Supporting Information

Colorimetric and Turn-on fluorescent chemosensor for selective detection of Hg^{2+}: Theoretical studies and Intracellular applications

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Table of Contents

1. Synthetic procedure of SBPH:

A mixture of salicylaldehyde **1b** (0.200 g, 1.64 mmol) and 1-(diphenylmethylene)hydrazine or benzophenonehydrazone **2** (0.322 g, 1.64 mmol) was dissolved in 12 mL of dry ethanol in presence of 4 drops of acetic acid and the resulting solution was stirred under reflux for 4 h at an ambient temperature. After completion of the reaction, monitored by TLC, the solvent was removed under reduced pressure, and the resulted mixture was diluted with dichloromethane (30 mL). The organic layer was then washed twice with water and dried over anhydrous Na_2SO_4. Evaporation of the solvent followed by purification gave the product as a light yellow solid (0.433 g, 1.44 mmol, yield = 88%)

M.p.: 65–66 °C;

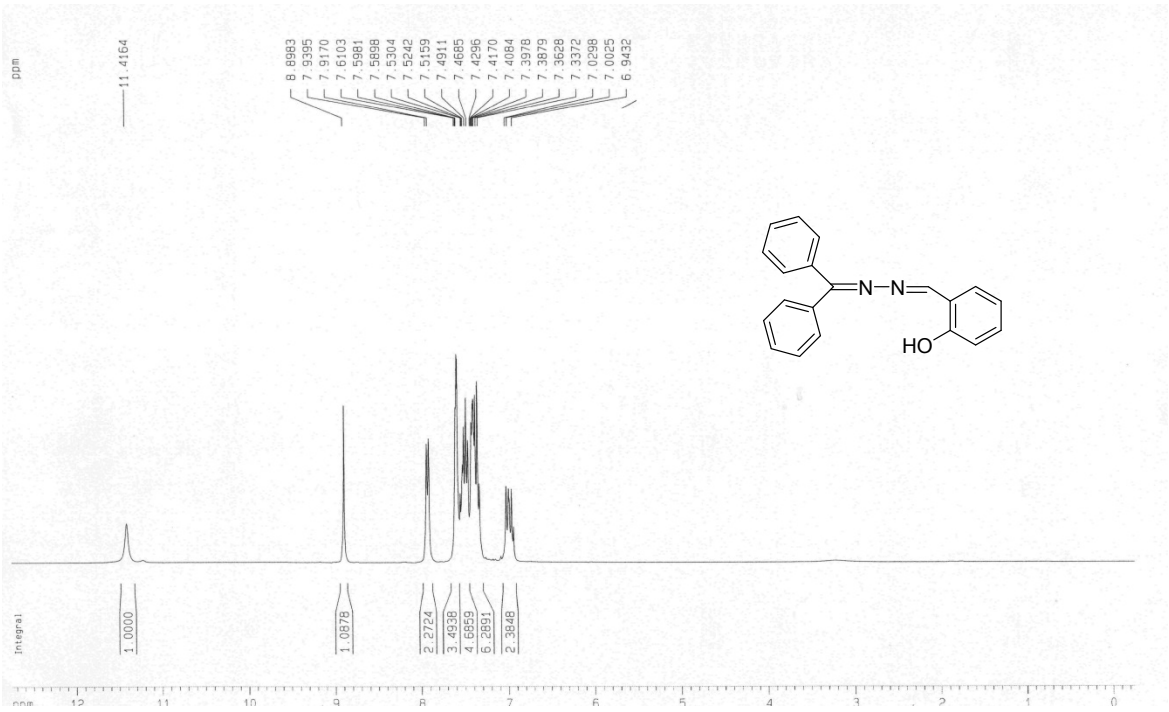
^{1}H-NMR (300 MHz, $CDCl_3$): δ 6.94–7.03 (m, 2H), 7.34–7.61 (m, 10H), 7.93 (d, J = 6.8 Hz, 2H), 8.90 (s, 1H), 11.42 (broad s, 1H).

^{13}C-NMR (75 MHz, $CDCl_3$): δ 76.14, 117.17, 118.22, 119.47, 126.80, 127.58, 128.60, 128.70, 128.78, 129.37, 131.18, 132.49, 133.05, 135.94, 137.35, 144.38, 159.98, 164.33, 168.95.

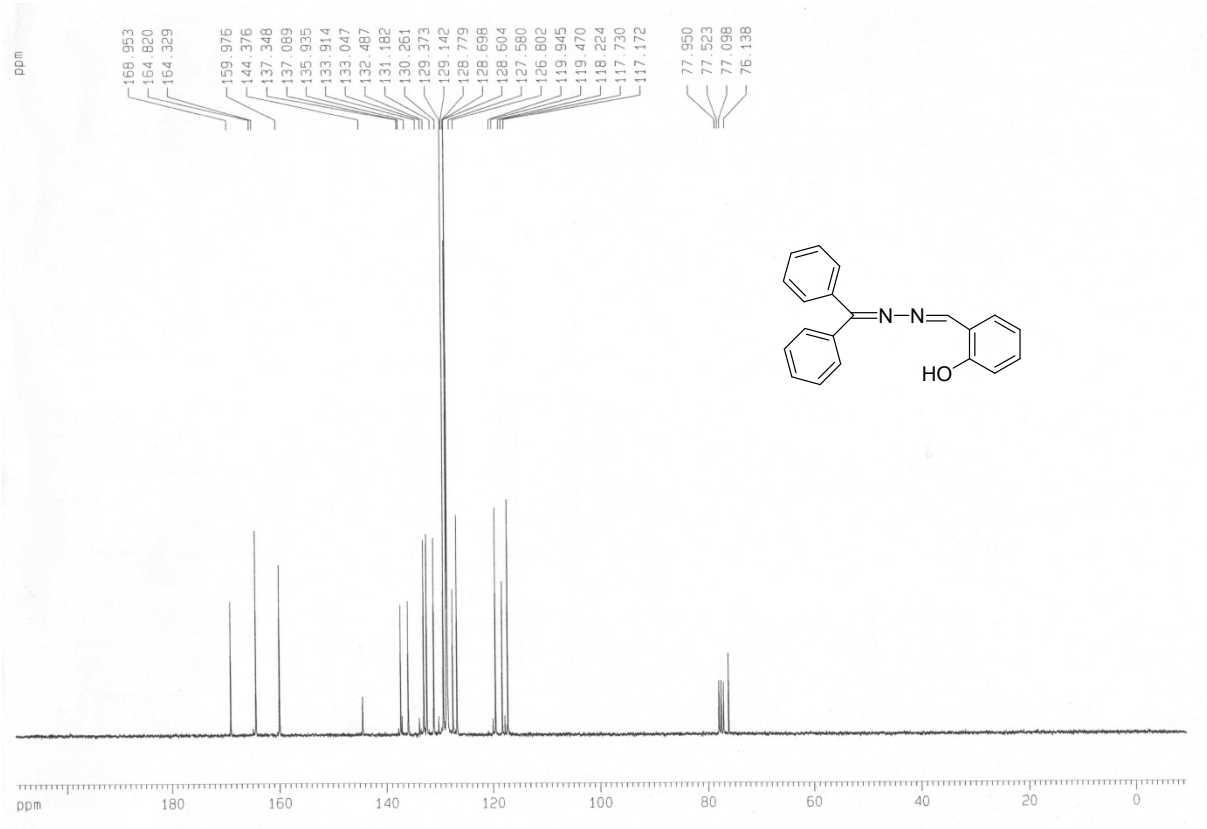
HRMS (ESI-TOF, *m/z*): calcd for $C_{20}H_{17}N_2O$ [M + H^+] 301.1342, found, 301.1340.

2. ^{1}H NMR, ^{13}C NMR and HRMS spectra of SBPH:

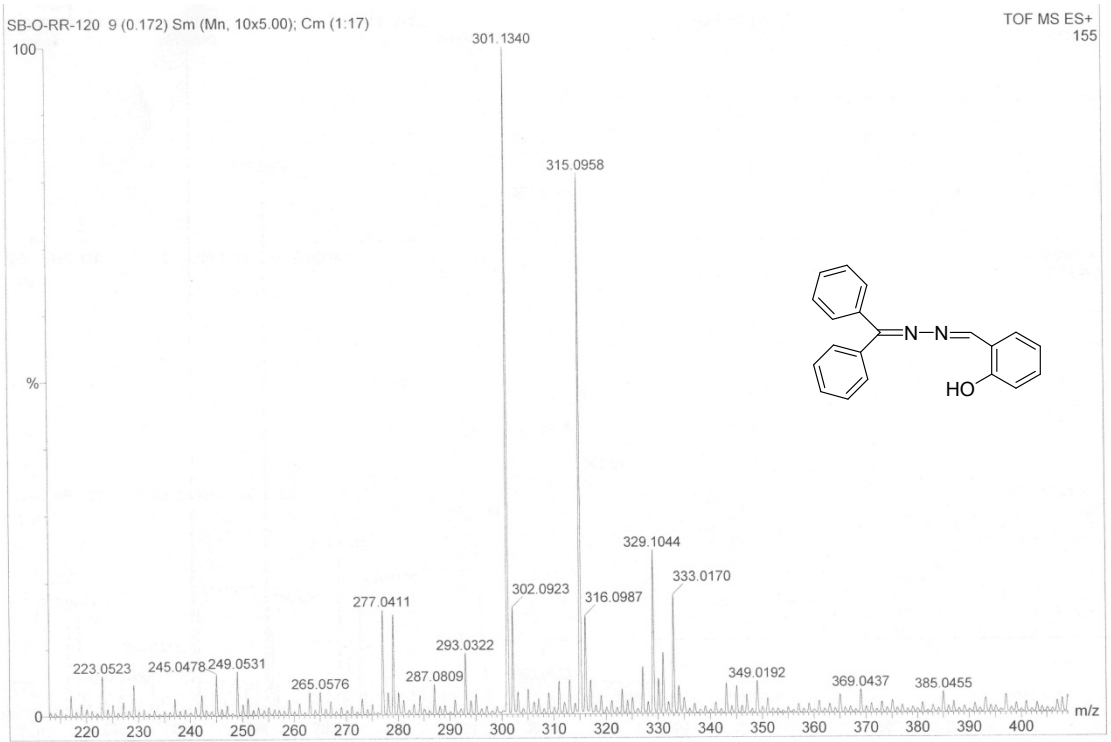
(a) ^{1}H NMR (300 MHz, $CDCl_3$) spectra of SBPH:



(b) ^{13}C NMR (75 MHz, $CDCl_3$) spectra of SBPH:



(c) HRMS spectra (ESI-TOF) of SBPH:



3. ^{1}H NMR spectra of DEAS–BPH:

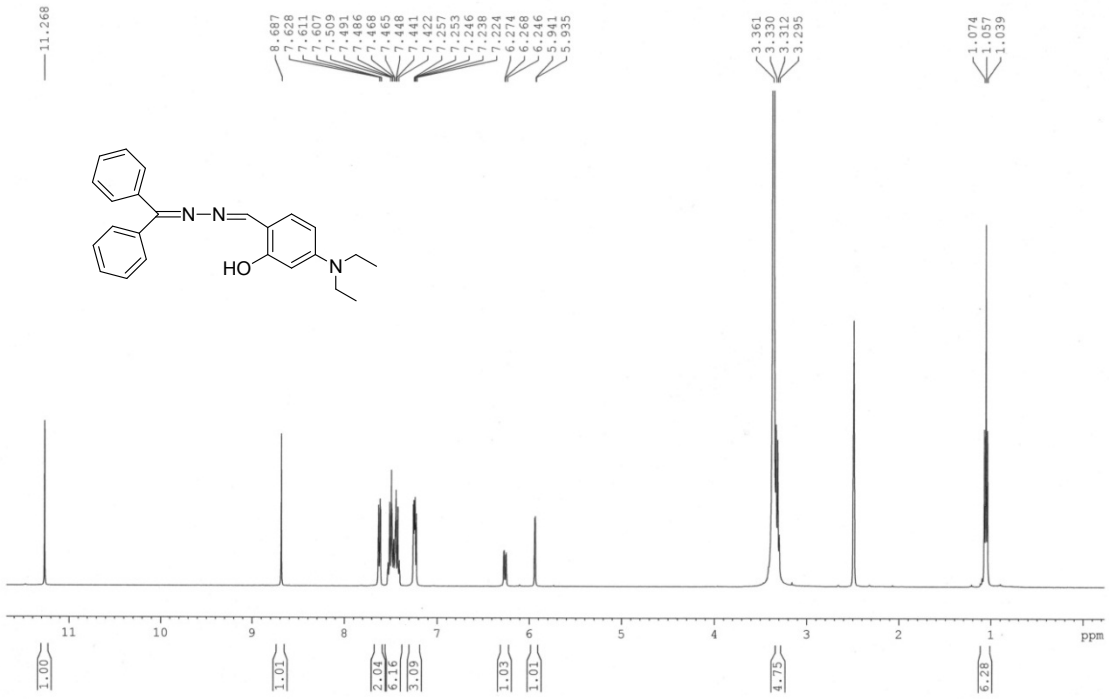


Fig.S1 ^{1}H NMR spectra (400 MHz) of **DEAS–BPH** in DMSO-d_6.

4. ^{13}C NMR spectra of DEAS–BPH:

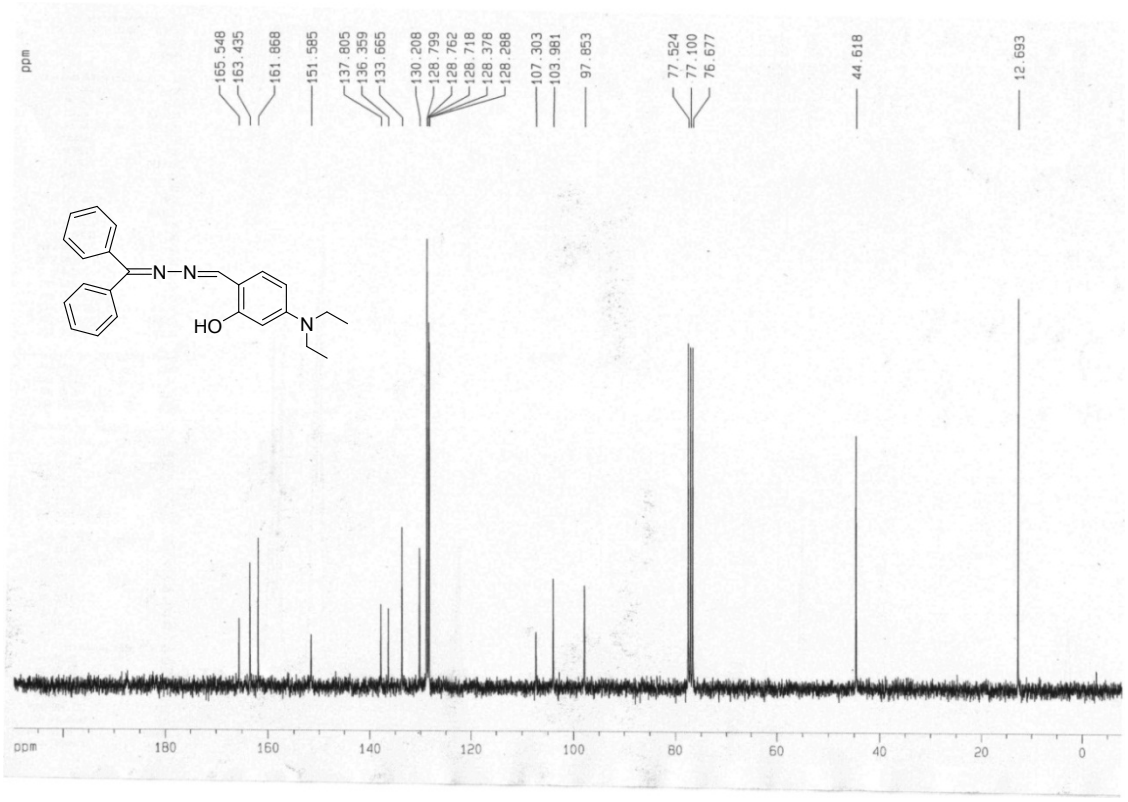


Fig.S2 ^{13}C NMR spectra (75 MHz) of **DEAS–BPH** in $CDCl_3$.

5. FT-IR spectra of DEAS–BPH and its complex with Hg^{2+}:

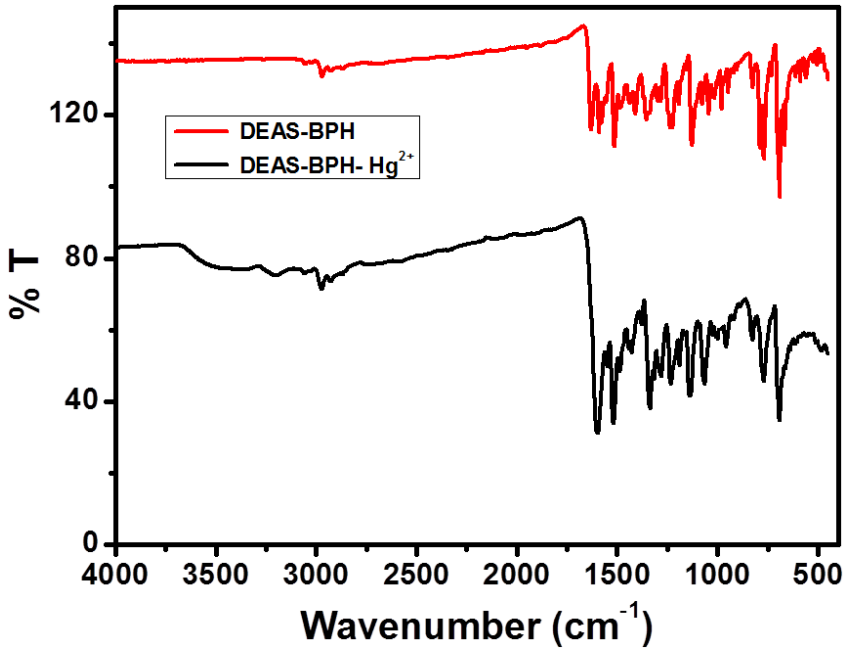


Fig.S3 FT-IR spectra of the receptor and its complex with Hg^{2+}.

6. HRMS spectra (ESI-TOF) of DEAS–BPH and the complex with Hg^{2+}:

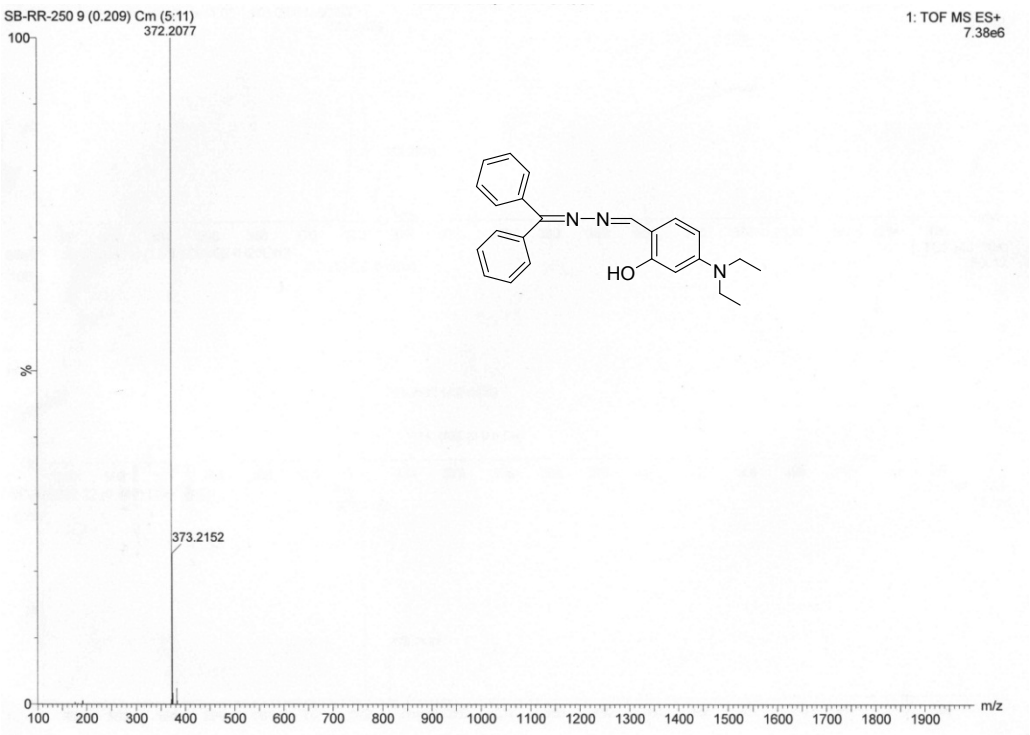


Fig.S4a HRMS spectra (ESI-TOF) of **DEAS–BPH**.

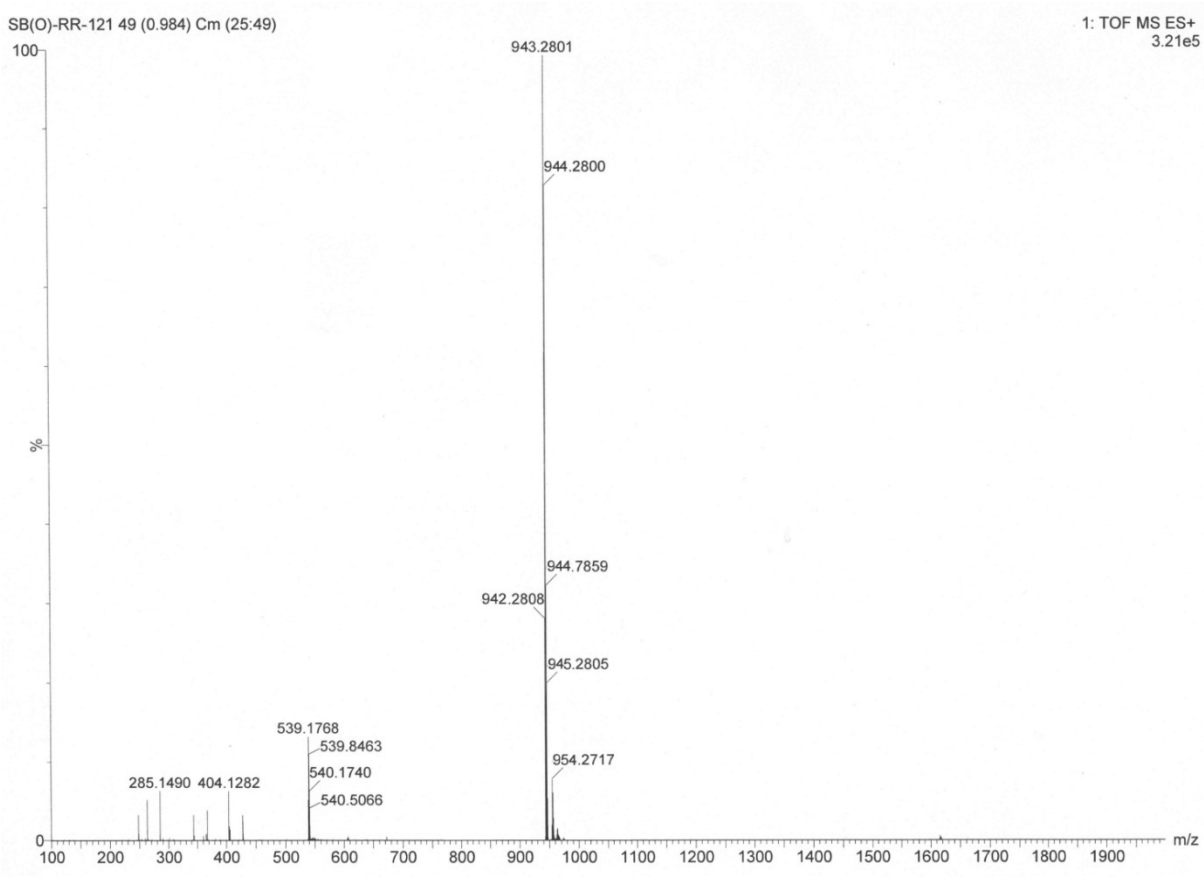


Fig.S4b HRMS spectra (ESI-TOF) of the complex of **DEAS–BPH** with Hg^{2+}.

7. UV-vis Absorption titration spectra of the receptor with different guest cations in CH_3CN–H_2O (4:1, v/v, pH = 7.2):

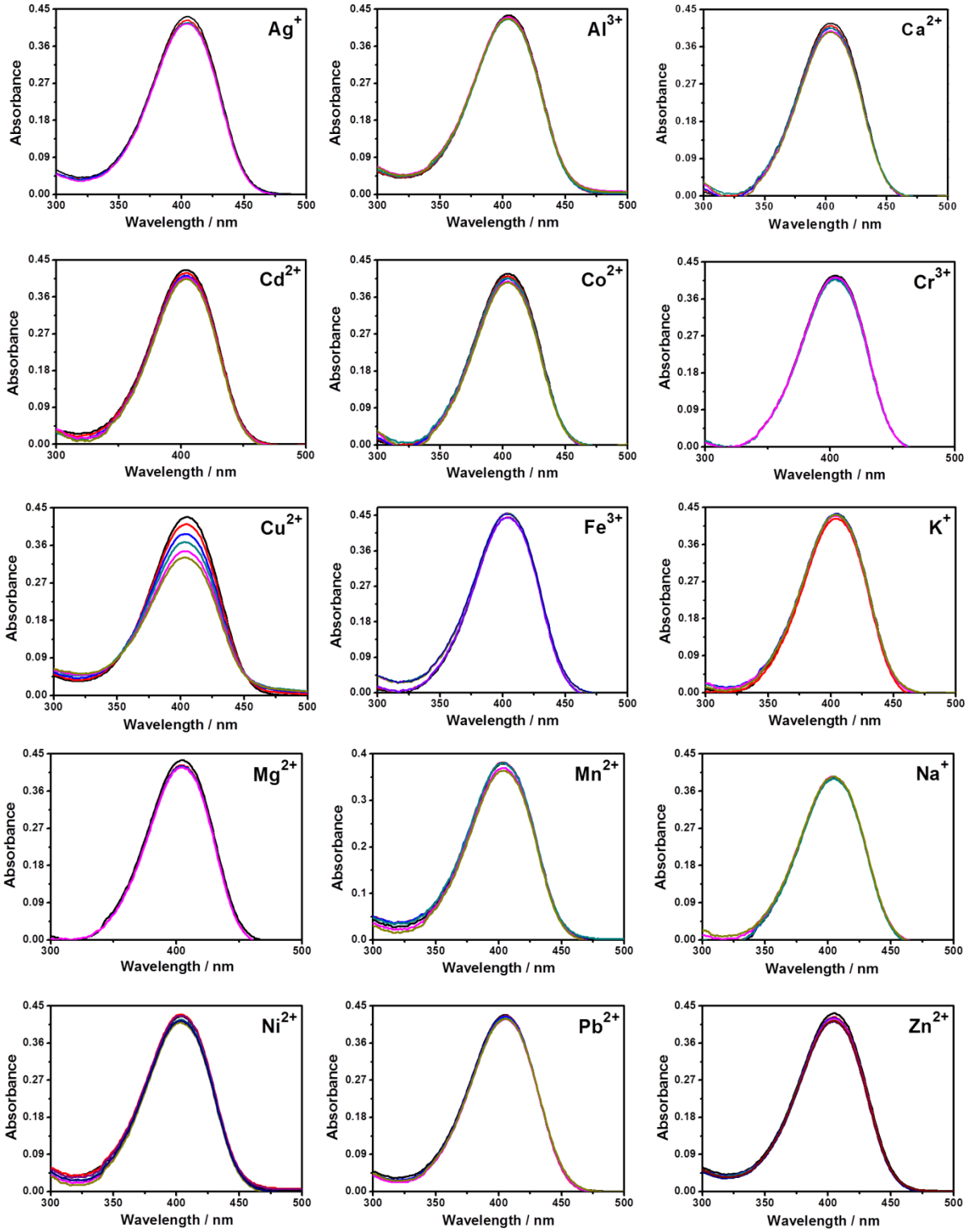


Fig. S5 UV-vis Absorption titration spectra of the receptor with different guest cations in CH_3CN–H_2O (4:1, v/v, pH = 7.2).

8. UV-vis spectra of SBPH with different cations:

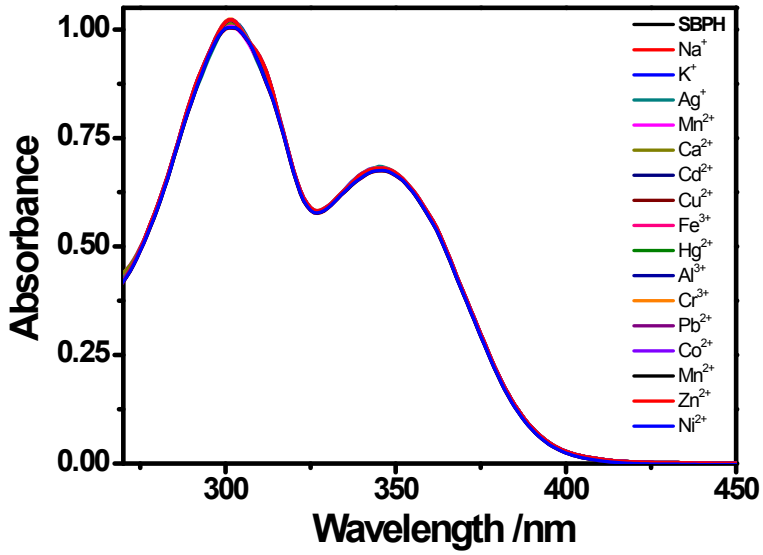


Fig. S6 UV-vis spectra of **SBPH** in the presence of 4 equivalents of various metal ions in CH_3CN–H_2O (4:1, v/v, pH = 7.2).

9. Emission spectra of SBPH with different cations:

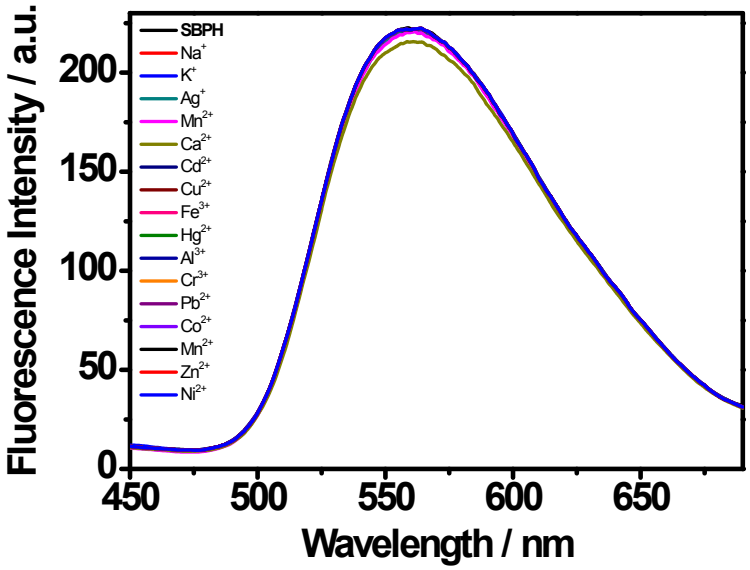


Fig. S7 Emission spectra of **SBPH** in the presence of 3 equivalents of various metal ions in CH_3CN–H_2O (4:1, v/v, pH = 7.2).

10. Difference in spectrofluorometric response upon excitation at the isosbestic point and the absorption maxima of the complex:

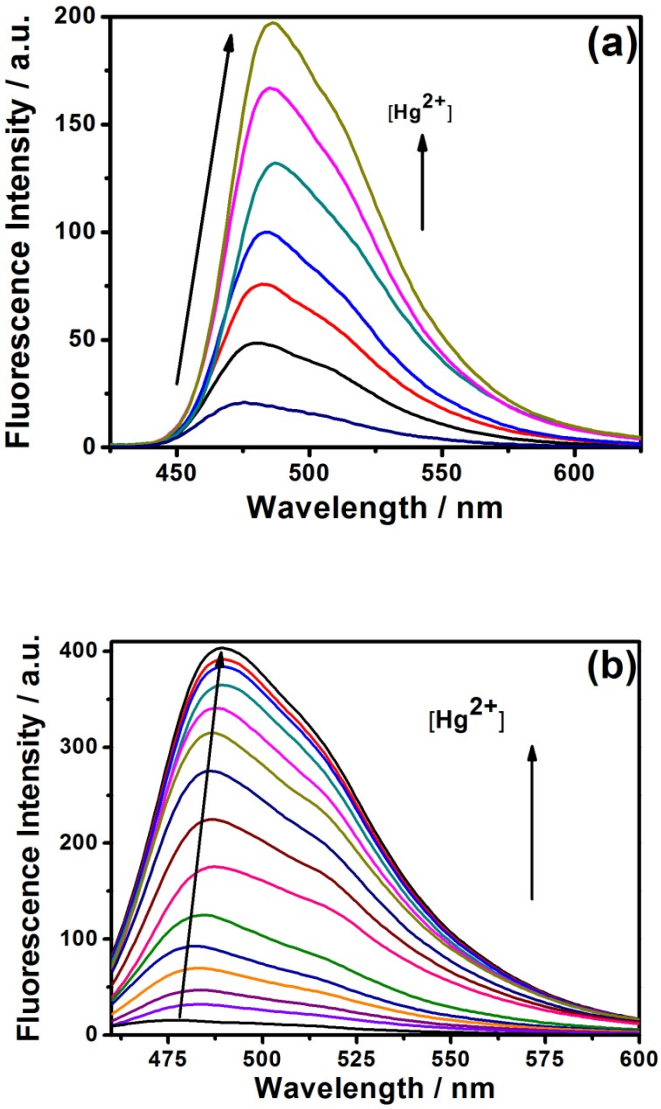


Figure S8: Fluorescence spectra of **DEAS–BPH** upon addition of Hg^{2+} up to saturation when excited (a) at isosbestic point (λ_{ex}= 416 nm), (b) at complex absorption maxima (λ_{ex}= 450 nm).

11. Fluorescence titration spectra of the receptor with different guest cations in $CH_3CN–H_2O$ (4:1, v/v, pH = 7.2):

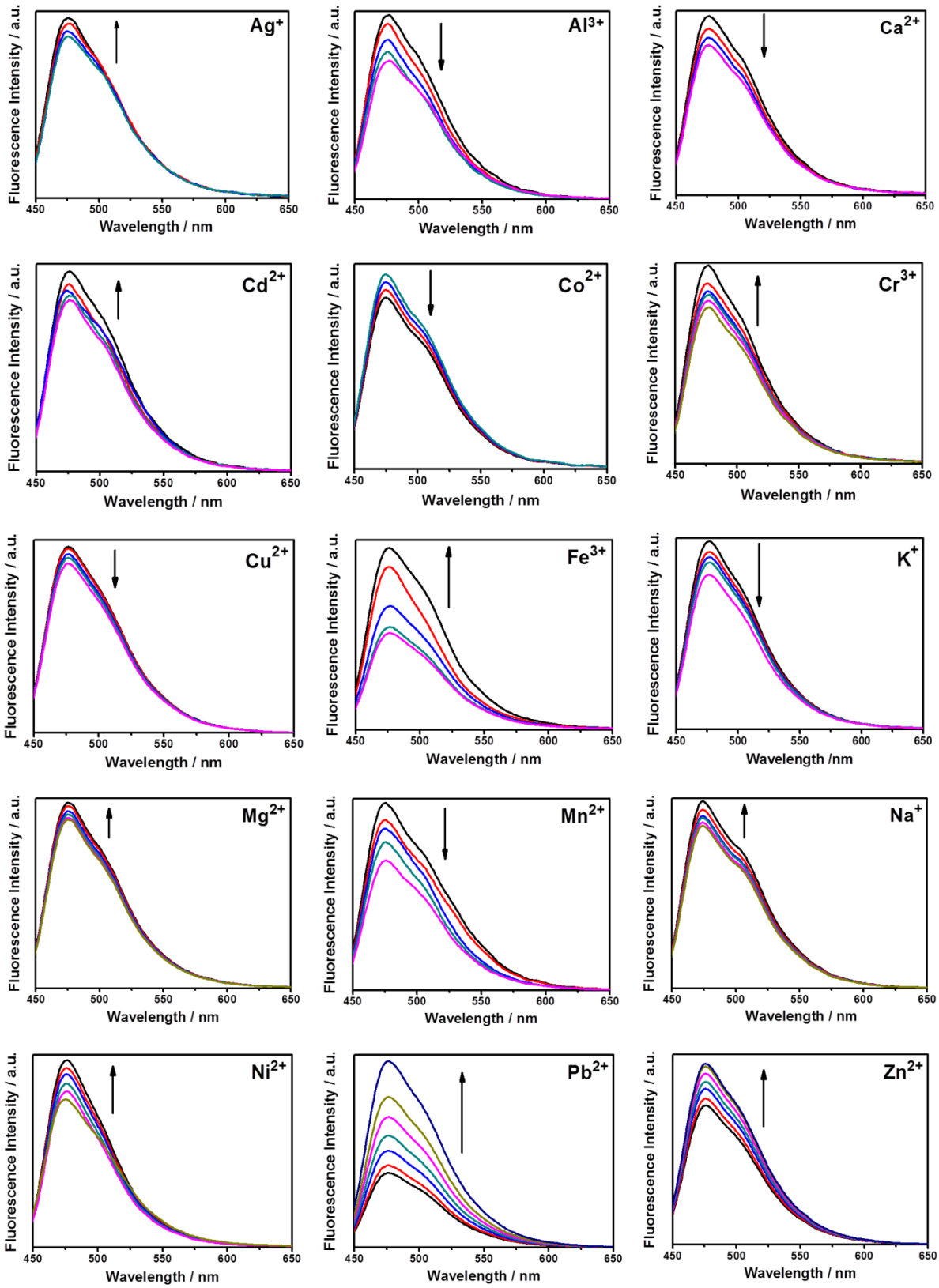


Fig. S9 Fluorescence titration spectra of the receptor with different guest cations in $CH_3CN–H_2O$ (4:1, v/v, pH = 7.2).

12. Effect of pH:

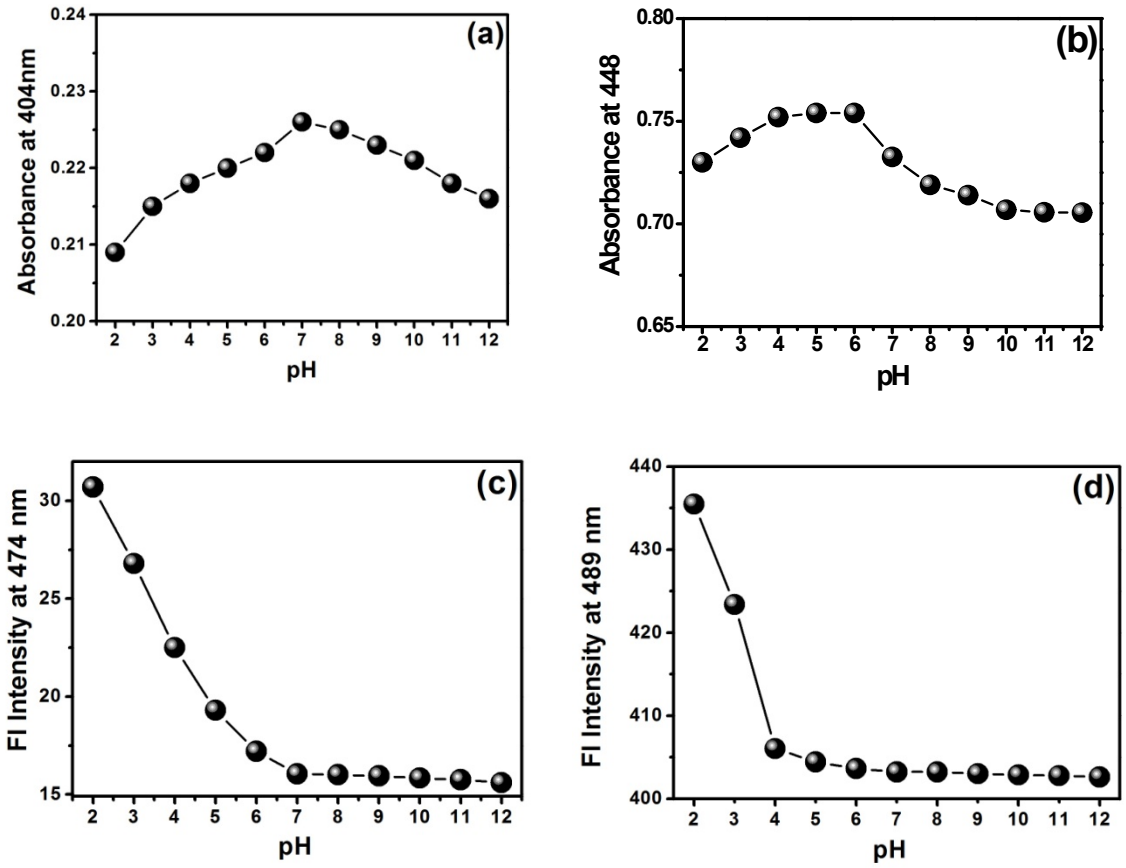


Fig. S10 (a) Effect of pH on the absorbance of the probe **DEAS–BPH** at 404 nm, (b) effect of pH on the absorbance at 448 nm for the complex of **DEAS–BPH** with Hg^{2+} in the pH range of 2.0–12.0 in $CH_3CN–H_2O$ (4:1, v/v), (c) fluorescence response of the probe **DEAS–BPH** at 474 nm, (d) fluorescence response of the complex of **DEAS–BPH** with Hg^{2+} at 489 nm as a function of pH (2.0–12.0) in $CH_3CN–H_2O$ (4:1, v/v). pH is adjusted by using aqueous solutions of 1 M HCl or 1 M NaOH.

The pKa value for the probe is calculated according to the reference – G. K. Vegesna, J. Janjanam, J. Bi, F.-T. Luo, J. Zhang, C. Olds, A. Tiwari and H. Liu, *J. Mater. Chem. B*, 2014, **2**, 4500.

The calculated pKa value is 7.1.

13. General procedure for drawing Job plot by UV–vis method:

Job plots were drawn by plotting ΔAX_{host} vs X_{host} (Fig. 7a, ΔA = change of intensity of the absorbance spectrum during titration and X_{host} is the mole fraction of the host in each case, respectively) and ΔAX_{metal} vs X_{metal} (Fig. 7b, ΔA = change of intensity of the absorbance spectrum during titration and X_{metal} is the mole fraction of the Hg^{2+} in each case, respectively).

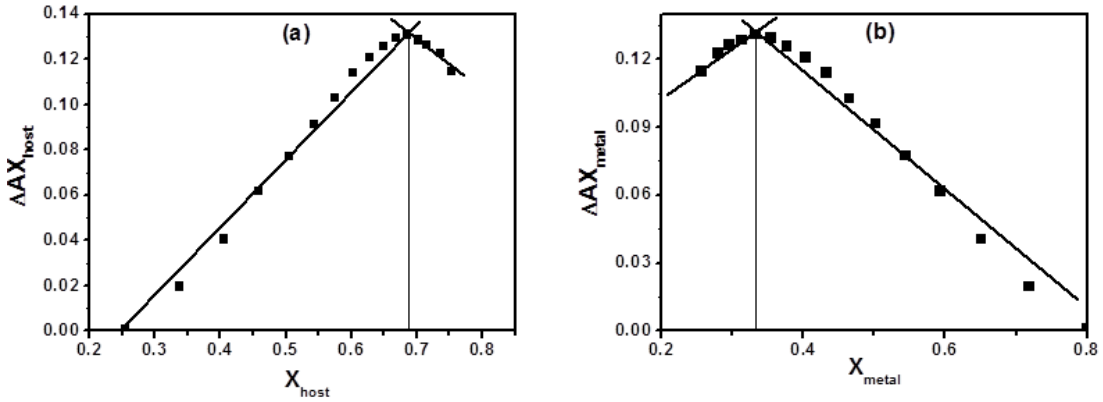


Fig. S11 Job's plot diagram of receptor for Hg^{2+} ion

14. Determination of Association constant:

By UV-vis method: The association constant (K_a) was calculated according to the Benesi-Hildebrand equation for 2:1 complex formation stated below.

$$1/(A - A_0) = 1/\{K_a(A_{max} - A_0)[Hg^{2+}]^2\} + 1/[A_{max} - A_0]$$

Here, A_0 is the absorbance of receptor in the absence of guest, A is the absorbance recorded in the presence of added guest and A_{max} is absorbance in presence of added $[Hg^{2+}]_{max}$. The association constant (K_a) could be determined from the slope of the straight line of the plot of $1/(A–A_0)$ against $1/[Hg^{2+}]^2$ and is found to be 1.15×10^{10} M^{-2}.

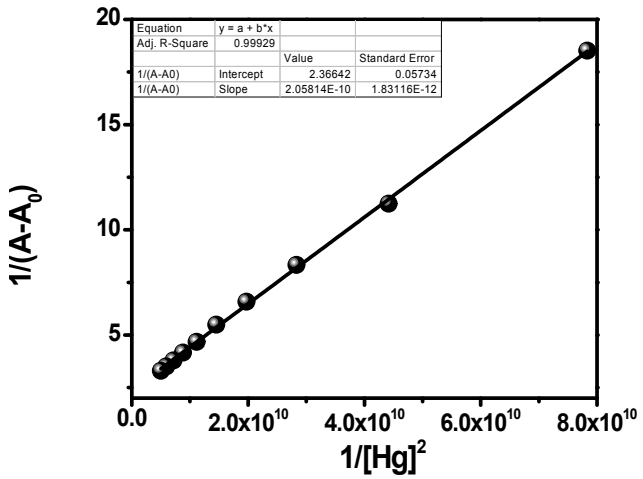


Fig. S12a: Benesi-Hildebrand plot from absorption titration data of receptor (20 μM) with Hg^{2+}.

By fluorescence method: The association constant (^{K_a}) value of Hg^{2+} with receptor has been determined from the emission intensity data following the modified Benesi–Hildebrand equation,

$$^{1}/\Delta I = {}^{1}/\Delta I_{max} + \{(^{1}/K_a[Hg^{2+}]^2) \times (^{1}/\Delta I_{max})\}$$

Here $\Delta I = {}^{I_A - I_{A_0}}$ and $\Delta I_{max} = {}^{I_{A_{max}} - I_{A_0}}$; where $^{I_{A_0}}$, ^{I_A} and $^{I_{A_{max}}}$ are the emission intensities of receptor considered in the absence of Hg^{2+}, at an intermediate Hg^{2+} concentration, and at a concentration of complete saturation, respectively. From the plot of $^{1/\Delta I}$ against $^{1/[Hg^{2+}]^2}$, the value of ^{K_a} has been determined from the slope. The association constant (^{K_a}) as determined by fluorescence titration method for the receptor with Hg^{2+} is found to be 1.36×10^{11} M^{-2}.

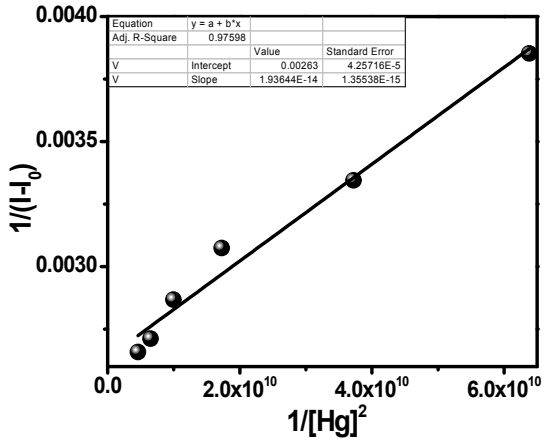


Fig. S12b: Benesi-Hildebrand plot from fluorescence titration data of receptor (20 μM) with Hg^{2+}.

15. Determination of detection limit:

Detection Limit of **DEAS–BPH** for Hg^{2+} was determined from the following equation

$$DL = (K \times SD)/S$$

Where K = 2 or 3 (we take 3 in this case); SD is the standard deviation of the blank solution; S is the slope of the calibration curve.

For UV–vis:

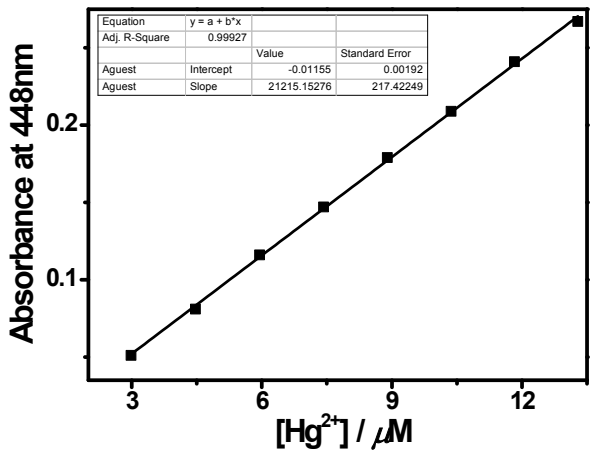


Fig. S13a

From the graph, we got *SD* = 0.027 and *S*= 2.1215× 10^4.

Thus using the formula we get the Detection limit = 3.82 × 10^{-6} M i.e. **DEAS–BPH** can detect Hg^{2+} in this minimum concentration through UV–vis method.

For Fluorescence:

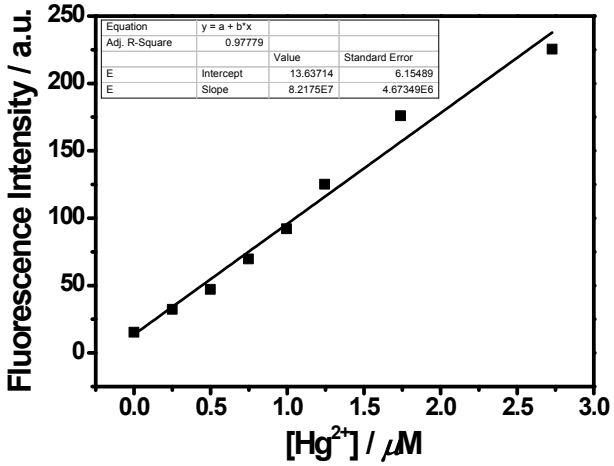


Fig. S13b

From the graph, we got *S* = 8.2175×$10^7$and *SD*=15.26.

Thus using the formula we get the Detection Limit = 5.57×10^{-7} M i.e. **DEAS–BPH** can detect Hg^{2+} in this minimum concentration through fluorescence method.

16. Theoretical and computational study:

Table S1: Selected optimized geometrical parameters for **DEAS–BPH** and the complex with Hg^{2+} in the ground state calculated at B3LYP levels

DEAS–BPH			
Bond	**Bond Distance (Å)**	**Bond**	**Bond Angle (°)**
14O–15H	0.9686	15H–14O–5C	108.977
14O–5C	1.3592	13N–12N–10C	110.774
12N–10C	1.2987	12N–10C–11H	118.386
12O–5C	1.359	12N–10C–4C	126.708

DEAS–BPH& Hg^{2+}complex			
Bond	**Bond Distance (Å)**	**Bond**	**Bond Angle (°)**
105Hg–14O	2.227	12N–105Hg–14O	89.384
105Hg–66O	2.382	64N–105Hg–66O	80.648
105Hg–12N	2.276	66O–105Hg–14O	106.157
105Hg–64N	2.508	64N–105Hg–12N	164.449
14O–5C	1.359	105Hg–14O–5C	127.958
12N–10C	1.369	13N–12N–10C	112.074

	12N–10C–4C	132.064

Table S2: Dominant electronic transitions with oscillator strengths of the **DEAS–BPH** and Hg^{2+} complex calculated by TDDFT method

Excited State	Excitation Energy (eV)	Wavelenth λ (nm)	Oscillator Strength (f)	Key Transitions
1	2.311	536.59	0.0124	HOMO → LUMO (99%)
2	2.647	468.38	0.3044	HOMO-1 → LUMO (99%)
3	2.940	421.80	0.2398	HOMO → LUMO+1 (96%)
4	2.858	433.77	0.8575	HOMO → LUMO+3 (80%)

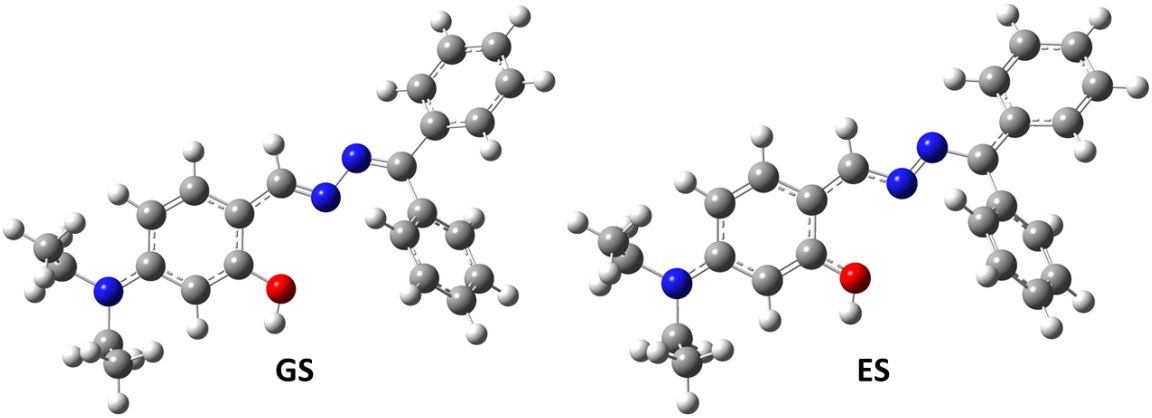


Fig. S14 Optimized structures of the receptor by DFT/B3LYP/6-31+G(d,p) method.

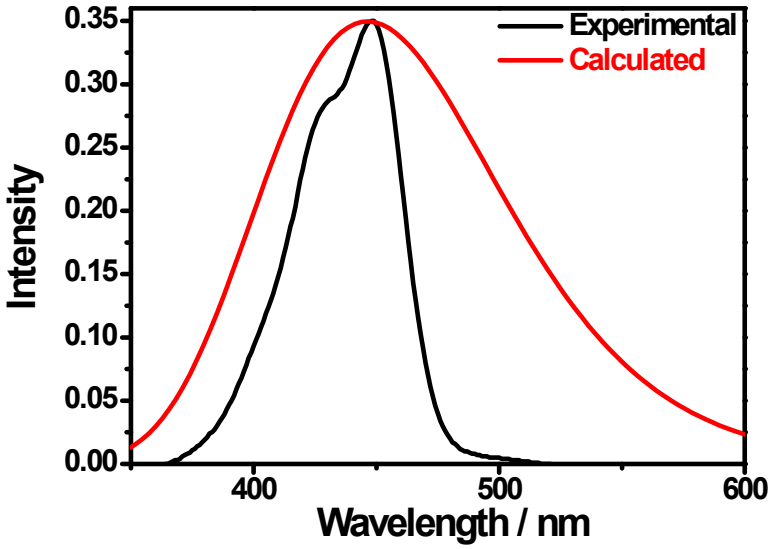


Fig. S15 UV-vis spectrum of [Hg(**DEAS–BPH**)$_2$] by TD-DFT method in CH_3CN.

Molecular orbital plots of DEAS–BPH and its complex:

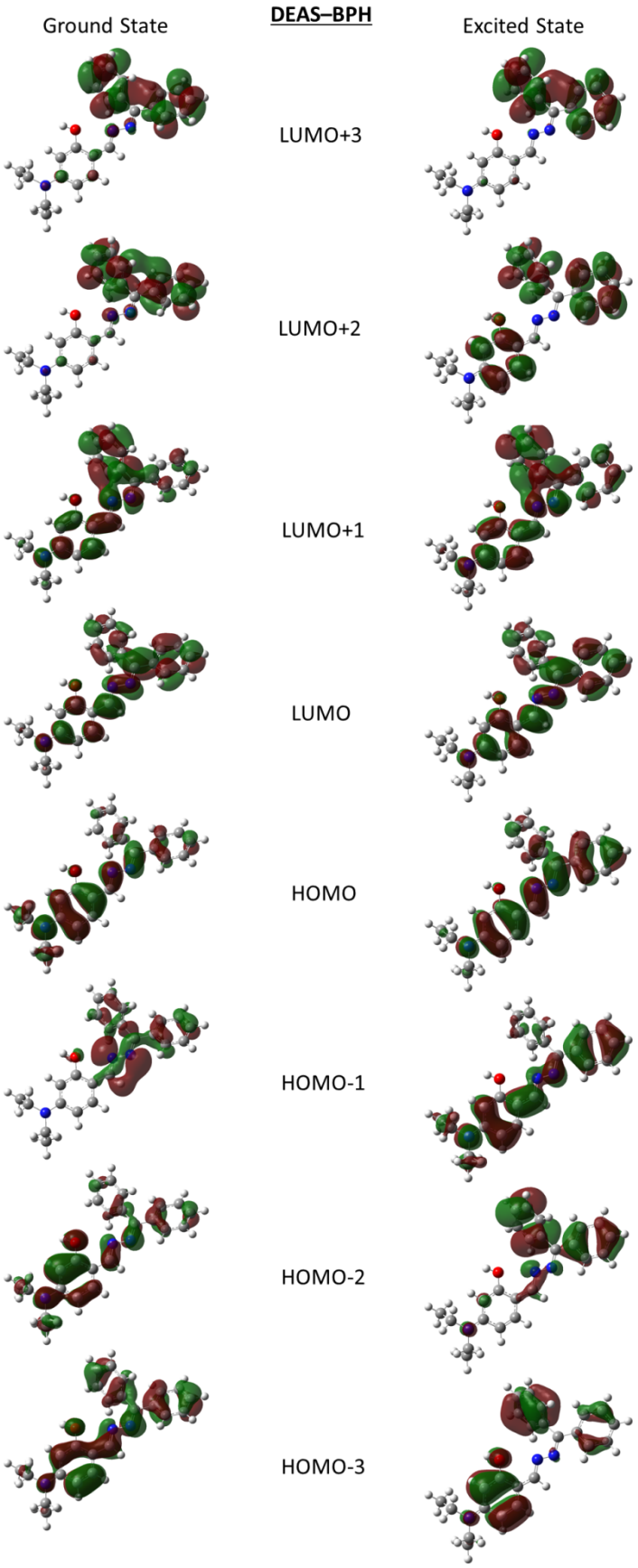


Fig. S16 Molecular Orbital (MO) diagram of the receptor **DEAS–BPH**.

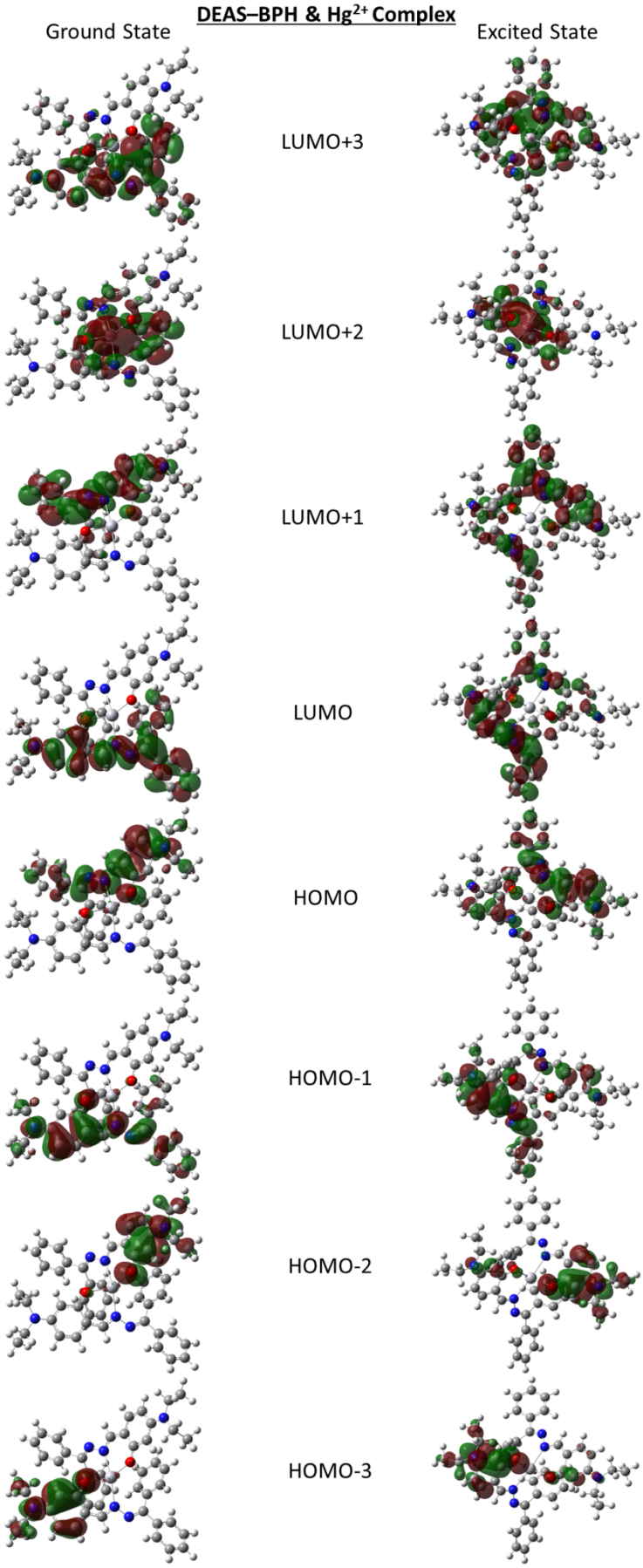


Fig. S17 Molecular Orbital (MO) diagram of the **DEAS–BPH** and Hg^{2+} complex.

Cartesian Coordinates:

Ground State of DEAS–BPH:

ATOM	X	Y	Z
C	4.42733	-0.49003	-0.29192
C	3.86471	-1.75161	0.05130
C	2.49509	-1.91329	0.09786
C	1.57277	-0.87700	-0.17139
C	2.13864	0.38262	-0.50669
C	3.51789	0.56385	-0.55630
H	4.49692	-2.59719	0.28417
H	2.09806	-2.89005	0.36195
H	3.88271	1.55222	-0.80826
C	0.16650	-1.19575	-0.07241
H	-0.05371	-2.24016	0.17988
N	-0.82857	-0.37906	-0.24423
N	-2.04296	-1.04408	-0.10321
O	1.30091	1.41696	-0.78195
H	1.82807	2.20133	-0.99427
C	-3.10092	-0.29596	-0.00392
C	-4.40607	-1.01039	0.03296
C	-4.52492	-2.30257	-0.51399
C	-5.53871	-0.43272	0.63335
C	-5.73416	-2.98966	-0.46269
H	-3.65555	-2.75216	-0.98023
C	-6.74892	-1.12528	0.68818
H	-5.46898	0.55750	1.07009
C	-6.85309	-2.40427	0.13933
H	-5.80802	-3.98190	-0.89833
H	-7.60987	-0.66403	1.16297
H	-7.79665	-2.94050	0.17701
C	-3.09301	1.19605	0.08379
C	-3.88590	1.95772	-0.79001
C	-2.31043	1.86371	1.03976
C	-3.88326	3.35154	-0.72219
H	-4.50032	1.45529	-1.53093

C	-2.32193	3.25563	1.11889
H	-1.69808	1.28642	1.72326
C	-3.10400	4.00425	0.23515
H	-4.49344	3.92557	-1.41321
H	-1.71845	3.75673	1.87004
H	-3.10795	5.08859	0.29484
N	5.78706	-0.30389	-0.38124
C	6.72096	-1.39667	-0.08754
C	6.99760	-1.62499	1.40372
H	7.65779	-1.16360	-0.60039
H	6.34725	-2.31733	-0.54667
H	7.67861	-2.47312	1.52980
H	7.46321	-0.74617	1.85845
H	6.07729	-1.84426	1.95238
C	6.35569	1.01164	-0.69263
C	6.42650	1.98063	0.49482
H	5.78681	1.46154	-1.51334
H	7.36205	0.84128	-1.08354
H	6.83722	2.94113	0.16672
H	5.43723	2.16365	0.92366
H	7.07160	1.58796	1.28567

Excited State of DEAS–BPH:

ATOM	X	Y	Z
C	4.42733	-0.49003	-0.29192
C	3.86471	-1.75161	0.05130
C	2.49509	-1.91329	0.09786
C	1.57277	-0.87700	-0.17139
C	2.13864	0.38262	-0.50669
C	3.51789	0.56385	-0.55630
H	4.49692	-2.59719	0.28417
H	2.09806	-2.89005	0.36195
H	3.88271	1.55222	-0.80826
C	0.16650	-1.19575	-0.07241
H	-0.05371	-2.24016	0.17988
N	-0.82857	-0.37906	-0.24423

N	-2.04296	-1.04408	-0.10321
O	1.30091	1.41696	-0.78195
H	1.82807	2.20133	-0.99427
C	-3.10092	-0.29596	-0.00392
C	-4.40607	-1.01039	0.03296
C	-4.52492	-2.30257	-0.51399
C	-5.53871	-0.43272	0.63335
C	-5.73416	-2.98966	-0.46269
H	-3.65555	-2.75216	-0.98023
C	-6.74892	-1.12528	0.68818
H	-5.46898	0.55750	1.07009
C	-6.85309	-2.40427	0.13933
H	-5.80802	-3.98190	-0.89833
H	-7.60987	-0.66403	1.16297
H	-7.79665	-2.94050	0.17701
C	-3.09301	1.19605	0.08379
C	-3.88590	1.95772	-0.79001
C	-2.31043	1.86371	1.03976
C	-3.88326	3.35154	-0.72219
H	-4.50032	1.45529	-1.53093
C	-2.32193	3.25563	1.11889
H	-1.69808	1.28642	1.72326
C	-3.10400	4.00425	0.23515
H	-4.49344	3.92557	-1.41321
H	-1.71845	3.75673	1.87004
H	-3.10795	5.08859	0.29484
N	5.78706	-0.30389	-0.38124
C	6.72096	-1.39667	-0.08754
C	6.99760	-1.62499	1.40372
H	7.65779	-1.16360	-0.60039
H	6.34725	-2.31733	-0.54667
H	7.67861	-2.47312	1.52980
H	7.46321	-0.74617	1.85845
H	6.07729	-1.84426	1.95238
C	6.35569	1.01164	-0.69263
C	6.42650	1.98063	0.49482

H	5.78681	1.46154	-1.51334
H	7.36205	0.84128	-1.08354
H	6.83722	2.94113	0.16672
H	5.43723	2.16365	0.92366
H	7.07160	1.58796	1.28567

Ground State of DEAS–BPH & Hg^{2+} Complex:

ATOM	X	Y	Z
C	4.42733	-0.49003	-0.29192
C	3.86471	-1.75161	0.05130
C	2.49509	-1.91329	0.09786
C	1.57277	-0.87700	-0.17139
C	2.13864	0.38262	-0.50669
C	3.51789	0.56385	-0.55630
H	4.49692	-2.59719	0.28417
H	2.09806	-2.89005	0.36195
H	3.88271	1.55222	-0.80826
C	0.16650	-1.19575	-0.07241
H	-0.05371	-2.24016	0.17988
N	-0.82857	-0.37906	-0.24423
N	-2.04296	-1.04408	-0.10321
O	1.30091	1.41696	-0.78195
C	-3.10092	-0.29596	-0.00392
C	-4.40607	-1.01039	0.03296
C	-4.52492	-2.30257	-0.51399
C	-5.53871	-0.43272	0.63335
C	-5.73416	-2.98966	-0.46269
H	-3.65555	-2.75216	-0.98023
C	-6.74892	-1.12528	0.68818
H	-5.46898	0.55750	1.07009
C	-6.85309	-2.40427	0.13933
H	-5.80802	-3.98190	-0.89833
H	-7.60987	-0.66403	1.16297
H	-7.79665	-2.94050	0.17701
C	-3.09301	1.19605	0.08379
C	-3.88590	1.95772	-0.79001

C	-2.31043	1.86371	1.03976
C	-3.88326	3.35154	-0.72219
H	-4.50032	1.45529	-1.53093
C	-2.32193	3.25563	1.11889
H	-1.69808	1.28642	1.72326
C	-3.10400	4.00425	0.23515
H	-4.49344	3.92557	-1.41321
H	-1.71845	3.75673	1.87004
H	-3.10795	5.08859	0.29484
N	5.78706	-0.30389	-0.38124
C	6.72096	-1.39667	-0.08754
C	6.99760	-1.62499	1.40372
H	7.65779	-1.16360	-0.60039
H	6.34725	-2.31733	-0.54667
H	7.67861	-2.47312	1.52980
H	7.46321	-0.74617	1.85845
H	6.07729	-1.84426	1.95238
C	6.35569	1.01164	-0.69263
C	6.42650	1.98063	0.49482
H	5.78681	1.46154	-1.51334
H	7.36205	0.84128	-1.08354
H	6.83722	2.94113	0.16672
H	5.43723	2.16365	0.92366
H	7.07160	1.58796	1.28567
C	-3.52650	7.80755	-3.96098
C	-2.90254	8.90361	-4.62070
C	-1.54140	9.10040	-4.50783
C	-0.68818	8.26776	-3.74902
C	-1.31619	7.17888	-3.08630
C	-2.68820	6.96681	-3.18764
H	-3.48155	9.59815	-5.21341
H	-1.09619	9.94614	-5.02547
H	-3.10419	6.12425	-2.64867
C	0.71641	8.60703	-3.71723
H	0.99453	9.47975	-4.32051
N	1.64852	7.99299	-3.05330

N	2.88905	8.57865	-3.28771
O	-0.54557	6.33935	-2.34552
C	3.85449	8.21884	-2.49568
C	5.20248	8.76027	-2.81966
C	5.50547	9.17578	-4.13059
C	6.19234	8.89669	-1.83042
C	6.75445	9.70669	-4.43913
H	4.74695	9.07090	-4.89802
C	7.44231	9.43386	-2.14075
H	5.97896	8.59266	-0.81151
C	7.72987	9.83883	-3.44505
H	6.97195	10.01303	-5.45826
H	8.19038	9.53744	-1.36032
H	8.70475	10.25135	-3.68735
C	3.70237	7.32808	-1.30519
C	4.53008	6.20336	-1.15604
C	2.74683	7.5988	-0.31234
C	4.39447	5.36062	-0.05208
H	5.27710	5.98422	-1.91291
C	2.62392	6.76653	0.79944
H	2.10551	8.46703	-0.41374
C	3.44338	5.64211	0.93075
H	5.03491	4.48863	0.04177
H	1.88650	6.99481	1.56339
H	3.34293	4.99206	1.79486
N	-4.87455	7.56273	-4.08067
C	-5.73732	8.44987	-4.86884
C	-6.18219	9.72670	-4.14477
H	-6.61733	7.86834	-5.15586
H	-5.22703	8.70484	-5.80301
H	-6.79542	10.33906	-4.81407
H	-6.77894	9.49136	-3.25911
H	-5.32432	10.3261	-3.82717
C	-5.51335	6.45616	-3.36071
C	-5.82255	6.74053	-1.88507
H	-4.88593	5.56281	-3.44936

H	-6.44178	6.22402	-3.88865
H	-6.27159	5.85564	-1.42222
H	-4.91702	6.99288	-1.32615
H	-6.52651	7.57111	-1.78313
Hg	0.24176	3.40339	-1.12333

Excited State of DEAS–BPH & Hg^{2+} Complex:

ATOM	X	Y	Z
C	4.75957576	-2.61286690	-2.06024641
C	4.86646751	-3.42839722	-0.87047186
C	3.94425950	-3.28794667	0.14576132
C	2.85734834	-2.34782888	0.10975915
C	2.74624311	-1.51014736	-1.07974481
C	3.70956295	-1.67269265	-2.11688034
H	5.65990951	-4.15800475	-0.76523657
H	4.03952756	-3.92170846	1.02715858
H	3.57356468	-1.01927201	-2.96992545
C	1.99694325	-2.36850633	1.24370411
H	2.25825213	-3.11181029	2.00143052
N	0.90475464	-1.65078317	1.56341394
N	0.38913228	-2.13131896	2.78746654
O	1.80110039	-0.59974921	-1.23828933
C	-0.67972451	-1.62702668	3.35213592
C	-1.12925963	-2.30953332	4.60600961
C	-0.63902277	-3.59823683	4.94047444
C	-2.04151306	-1.68487982	5.49085971
C	-1.04660837	-4.23627461	6.12088677
H	0.05757029	-4.07803800	4.26125287
C	-2.44616081	-2.32538080	6.67622083
H	-2.42960860	-0.69749550	5.25957033
C	-1.95277564	-3.60304528	6.99773786
H	-0.66445972	-5.22660250	6.35849222
H	-3.14334664	-1.82685000	7.34576017
H	-2.26915474	-4.09944305	7.91227347
C	-1.48068871	-0.44734773	2.87906814
C	-2.80614227	-0.62945796	2.42229596

C	-0.96291721	0.86570851	2.97658057
C	-3.60007688	0.47635221	2.07548339
H	-3.20553413	-1.63554311	2.33050317
C	-1.76595706	1.97384563	2.63985933
H	0.04843192	1.02110404	3.34268412
C	-3.08544797	1.78234684	2.19245187
H	-4.61053506	0.31921944	1.70748024
H	-1.35918138	2.97764078	2.72389274
H	-3.70011071	2.63827487	1.92544712
N	5.65976134	-2.77453658	-3.11179097
C	6.78508317	-3.72734584	-3.02666285
C	8.00286099	-3.21596867	-2.22104421
H	7.10409905	-3.95160694	-4.05173847
H	6.43197155	-4.67579060	-2.60238999
H	8.78353470	-3.98829111	-2.18366134
H	8.43194585	-2.31875446	-2.68264015
H	7.71942212	-2.96426800	-1.19290767
C	5.55591073	-1.94500437	-4.32953033
C	6.18037709	-0.53562979	-4.20052129
H	4.50032371	-1.85694390	-4.61438825
H	6.05309429	-2.48598865	-5.14429098
H	6.03154805	0.02947975	-5.13065610
H	5.71831391	0.02617125	-3.38158229
H	7.25801390	-0.59783711	-4.00695807
C	-4.55647429	-0.92341898	-3.32630485
C	-4.50583942	0.45339380	-3.76661259
C	-3.58366334	1.31857006	-3.21603678
C	-2.64100533	0.93698827	-2.19880837
C	-2.69558836	-0.44429638	-1.73478294
C	-3.65897676	-1.31940066	-2.31340854
H	-5.18225769	0.82002305	-4.52899256
H	-3.56136912	2.34939231	-3.56869889
H	-3.64976952	-2.32820163	-1.91929191
C	-1.78443010	1.98013604	-1.74899958
H	-1.97734759	2.95202619	-2.20981993
N	-0.77314257	2.01895778	-0.85534945

N	-0.33848211	3.36161884	-0.76218714
O	-1.90887609	-0.92141778	-0.78597682
C	0.62457606	3.79461408	0.01367399
C	0.82366800	5.28237256	-0.01763439
C	-0.23282740	6.14068509	-0.41359573
C	2.06999883	5.86140873	0.32368795
C	-0.04874502	7.53079673	-0.46344832
H	-1.18599058	5.69673443	-0.68137067
C	2.25493254	7.25487588	0.26743035
H	2.89861657	5.22516408	0.62038472
C	1.19750628	8.09705602	-0.12333547
H	-0.87280389	8.17421430	-0.76392781
H	3.22255691	7.67964551	0.52469482
H	1.33953641	9.17463939	-0.16203895
C	1.52736996	3.00072526	0.90989574
C	2.35210764	1.97084316	0.40535086
C	1.62310121	3.34116885	2.28198069
C	3.24454338	1.28883051	1.25858874
H	2.32282934	1.70682946	-0.64780899
C	2.50858184	2.65844928	3.13137624
H	1.01425678	4.15216544	2.67467864
C	3.32517278	1.62766428	2.62051982
H	3.86705010	0.49719418	0.85230535
H	2.56923118	2.93223107	4.18220653
H	4.01351278	1.09943004	3.27568002
N	-5.45497996	-1.81884942	-3.90460243
C	-6.43209173	-1.38412598	-4.92308545
C	-7.68787575	-0.68405794	-4.35163953
H	-6.74256219	-2.27480193	-5.48292512
H	-5.93870200	-0.72470067	-5.64799990
H	-8.35014896	-0.36675337	-5.16903979
H	-8.25192790	-1.35940049	-3.69756796
H	-7.41374283	0.20171766	-3.76764495
C	-5.51007118	-3.22594290	-3.46010211
C	-6.32734728	-3.45984477	-2.16747119
H	-4.48743406	-3.59835580	-3.32304201

H	-5.94875827	-3.81543176	-4.27484487
H	-6.28199230	-4.51875723	-1.87859937
H	-5.93178337	-2.86191333	-1.33937149
H	-7.38052854	-3.18990897	-2.31135145
Hg	-0.00193655	-0.04225583	0.07802175

17. Reversibility Study:

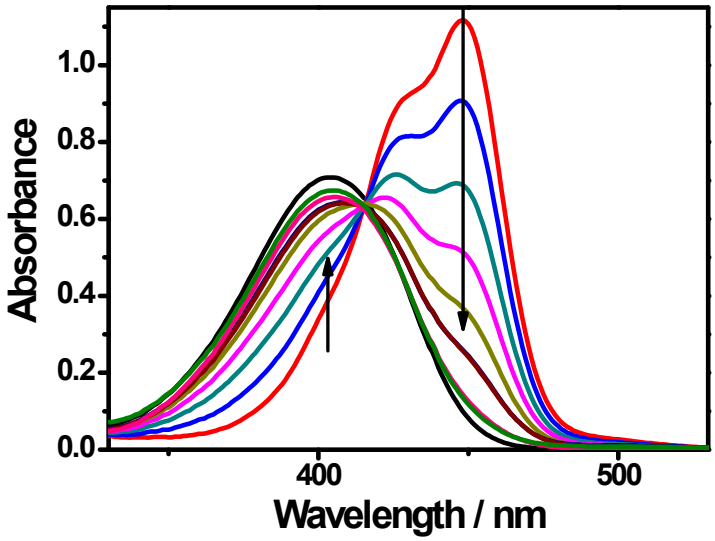


Fig. S18 Absorption titration spectra of **DEAS–BPH** (6 μM) containing Hg^{2+} (20 μM) upon increasing the concentration of the Na_2EDTA solution (0 to 10 equivalents).

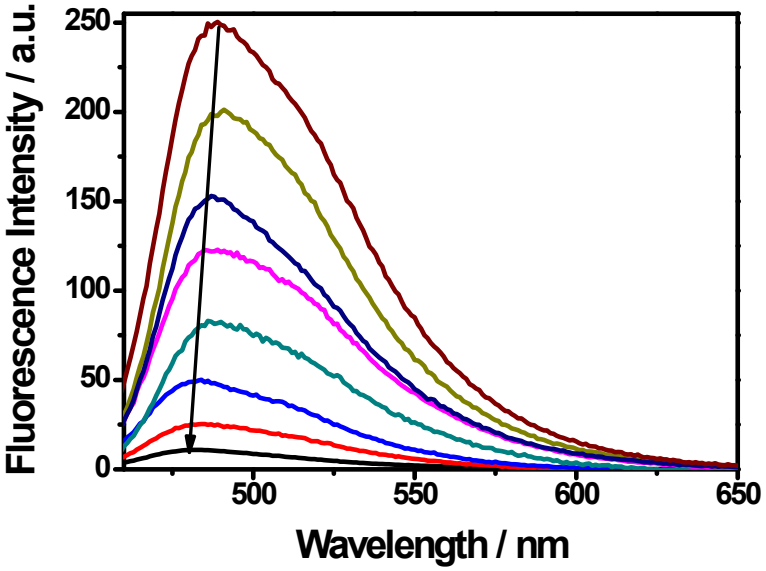


Fig. S19 Fluorescence titration spectra of **DEAS–BPH** (6 μM) containing Hg^{2+} (20 μM) upon increasing the concentration of Na_2EDTA (0 to 10 equivalents), λ_{ex} = 505 nm.