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A novel ditopic chemosensor for cadmium and fluoride and its possible application as a pH sensor

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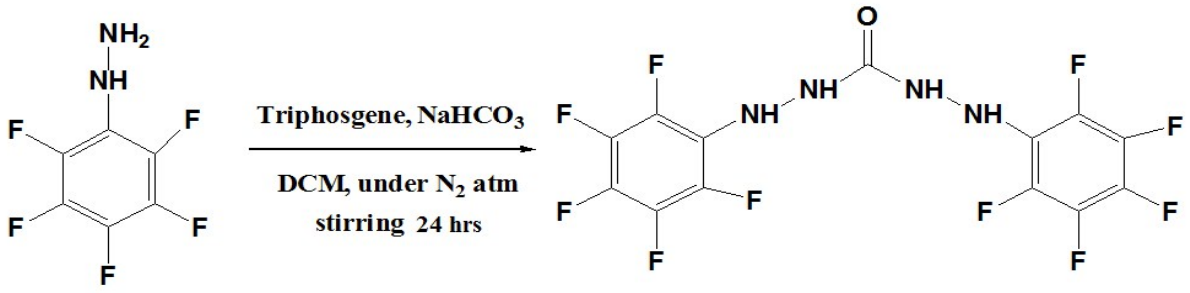

Scheme S1 Synthesis of **BPC**.

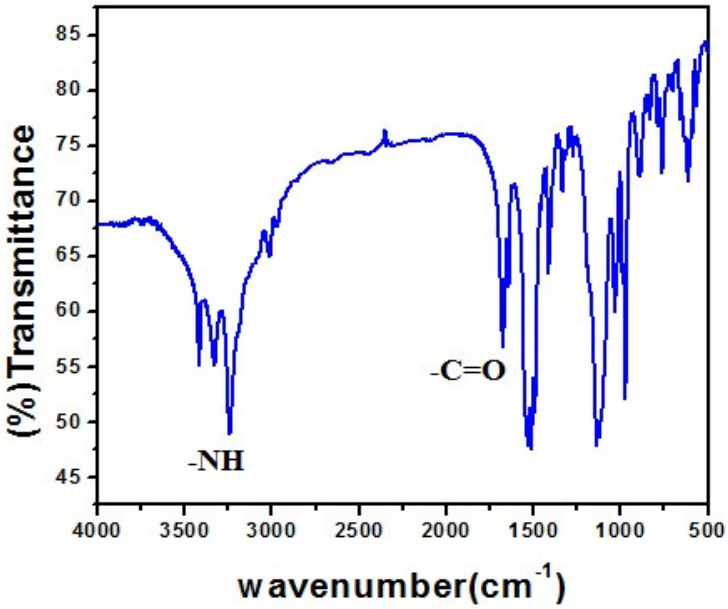

Fig. S1 IR data of **BPC**.

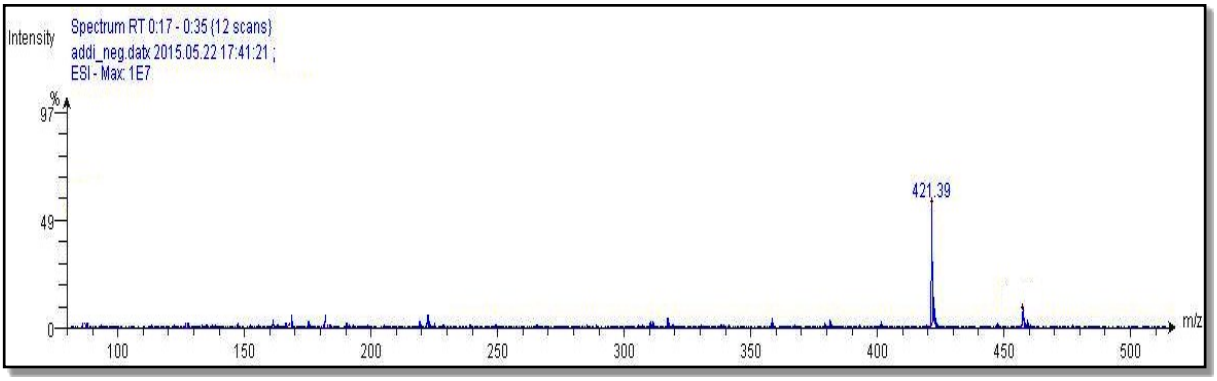

Fig. S2 ESI-Mass data of **BPC**.

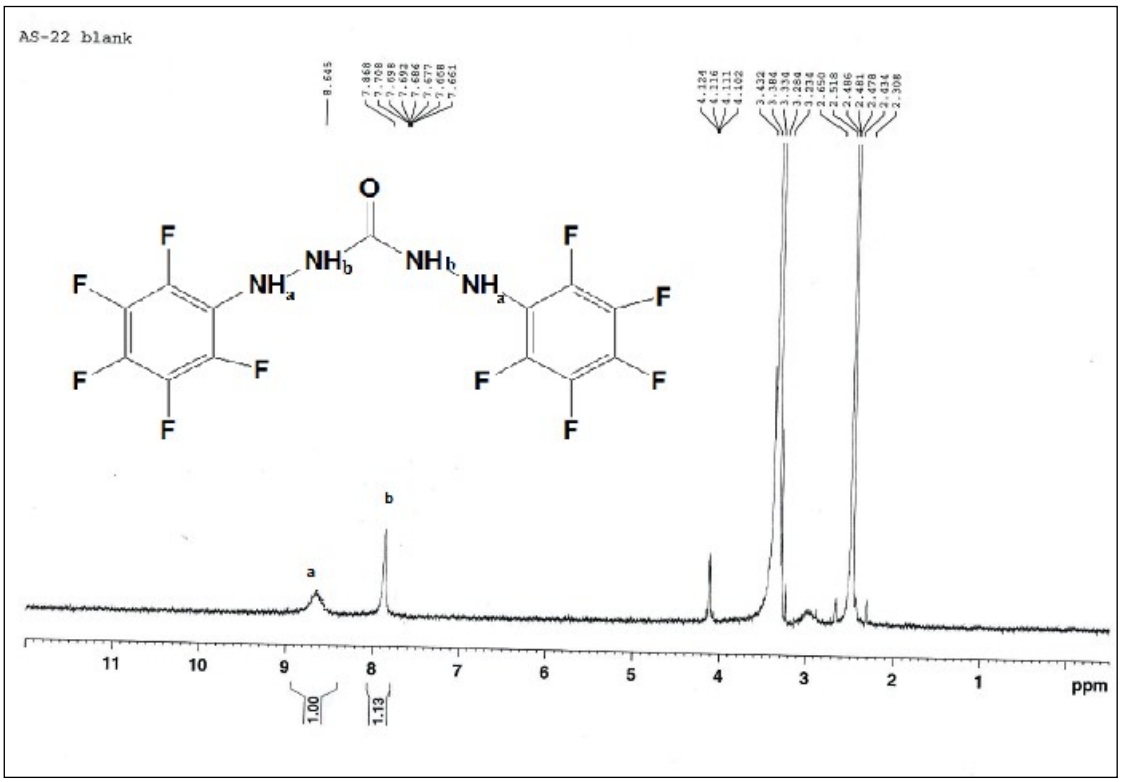

Fig. S3 ^{1}H NMR data of **BPC** in DMSO-d_6.

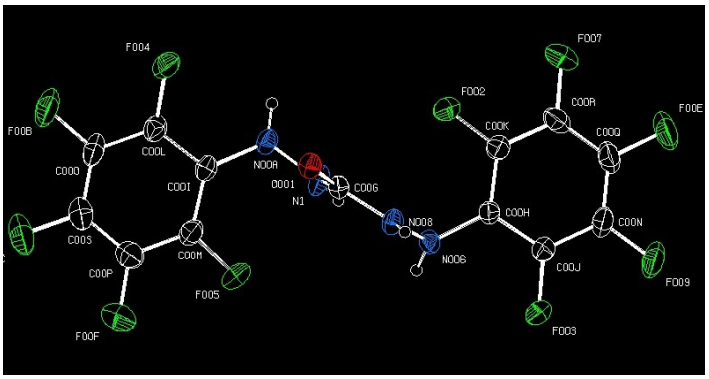

Fig. S4 ORTEP diagram of **BPC** crystal.

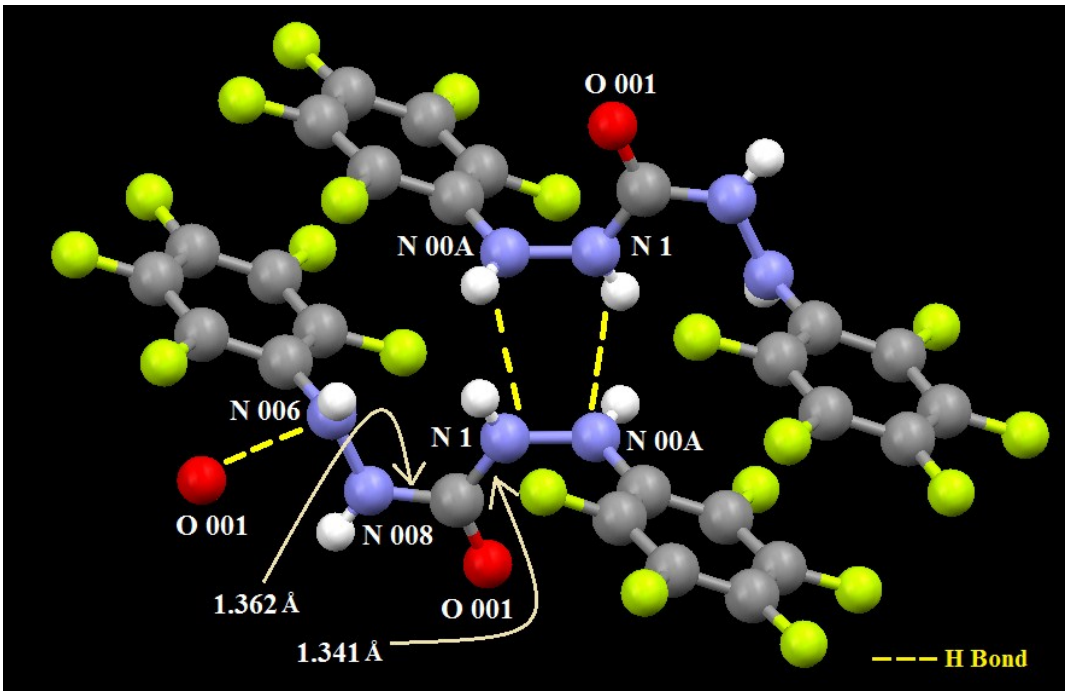

Fig. S5 Intermolecular H-bonding network in **BPC** molecule.

Table S1 Crystallographic data of **BPC**.

Crystal Data	
Formula	C13 H4 F10 N4 O
Formula Weight	422.20
Crystal System	monoclinic
Space group	P21/c (No. 14)
a, b, c [Angstrom]	14.6959(10) 7.2819(6) 13.7456(10)
alpha, beta, gamma [deg]	90 94.301(5) 90
V [Ang**3]	1466.83(19)
Z	4
D(calc) [g/cm**3]	1.912
Mu(MoKa) [/mm]	0.212
F(000)	832
Crystal Size [mm]	0.00 x 0.00 x 0.00
Data Collection	
Temperature (K)	296
Radiation [Angstrom]	MoKa 0.71073
Theta Min-Max [Deg]	1.4, 26.6
Dataset	-16: 18 ; -9: 9 ; -16: 17
Tot., Uniq. Data, R(int)	22742, 3056, 0.060
Observed Data [I > 2.0 sigma(I)]	1752
Refinement	
Nref, Npar	3056, 253
R, wR2, S	0.0558, 0.1965, 1.02
w = ^2^(FO^2^)+(0.1077P)^2^+0.3645P] WHERE P=(FO^2^+2FC^2^)/3'	
Max. and Av. Shift/Error	0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-0.43, 0.49

Table S2 Selected bond distances (angstrom) of **BPC**.

F002	-C00K 1.358(3)	N1	-H1 0.8600
F003	-C00J 1.340(3)	N006	-H006 0.8600
F004	-C00L 1.349(4)	N008	-H008 0.8600
F005	-C00M 1.350(4)	N00A	-H00A 0.8600
F007	-C00R 1.340(5)	C00H	-C00K 1.382(4)
F00B	-C00O 1.339(5)	C00I	-C00M 1.391(4)
F00C	-C00S 1.334(4)	C00I	-C00L 1.378(4)
F00E	-C00Q 1.334(4)	C00J	-C00N 1.385(4)
F00F	-C00P 1.340(5)	C00K	-C00R 1.374(4)
O001	-C00G 1.236(4)	C00L	-C00O 1.377(4)
N1	-N00A 1.401(3)	C00M	-C00P 1.386(5)
N1	-C00G 1.341(4)	C00N	-C00Q 1.366(5)
N006	-N008 1.406(3)	C00O	-C00S 1.369(5)
N006	-C00H 1.412(4)	C00P	-C00S 1.365(6)
N008	-C00G 1.362(4)	C00Q	-C00R 1.362(5)
N00A	-C00I 1.408(4)		

Table S3 Selected bond angles (degrees) of **BPC**.

N00A	-N1	-C00G 121.0(2)	F002	-C00K	-C00R 118.8(3)
N008	-N006	-C00H 115.4(2)	F004	-C00L	-C00O 118.8(3)
N006	-N008	-C00G 121.9(2)	C00I	-C00L	-C00O 123.2(3)
N1	-N00A	-C00I 117.2(2)	F004	-C00L	-C00I 117.9(3)
N00A	-N1	-H1 119.00	F005	-C00M	-C00P 116.7(3)
C00G	-N1	-H1 120.00	C00I	-C00M	-C00P 122.4(3)
N008	-N006	-H006 122.00	F005	-C00M	-C00I 120.9(3)
C00H	-N006	-H006 122.00	F009	-C00N	-C00Q 120.6(3)

C00G	-N008	-H008	119.00	C00J -C00N -C00Q	120.1(3)
N006	-N008	-H008	119.00	F009 -C00N -C00J	119.3(3)
C00I	-N00A	-H00A	121.00	F00B -C00O -C00L	119.3(3)
N1	-N00A	-H00A	121.00	F00B -C00O -C00S	120.5(3)
O001	-C00G	-N008	120.7(3)	C00L -C00O -C00S	120.3(3)
N1	-C00G	-N008	115.7(2)	F00F -C00P -C00M	119.2(3)
O001	-C00G	-N1	123.6(3)	F00F -C00P -C00S	120.4(4)
N006	-C00H	-C00J	120.3(2)	C00M -C00P -C00S	120.4(3)
N006	-C00H	-C00K	123.6(3)	F00E -C00Q -C00N	120.6(3)
C00J	-C00H	-C00K	116.0(3)	C00N -C00Q -C00R	119.2(3)
N00A	-C00I	-C00L	119.0(3)	F00E -C00Q -C00R	120.2(3)
N00A	-C00I	-C00M	125.7(3)	F007 -C00R -C00Q	120.4(3)
C00L	-C00I	-C00M	114.9(3)	C00K -C00R -C00Q	120.4(3)
F003	-C00J	-C00N	119.1(3)	F007 -C00R -C00K	119.2(3)
F003	-C00J	-C00H	119.0(3)	F00C -C00S -C00P	120.7(4)
C00H	-C00J	-C00N	121.9(3)	C00O -C00S -C00P	118.7(3)
C00H	-C00K	-C00R	122.3(3)	F00C -C00S -C00O	120.6(3)
F002	-C00K	-C00H	118.9(3)		

Table S4 Hydrogen bonding in **BPC**.

N1	-- H1	.. N006	0.8600	2.3300 2.691(3)	106.00
N1	-- H1	.. N00A	0.8600	2.3600 3.057(3)	139.00 3_666
N006	-- H006	.. O001	0.8600	2.3700 2.913(3)	122.00 2_645
N008	-- H008	.. F005	0.8600	2.2000 2.949(3)	146.00 2_655
N00A	-- H00A	.. O001	0.8600	2.5300 3.014(3)	117.00 3_676

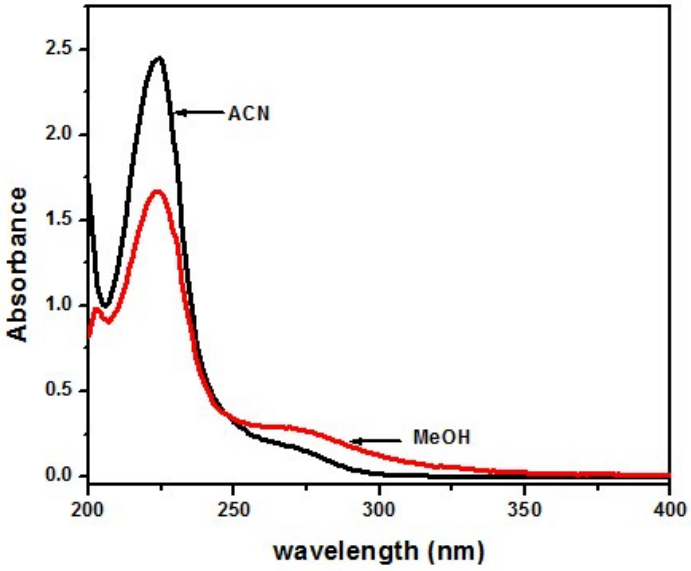

Fig. S6 UV-Spectra of **BPC** (1X 10^{-5} M) in ACN and MeOH.

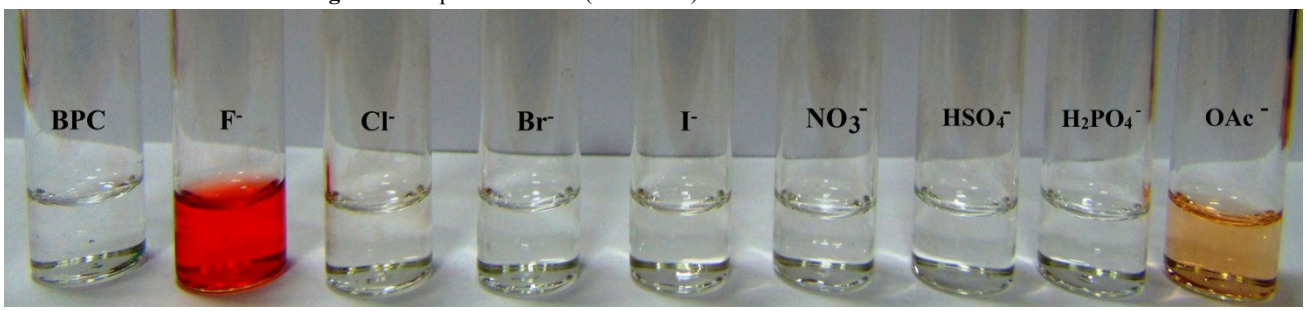

Fig. S7 Solutions of **BPC** in ACN-H_2O (9:1v/v) medium in presence of various anions.

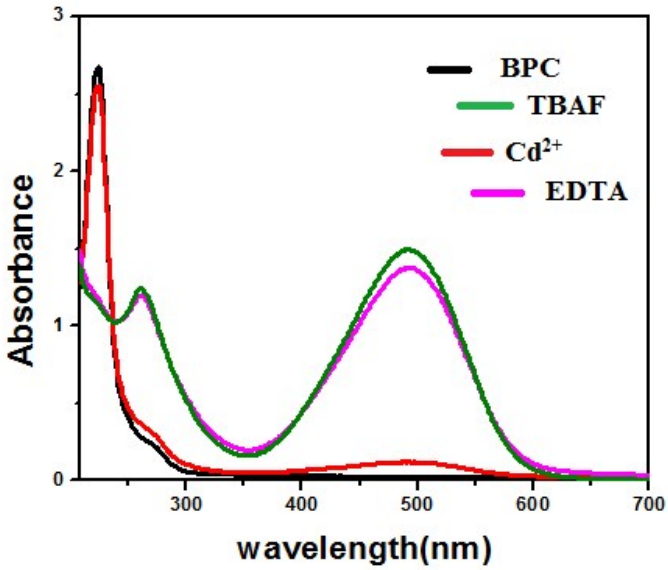

Fig. S8 Reversible UV-Vis response of **BPC** with F^-, Cd^{2+} and EDTA.

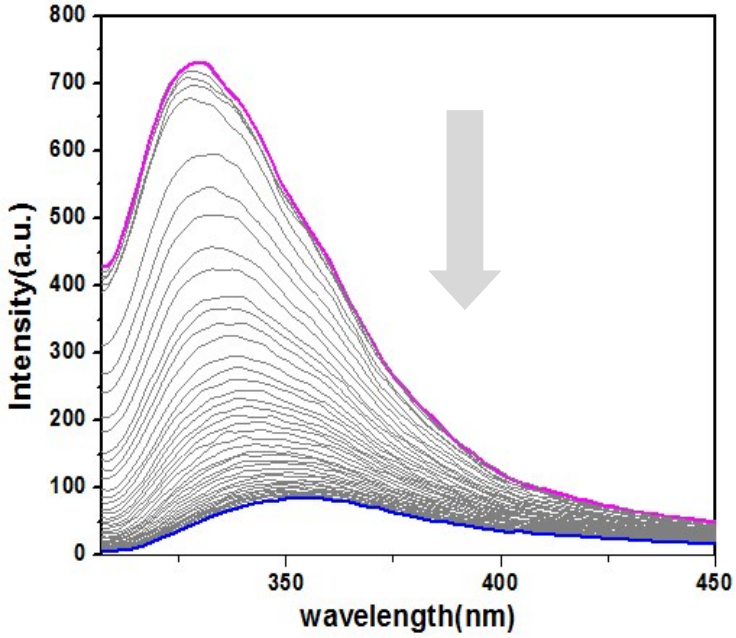

Fig. S9 Emission of **BPC** ($2x10^{-6}$ M) on titrating with Cd^{2+} ($1x\ 10^{-5}$ M) in ACN-H_2O (7:3 v/v) medium.

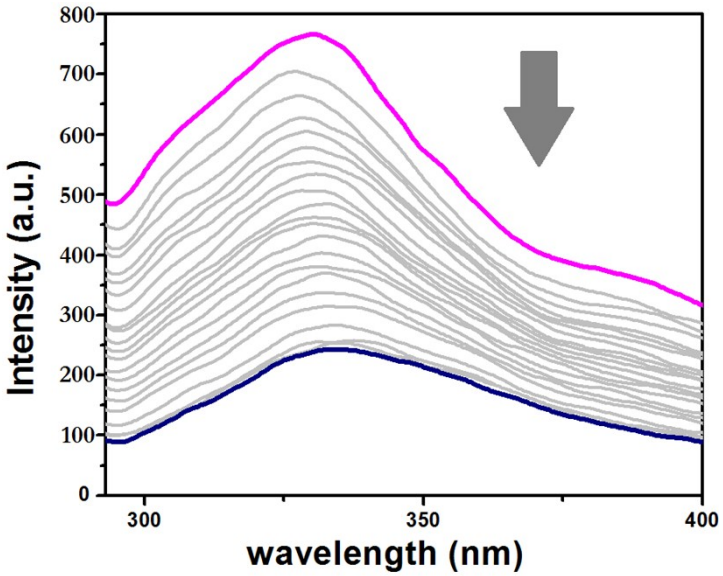

Fig. S10 Emission of **BPC** ($2x10^{-6}$ M) with F^- (0-2eq) in ACN-H_2O (9:1v/v) medium.

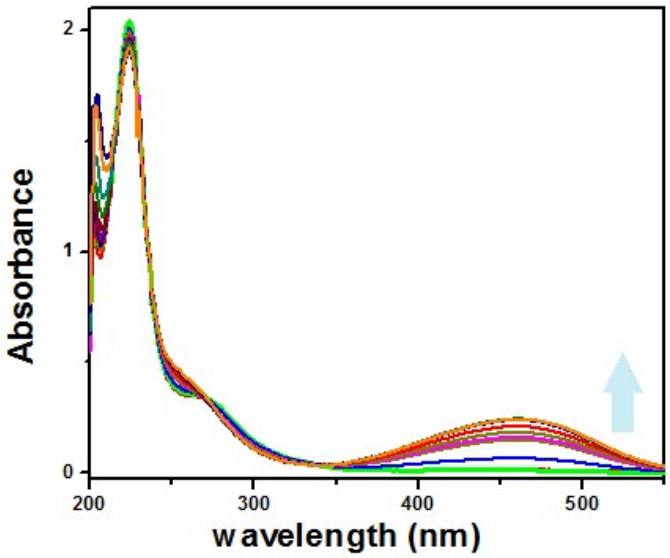

Fig. S11 UV-Vis titration curve of **BPC** with NaOH (10^{-2}M) in methanol.

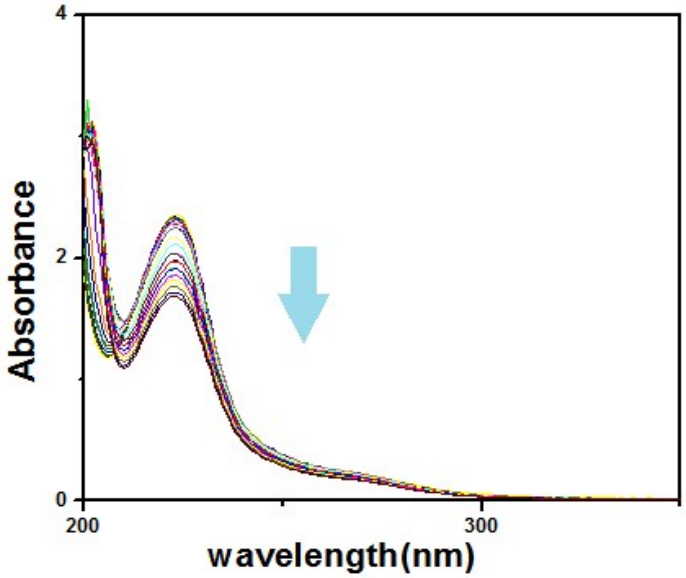

Fig. S12 UV-Vis titration curve of **BPC** with HCl in methanol (pH 1).

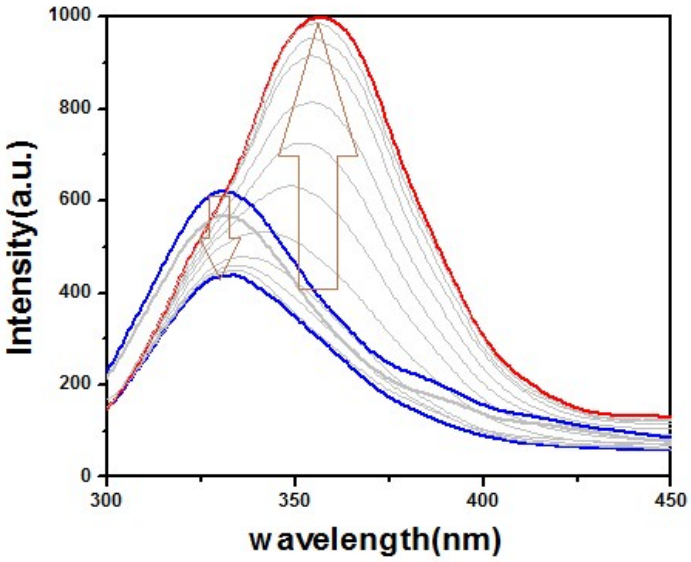

Fig. S13 Emission curve of **BPC** with NaOH (10^{-2}M) in ACN-H_2O medium.

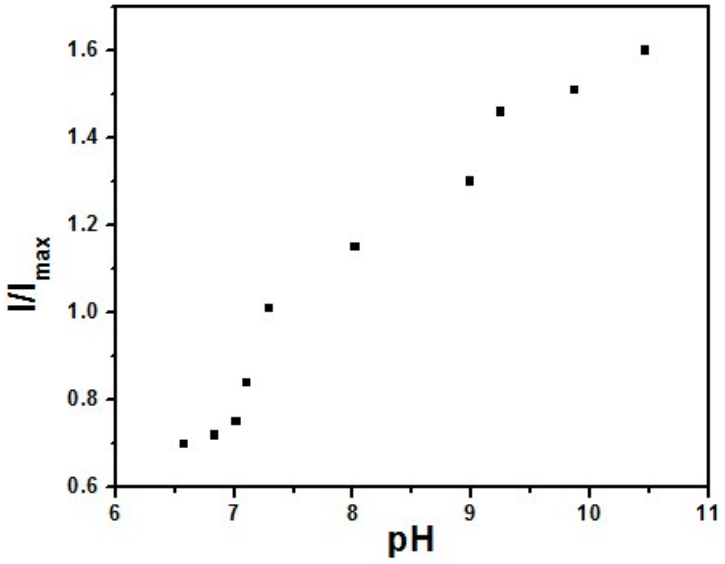

Fig. S14 The ratio of emission intensity as a function of pH.

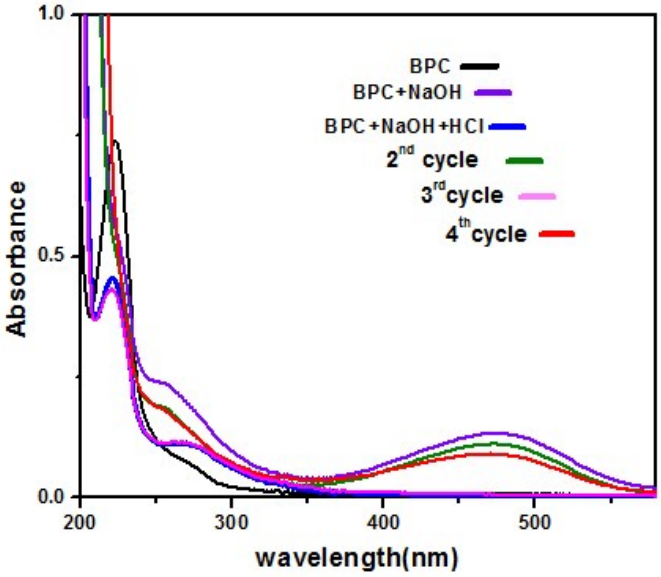

Fig. S15 Reversible UV-Vis response of **BPC** with NaOH and HCl.

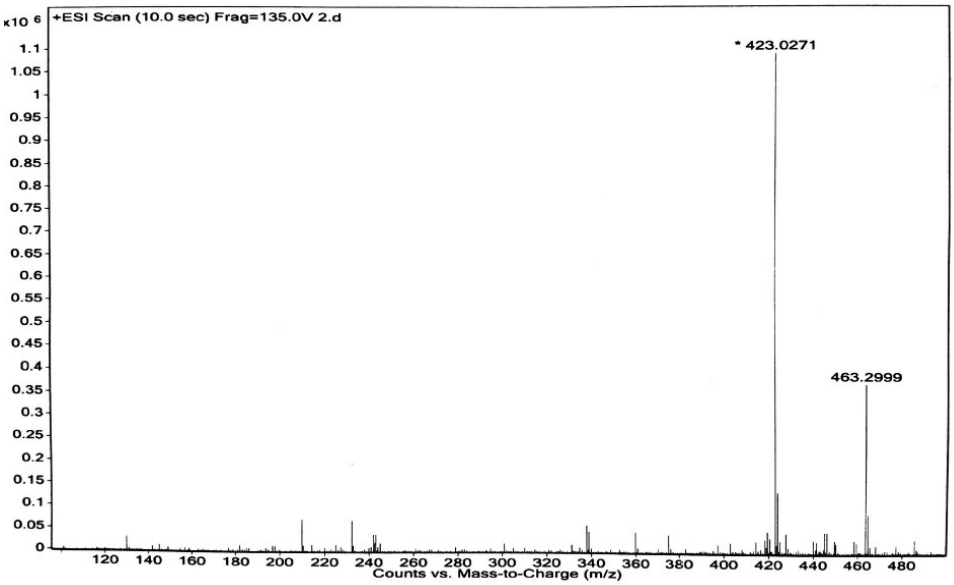

Fig. S16 ESI-Mass data of **BPC** with NaOH showing adduct at 463.

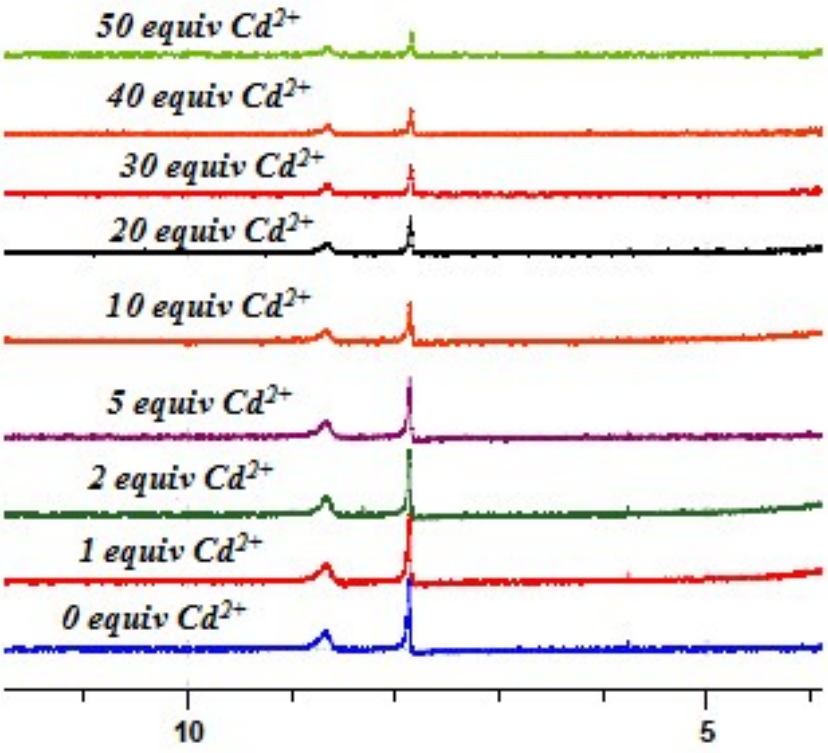

Fig. S17 ^{1}H-NMR titration of **BPC** ($1x10^{-3}$ M) with $Cd(NO_3)_2$ solution in DMSO-d_6.

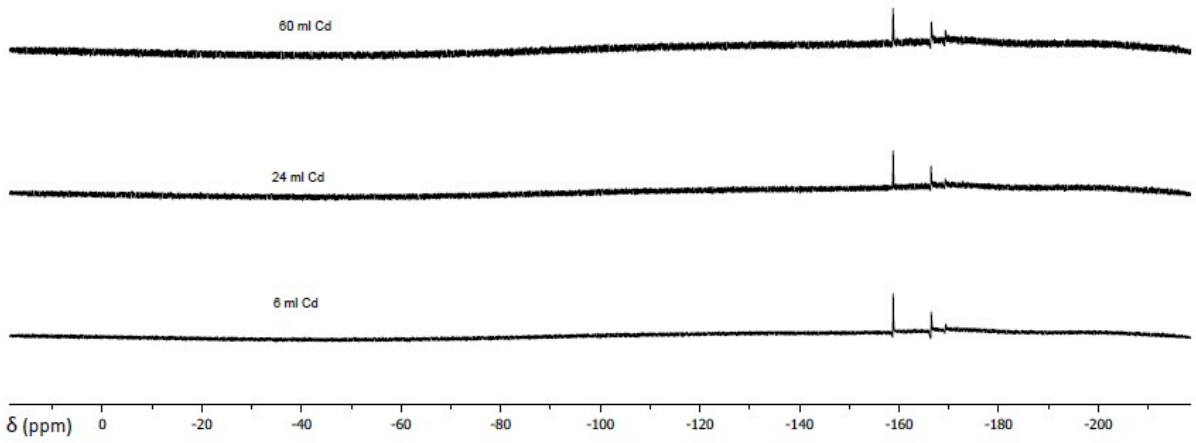

Fig. S18 ^{19}F-NMR titration of **BPC** ($1x10^{-3}$ M) with $Cd(NO_3)_2$ solution in DMSO-d_6.

Benesi-Hildebrand Equation and Plot:

The association constant of a complex formed in between the receptors and the incoming anions has been determined from the following complex equilibrium.

$$L + mX^{n-} \longleftrightarrow (X_mL)^{mn-}$$

$$K = \frac{[(XmL)]^{mn-}}{[L][X^{n-}]^m}$$

For 1:1 type complex formation with m=1 following the Benesi-Hildebrand relation, can be expressed in terms of optical density (A) as follows:

$$A = \frac{A_o + A_1K[X^{n-}]}{1 + K[X^{n-}]}$$

Or,

$$\frac{1}{A - A_0} = \frac{1}{(A_1 - A_0)} + \frac{1}{(A_1 - A_0)K[X^{n-}]}$$

Where $[X^{n-}]$, [L] and $[(X_mL)^{mn-}]$ are the concentration of the added anions, receptors and the complexation between anions and receptors, respectively. A_o, A and A_1 indicates the optical density or absorbance at a particular wavelength of receptor **1** or receptor **2** without adding any anion, absorbance after adding anion at every successive step and excess amount of added anion, respectively. The binding constant or association constant K (M^{-1} or M^{-2}) is determined from the ratio of intercept and slope of Benesi-Hildebrand plot of optical density.

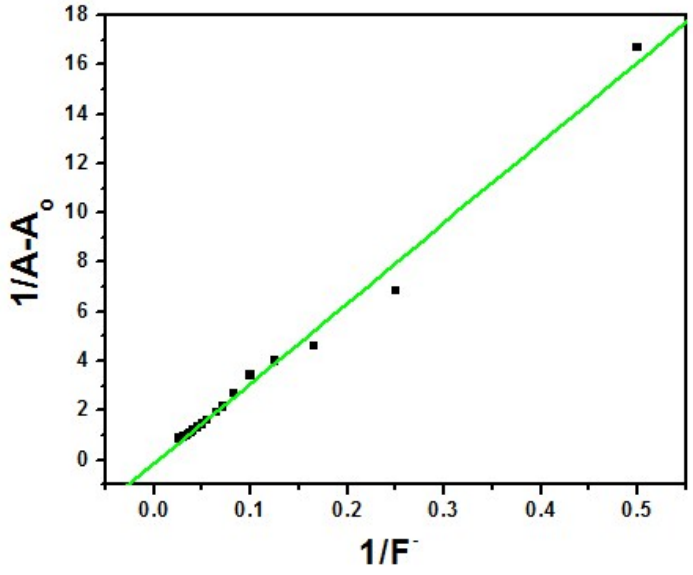

Fig. S19 B-H Plot of **BPC** with F^-.

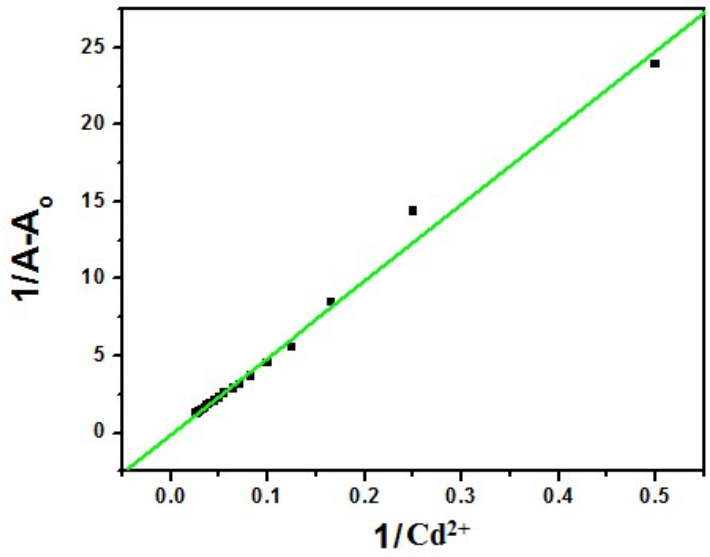

Fig. S20 B-H Plot of **BPC** with Cd^{2+}.

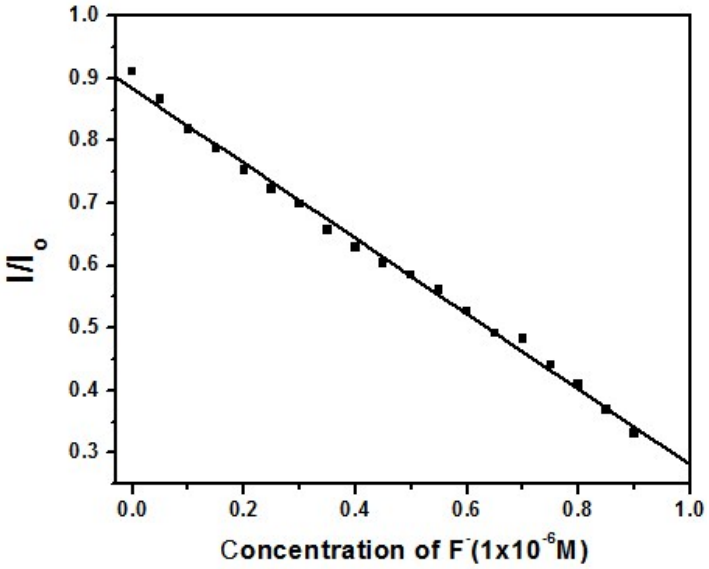

Fig. S21 Ratio of emission intensity of **BPC** with Cd^{2+}.

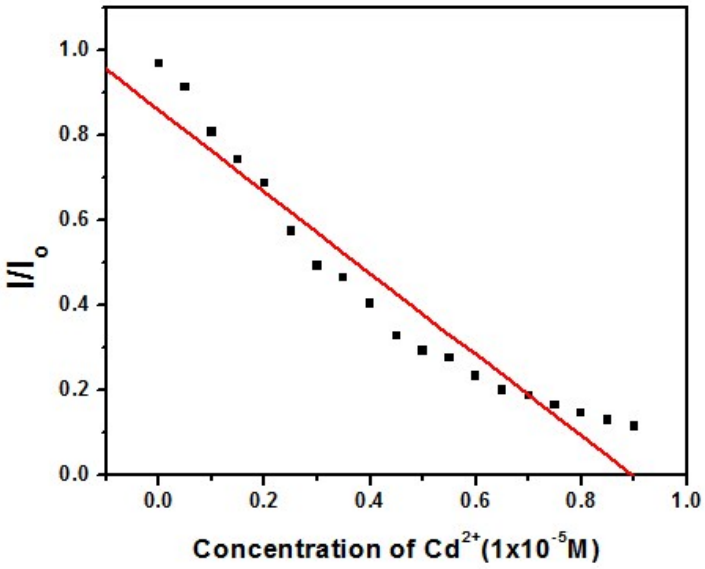

Fig. S22 Ratio of emission intensity of **BPC** with F^-.

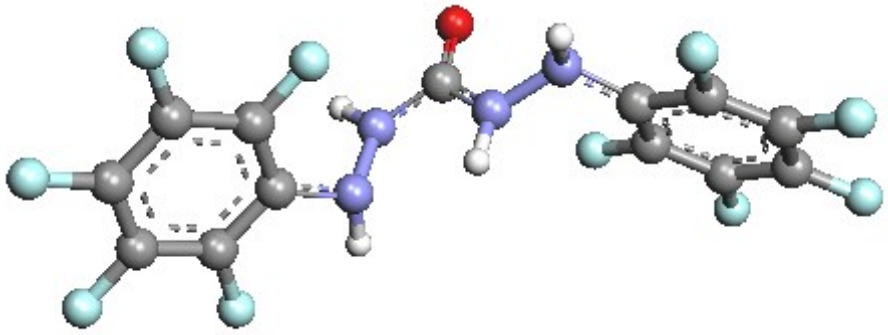

Fig. S23 Geometry optimized structure of **BPC** (Final Single Point Energy -1789.692685643 Eh).

Table S5 Cartesian coordinates of Geometry optimized structure of **BPC**.

O	7.218614	7.706984	4.964527
F	3.925713	6.051074	5.953497
F	3.947167	3.479408	1.959402
F	8.874752	4.939706	9.348283
F	9.768018	5.637518	4.725993
N	5.431533	4.835981	3.886087
F	1.230862	5.913203	6.021888
N	5.999037	6.111108	3.920117
F	1.240915	3.301052	2.067827
N	7.962640	5.907551	6.933060
F	11.366755	3.909770	9.661223
F	13.057044	3.696766	7.506165
N	7.169558	5.581196	5.846214
F	-0.142139	4.525014	4.098327
F	12.210494	4.560019	5.044880
C	6.824244	6.543416	4.933322
C	4.021559	4.786457	3.937849
C	9.224738	5.309347	7.030605
C	3.290008	4.078842	2.971204
C	3.287881	5.392113	4.971318
C	9.692296	4.857366	8.277455
C	10.116005	5.195197	5.947793
C	1.899409	3.978923	3.017920
C	10.969112	4.326383	8.450330
C	11.390643	4.646944	6.103354
C	1.194358	4.606417	4.046016
C	1.895560	5.318061	5.021877
C	11.827404	4.212447	7.355515
H	5.804268	4.292786	3.100218
H	5.696727	6.814991	3.239624
H	7.437547	5.890492	7.812344
H	6.786279	4.634468	5.770765

Table S6 Cartesian coordinates of Geometry optimized structure of **BPC** with TBAF (1:1) [Ref (Fig. 9a)].

O	7.529109	8.155624	4.987964
F	3.970187	6.274209	6.084233
F	4.627302	3.446772	2.307883
F	9.306590	6.126335	9.520715
F	9.787425	5.117537	4.886960
N	5.715104	5.302250	4.012257
F	1.452106	5.380354	6.301913
N	6.041206	6.636316	4.220307
F	2.088578	2.524704	2.575294
N	8.355411	6.501102	6.971122
F	11.511247	4.642905	10.057785
F	12.839990	3.346059	8.027028
N	7.406958	6.094347	6.024278
F	0.467766	3.488024	4.579256
F	11.916256	3.595247	5.454330
C	7.057690	7.014778	5.095970
C	4.390264	4.908201	4.162935
C	9.439958	5.663296	7.196321
C	3.851766	3.931298	3.305308
C	3.540750	5.372865	5.186084
C	9.946951	5.509119	8.502599
C	10.151229	4.996565	6.177946
C	2.551448	3.447149	3.433412
C	11.077536	4.749877	8.791794

C	11.273109	4.213783	6.458809
C	1.726058	3.938913	4.445039
C	2.230173	4.907433	5.314484
C	11.749971	4.087299	7.764205
N	6.459649	0.774204	6.394808
C	5.120938	1.158116	6.968057
C	6.519836	-0.708950	6.180660
C	7.541905	1.201361	7.351303
C	6.654875	1.494969	5.087077
F	6.316004	4.009714	6.874977
H	6.187730	4.884253	3.206159
H	5.931962	7.266057	3.418172
H	7.919042	6.824192	7.840924
H	6.855583	5.168229	6.290711
H	5.127773	2.252239	7.097080
H	4.992483	0.641070	7.930589
H	4.337643	0.838429	6.264441
H	5.719530	-0.997760	5.483673
H	7.502375	-0.966448	5.758951
H	7.386133	0.681136	8.307962
H	8.514205	0.915287	6.923031
H	7.454519	2.293860	7.468594
H	5.860881	1.177202	4.394441
H	6.598419	2.575339	5.302932
H	7.637035	1.213863	4.679179
H	6.378371	-1.210632	7.149229

Table S7 Cartesian coordinates of Geometry optimized structure of **BPC** with TBAF (1:2) [Ref (Fig. 9b)].

O	6.5638194	6.7828049	8.7654052
F	3.5874418	5.6092972	5.9118862
F	7.1561212	5.7302779	2.7076479
F	9.0478283	5.8518588	10.7412067
F	9.3212378	3.8747754	6.4297926
F	3.5874418	5.6092972	5.9118862
N	6.4413932	5.8965836	5.3567748
F	1.8290074	5.3887075	3.9197962
N	6.0790000	6.5745689	6.5298287
F	5.3451473	5.3799682	0.7180956
N	7.8149111	4.3155486	8.7162365
F	11.5254202	6.9760913	10.3814307
F	12.8617697	6.6161911	8.0096938
N	6.8784239	4.7341297	7.7497496
F	2.6502040	5.2065956	1.2861026
F	11.7517979	5.0844787	6.0306604
C	6.5294181	6.0930482	7.7348733
C	5.4719885	5.7244573	4.3940475
C	5.8539452	5.6108710	3.0255494
C	4.0777131	5.5852903	4.6477171
C	9.7067637	5.6544039	9.5843024
C	9.8337003	4.6675169	7.3779143
C	9.1058110	4.8839202	8.5686878
C	4.9237751	5.4501836	1.9902093
C	10.9734624	6.2321488	9.4083609
C	11.0834205	5.2698773	7.1732579
C	3.5489528	5.3547868	2.2744586
C	3.1380095	5.4620041	3.6118006
C	11.6597308	6.0450104	8.1951468
H	7.5203396	6.0502094	5.1197552
H	5.9577664	7.6333862	6.4738629
H	7.4318849	4.5075740	9.6487555
H	6.9924899	4.2821948	6.8354657
F	5.7085337	9.2574805	6.4698462

F	8.8822533	6.4468710	5.2544777
N	2.8745107	9.1467852	7.8061564
C	1.4824414	9.1397397	8.3552463
C	2.8715620	8.7626430	6.3413293
C	3.7451879	8.1725803	8.5708937
C	3.5008014	10.5168774	7.9188472
H	1.5097635	9.4306921	9.4248423
H	1.0626223	8.1188556	8.2540742
H	0.8607236	9.8587205	7.7845322
H	2.1981635	9.4596250	5.8020252
H	3.9372956	8.8686497	6.0150155
H	3.3616663	7.1473475	8.4065189
H	4.7785020	8.2629953	8.1779753
H	3.7086061	8.4367200	9.6465341
H	2.8574580	11.2448185	7.3835916
H	3.5748327	10.7869347	8.9917056
H	4.5064174	10.4170554	7.4364588
H	2.5201127	7.7177343	6.2428490
N	9.0984953	9.5087498	5.6021727
C	8.0421210	9.1767482	4.5669220
C	8.7030267	8.8277644	6.8992931
C	9.1765007	10.9867622	5.8004539
C	10.4159270	8.9379456	5.1425621
H	8.2723469	9.7369666	3.6372204
H	7.0524168	9.4364419	5.0094732
H	8.1262153	8.0753740	4.4296179
H	8.7161868	7.7407371	6.6486560
H	9.4436318	9.0980389	7.6792534
H	8.1803037	11.3464365	6.1267567
H	9.9350809	11.2118551	6.5776914
H	9.4618026	11.4719249	4.8444225
H	10.2368875	7.8400719	5.0299902
H	10.6950598	9.4120852	4.1790096
H	11.1867604	9.1493147	5.9119282
H	7.6698289	9.1530794	7.1451610

Table S8 Cartesian coordinates of Geometry optimized structure of **BPC** with TBAF (1:2) [Ref (Fig. 9c)].

O	7.5473570	7.8431771	7.4370598
F	5.3399197	5.5314621	6.2012542
F	6.8885206	5.7853035	1.6809157
F	10.2089289	6.0245243	9.6618052
F	8.3344402	3.5101475	6.0597724
N	6.5640552	7.0928053	4.0838442
F	4.7922856	2.9296526	5.8493138
N	6.7703854	7.7342947	5.2950321
F	6.2774428	3.1698823	1.3423798
N	9.4332066	6.0216784	7.0504346
F	10.1047838	3.8038523	11.2481543
F	9.1177003	1.4310910	10.2441554
N	8.5214477	6.3047568	6.0185803
F	5.2084162	1.6972755	3.4186150
F	8.2049598	1.3483453	7.6505925
C	7.6294240	7.2946859	6.3298010
C	6.2178108	5.7534929	3.9720611
C	9.2598550	4.8641952	7.8172300
C	6.3843807	5.0935097	2.7283771
C	5.6129987	4.9841997	4.9984870
C	9.7325626	4.8661895	9.1540249
C	8.7712888	3.6298985	7.3240862
C	6.0772457	3.7410056	2.5415301
C	9.6692192	3.7380163	9.9805746
C	8.6931939	2.4933494	8.1495382

C	5.5173463	2.9926941	3.5904016
C	5.3241525	3.6198166	4.8305366
C	9.1707695	2.5266437	9.4695382
N	4.3113751	9.7662258	1.5347280
C	4.6764770	9.9473110	2.9926114
C	4.5238878	8.3114569	1.1724242
C	2.8963287	10.1801093	1.2805852
N	4.3113751	9.7662258	1.5347280
C	5.2784973	10.5911237	0.7154032
N	10.6417112	8.0850675	2.1612977
C	9.8863703	8.6204437	3.3608459
C	11.2245727	9.2071728	1.3688620
C	9.6592454	7.2937847	1.3195067
C	11.7088729	7.1411952	2.6587089
H	6.9786953	7.5866499	3.2589108
H	5.9536630	8.2051247	5.7019790
H	9.5219179	6.8474203	7.6640804
H	8.8687987	6.0231817	4.9911293
H	5.1519051	11.6584960	0.9881375
H	5.0498458	10.4401408	-0.3590353
H	6.2909555	10.1982512	0.9936627
H	5.7466505	9.6250445	3.0581056
H	4.0127936	9.3055674	3.6053140
H	4.5380373	11.0145663	3.2597935
H	4.2772079	8.1765264	0.0999854
H	5.6037942	8.1168927	1.3865958
H	3.8601982	7.6872547	1.8029163
H	2.2198458	9.5543333	1.8968037
H	2.6624882	10.0382151	0.2061245
H	2.7733081	11.2474071	1.5546656
H	11.1465827	6.3593243	3.2335298
H	12.2415492	6.7125854	1.7847768
H	12.4158551	7.7067282	3.3002056
H	8.7780558	7.9448730	1.1348066
H	10.1759562	6.9677950	0.3930766
H	9.3512295	6.4418026	1.9718001
H	11.9250080	9.7829907	2.0079225
H	10.3989505	9.8633678	1.0279314
H	11.7673308	8.7954350	0.4933390
H	8.9976675	9.1737645	2.9872896
H	10.5782335	9.2377230	3.9695969
H	9.5503187	7.6988366	3.8862852
F	7.2097087	8.9197385	2.0612751
F	9.4084605	5.7774212	3.7349692

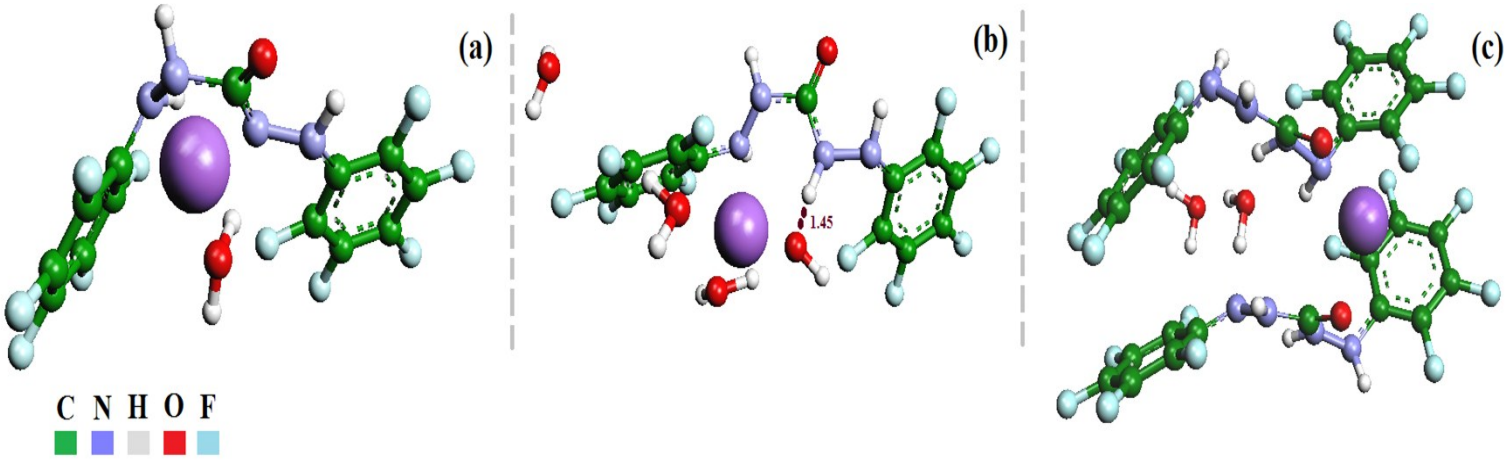

Fig. S24 (a) Energy minimized structure of **BPC** with NaOH, (b) **BPC** with one molecule of NaOH and three molecules of water considering and (c) two molecules of **BPC** with one molecule of NaOH and water.

Table S9 Cartesian coordinates of Geometry optimized structure of **BPC** with NaOH [Ref (Fig. S23a)].

O	6.4133997	7.9533900	7.3750196
F	2.9034221	6.0485256	5.8614985
F	6.0467584	4.4573015	2.6073206
F	10.7152040	6.8020694	8.2312555
F	8.2114234	3.5663668	5.7507584
N	5.3869490	6.4583631	4.3024242
F	1.4315025	3.8646610	5.4745217
N	5.3563892	7.2532098	5.4586678
F	4.4963819	2.2466045	2.2268147
N	8.3241098	6.1181517	7.1072441
F	12.8903404	5.1481418	8.1578978
F	12.7571605	2.7363213	6.8255730
F	4.4963819	2.2466045	2.2268147
N	7.3405584	6.1957809	6.1169084
F	2.1489936	1.9379840	3.6389095
F	10.3960813	2.0003777	5.6180495
C	6.4827424	7.1751401	6.3759124
N	7.3405584	6.1957809	6.1169084
C	4.5644916	5.3348780	4.2372589
C	9.3978544	5.2687035	6.9773062
C	4.9005135	4.3220844	3.3001115
C	3.3454331	5.1516330	4.9322200
C	10.6338353	5.6165177	7.5877537
C	9.3568420	4.0177727	6.3055128
C	4.1186407	3.1761697	3.1093405
C	11.7500167	4.7724327	7.5620578
C	10.4820498	3.1779955	6.2539287
C	2.9134574	3.0217299	3.8201171
C	2.5561668	4.0016986	4.7583107
C	11.6893353	3.5477730	6.8710400
O	5.4158627	4.6317625	7.3751082
Na	4.4621401	6.6187672	7.7240106
H	6.3521079	6.2646781	3.9885934
H	5.1765536	8.2404823	5.2204323
H	8.4668059	6.9820870	7.6487860
H	6.2036702	4.8987776	6.7982980
H	5.3389870	3.6585089	7.3230927

Table S10 Cartesian coordinates of Geometry optimized structure of **BPC** and NaOH with $3H_2O$ [Ref (Fig. S23b)].

O	7.0355884	7.2897394	7.0738738
F	3.2316474	4.8755599	6.3508242
F	5.0086588	4.9758421	1.9122836
F	10.4650897	6.4115457	8.6816212
F	9.0542436	3.0999982	5.5482736
N	5.4654191	5.3949821	4.5762813
F	0.8808275	4.0244962	5.3788070
N	5.5661678	6.2876103	5.6364124
F	2.6186633	4.0626307	0.9567715
N	8.3653680	5.0571307	7.5541190
F	13.0702108	5.8821170	8.0504566
F	13.6742512	3.9770768	6.1522689
N	7.3219868	5.0397320	6.6011004
F	0.5170346	3.5997501	2.6830476
F	11.6290280	2.6370848	4.8922445
C	6.7011877	6.2531742	6.4872588
C	4.2143239	4.9763594	4.1523516
C	9.6699765	4.8057588	7.1215549
C	3.9933821	4.7448410	2.7696008
C	3.1107053	4.7444526	5.0073068
C	10.7482273	5.4686412	7.7596298
C	10.0107367	3.8200706	6.1637921
C	2.7739423	4.2647872	2.2695704
C	12.0868509	5.2113696	7.4355224
C	11.3494549	3.5670370	5.8169783
C	1.6987944	4.0462319	3.1473238
C	1.8860321	4.2776962	4.5166742
C	12.3975558	4.2384644	6.4682221
Na	3.9895303	2.7457461	7.3672924
O	6.1309333	2.7722434	6.8698006
O	1.7826277	2.7190965	7.9133768
H	6.1561948	5.5026941	3.8210446
H	5.3141327	7.2654659	5.4245800
H	8.3051339	5.9316689	8.1036042
H	6.7562053	4.0539100	6.6107679
H	6.8805617	2.2117886	7.1567268
H	1.2824641	3.2819823	7.2781870
H	1.2144356	1.9357330	8.0715182
O	-0.5080080	6.1625557	3.7206491
H	-0.7497294	5.2904518	3.3405498
H	-0.3209541	6.7147327	2.9311157
O	4.4098295	1.8158940	5.3657368
H	5.3412535	2.1376622	5.7728181
H	4.4557498	1.8596137	4.3912667

Table S11 Cartesian coordinates of Geometry optimized structure of **2BPC** with NaOH and H_2O [Ref (Fig. S23c)].

O	6.357658402	6.376112402	8.411245602
F	2.310664100	6.684234202	6.396621302
F	5.191331402	4.768269702	3.130408700

F	9.273401102	4.712388402	9.337614802
F	8.580834802	3.775024300	4.713160602
N	4.867803102	6.606218002	5.180769802
F	0.295632700	5.069566402	5.563225602
N	5.137649002	6.785309102	6.529322302
F	3.142045400	3.178998500	2.257171300
N	7.439014702	4.088430800	7.316533102
F	11.928999002	5.001670502	8.871935302
F	12.928197704	4.703606102	6.331740702
N	6.622523402	4.992959002	6.552521202
F	0.680777800	3.318039300	3.478756900
F	11.250545302	4.089436200	4.261357502
C	6.058635602	6.040396602	7.249878402
C	3.816398800	5.751419902	4.797697202
C	8.840329502	4.245604602	7.028190202
C	3.986910100	4.849328302	3.726892500
C	2.541446000	5.813124902	5.402685402
C	9.733598502	4.562407102	8.068705402
C	9.381956702	4.087007100	5.733992102
C	2.937946700	4.038148800	3.277397000
C	11.112325902	4.712122902	7.856621402
C	10.757148202	4.244772002	5.491693802
C	1.681810000	4.093749200	3.902568300
C	1.490484000	4.984670302	4.973931902
C	11.622766002	4.559965002	6.555469402
O	5.582845602	3.014851700	10.301147102
F	1.533067100	3.475357500	8.534149202
F	3.176019200	0.128344900	5.493503802
F	8.041022402	0.797479300	12.233045202
F	8.015297302	0.871404400	7.463696802
N	3.812923900	1.916750100	7.415644302
F	-0.957094400	2.989300000	7.672078802
N	4.114089700	2.671441600	8.554026202
F	0.658515300	-0.233774300	4.576372402
N	6.582911102	0.466960100	9.924335402
F	10.710515702	1.380840000	12.216310302
F	12.031559902	1.734636400	9.820741602
N	5.694718502	1.068595000	9.051092902
F	-1.459087100	1.186408500	5.644445202
F	10.642990902	1.480287300	7.467989002
C	5.138282302	2.301710100	9.362805802
C	2.494007700	1.803562000	7.070252802
C	7.935801502	0.830091700	9.861286402
C	2.171126500	0.890699900	6.015734302
C	1.366646000	2.530091100	7.565523102
C	8.682567602	0.949135000	11.057580802
C	8.641875602	0.992805100	8.646750002
C	0.873221400	0.663021500	5.552019202
C	10.051512902	1.254728500	11.059965702
C	10.009898302	1.314049900	8.638645702
C	-0.208685000	1.381937900	6.094690402
C	0.051873700	2.288936200	7.134166702
C	10.728193702	1.432950000	9.839745802
Na	6.927460102	4.650437202	9.718890902
O	5.587245602	2.813776100	5.695066602
O	5.002116802	1.260944200	3.560674700
H	5.711615502	6.511887802	4.602323502
H	4.853391502	7.674824802	6.950791102
H	7.103605402	3.155851400	6.975327502
H	6.032290102	4.374591502	5.905684502
H	4.838220702	2.409391400	6.313521802
H	3.613009000	3.537111400	8.788434302
H	6.240249602	0.435500500	10.893546302
H	5.195658302	0.492044500	8.359443202

H	5.563091302	2.276701600	4.844291402
H	4.475599402	1.773529800	2.907005800
H	4.343023802	0.707897500	4.044778000

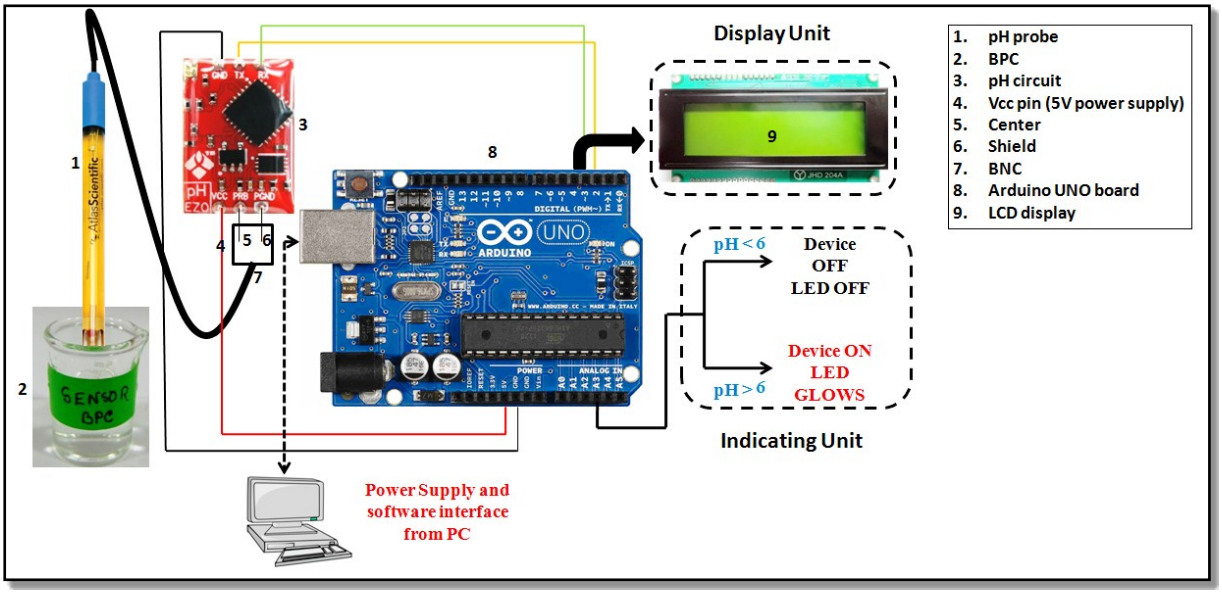

Fig. S25 Interfacing of pH sensor (**BPC**) with suitable circuitry.