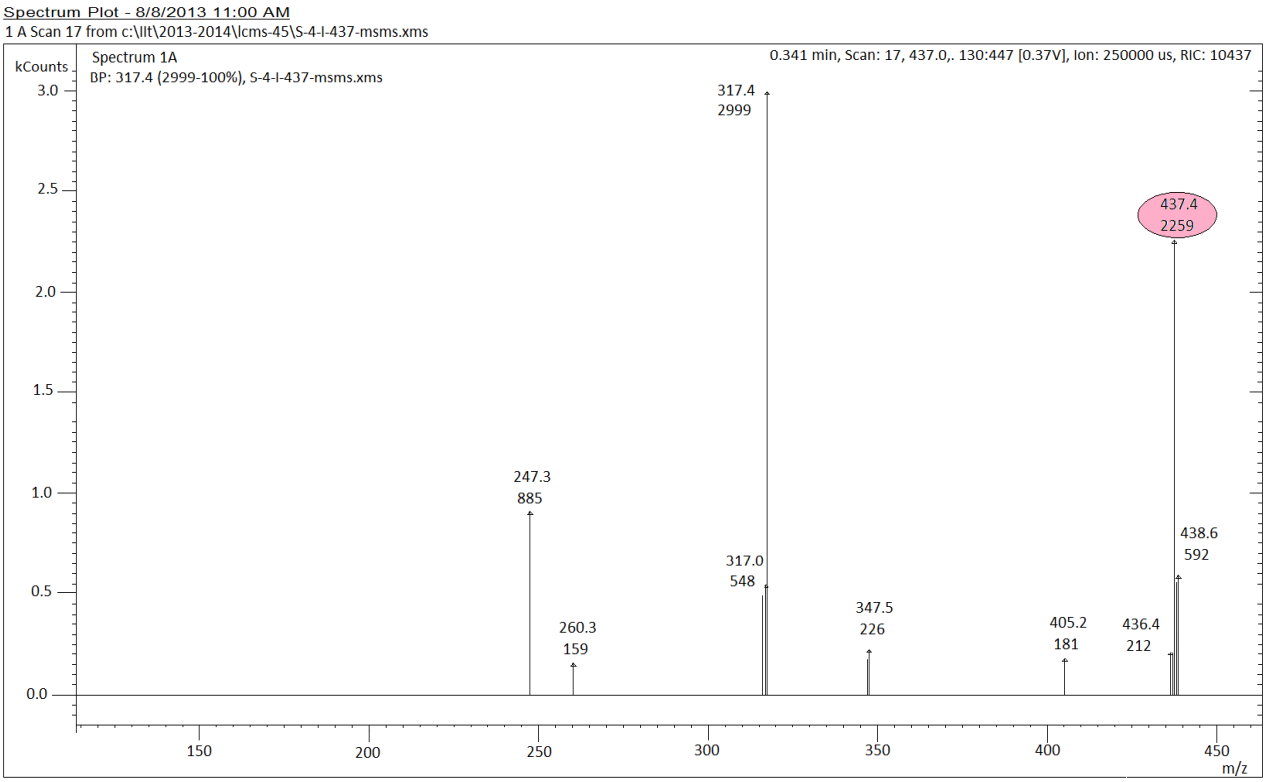

Figure S11. LC-MS spectrum of receptor **2.**I^- ion complex $[M+H^+.(H_2O)_{0.5}]$

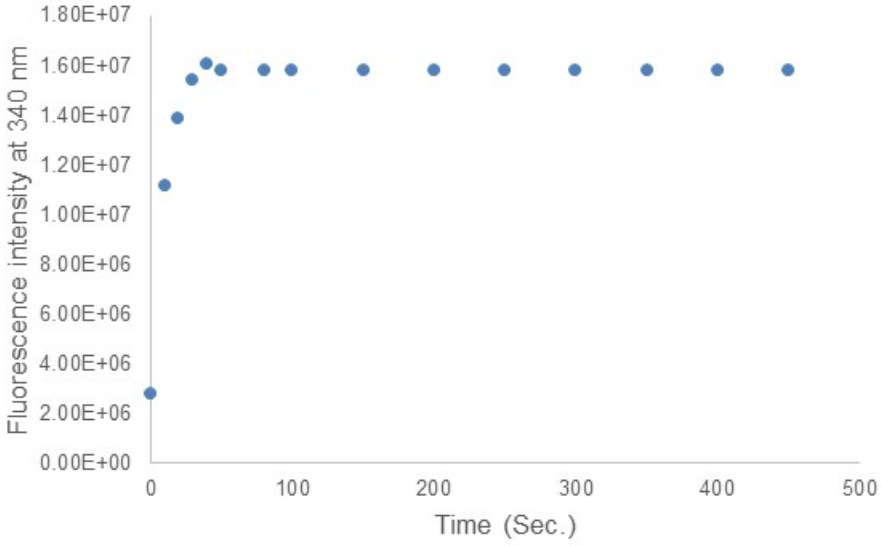

Figure S12. A change in fluorescence intensity of receptor **2** with time (sec.) upon addition of 3 equiv. of I^-.

Table S1. A comparison of literature reported synthesis with present methodology

Group	Synthetic strategy	Detection limit	Fluorescence response	Ref.
Singh *et al.*	Multistep tripodial	2.1 μM	quenching	1a
Wang *et al.*	Multistep Ag-complex	7.16 μM	quenching	21
Shang *et al.*	Capped CdSe nanoparticles	0.28 μM	quenching	22
Yang *et al.*	Multistep PVC membrane	0.5 μM	quenching	23
Wang *et al.*	Capped Au nanoclusters	118 nM	quenching	24
Lin *et al.*	Multistep Hg-complex	0.45 μM	enhancement	25
Present work	**Simple condensation & reduction**	**1.38 μM**	**enhancement**	-

Table S2 Crystallographic details for receptor **2**

Parameter	**Receptor 2**
Formula	$C_{18}H_{24}N_2O_2$
Formula weight	300.39
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Tetragonal
Space group	P 4_12_12
Unit cell dimensions	a = 7.5161(6) Å c = 29.023(2) Å
Volume	1639.6(3) $Å^3$
Z	4
Density (calculated)	1.217 Mg/m^3
Absorption coefficient	0.080 mm^{-1}
F(000)	648
Crystal size	0.23 x 0.23 x 0.27 mm^3
Theta range for data collection	2.799 to 24.988°
Index ranges	-8<=h<=8, -5<=k<=6, -33<=l<=34
Reflections collected	10916
Independent reflections	1434 [R(int) = 0.050]
Completeness to theta = 25.00°	99.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1434 / 0 / 109
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0590, wR2 = 0.1365
R indices (all data)	R1 = 0.0807, wR2 = 0.1539
Largest diff. peak and hole	0.500 and -0.222 $e/Å^3$

Table S3. Hydrogen bonds for receptor 2 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(8)-H(8A)...O	0.98	2.57	3.156(6)	118.6
N-H(1N)...O	1.10(5)	2.20(5)	2.993(5)	127(3)
O-H(1O)...N#2	0.95(7)	1.81(7)	2.760(5)	171(7)

Symmetry transformations used to generate equivalent atoms:
#1 y,x,-z #2 y,x+1,-z

Table S4: An optimized bond angles, dihedral angles, bond length and energy calculated at B3LYP/ LANL2DZ level.

Parameter	Ligand **2**	**2**.I^-
Dihedral angles (°)		
N25-C29-C30-N26	61.09	91.88
C29-C30-N26-C24	-135.57	-169.19
C5-C4-C23-N25	33.34	69.46
O21-C3-C4-C23	-0.50	-2.44
C27-C23-N25-C29	-66.67	-80.35
C3-C4-C23-N25	-147.43	-108.38
O22-C12-C11-C24	-2.34	0.35
C11-C24-N26-C30	157.50	-179.05
Bond angles (°)		
C23-N25-C29	116.22	112.14
C5-C4-C23	121.38	121.06
C30-N26-C24	120.29	114.74
N26-C24-C28	113.49	110.27
N25-C29-C30	109.24	112.12
Bond Length (Å)		
N25-C29	1.46	1.52
C30-N26	1.46	1.54
C24-N26	1.47	1.56
C23-N25	1.47	1.53
C12-O22	1.39	1.40
C3-O21	1.40	1.43
O22-H45	0.97	1.02
O21-H44	0.97	1.02
N25-H42	1.01	1.05
N26-H43	1.01	1.06
C23-C27	1.54	1.56
Energy (a.u.)	-960.28	-959.48