Electronic Supplementary Material (ESI) for Dalton Transactions.

A simple urea-based multianalyte and multichannel chemosensor for selective detection of F^-, Hg^{2+} and Cu^{2+} in solution and cells, extraction of Hg^{2+} and Cu^{2+} from real water sources: A logic gate mimic ensemble

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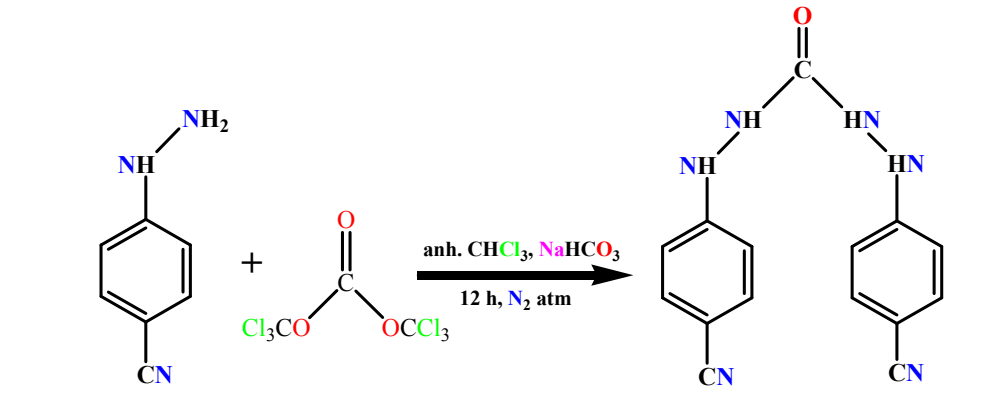


4-cyanophenyl hydrazine **triphosgene** **1, 5-bis (4-cyanophenyl) carbonohydrazide**

Scheme S1 Preparation of **BCC**.

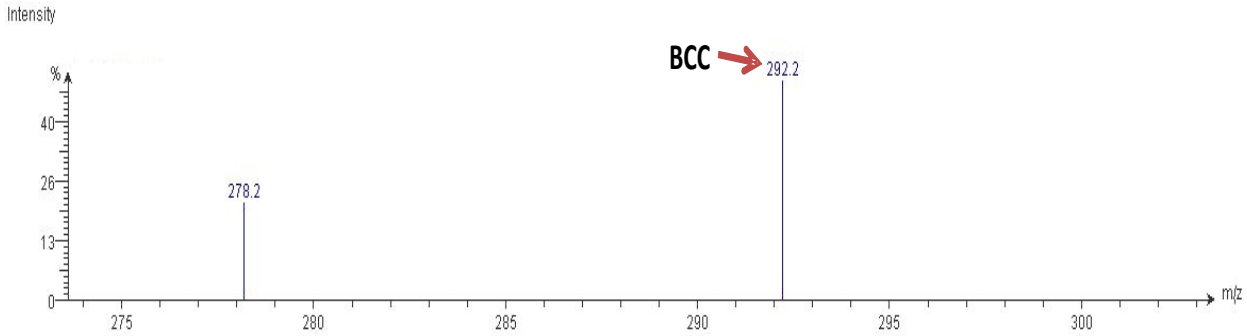


Fig.S1 ESI-Mass data of **BCC**

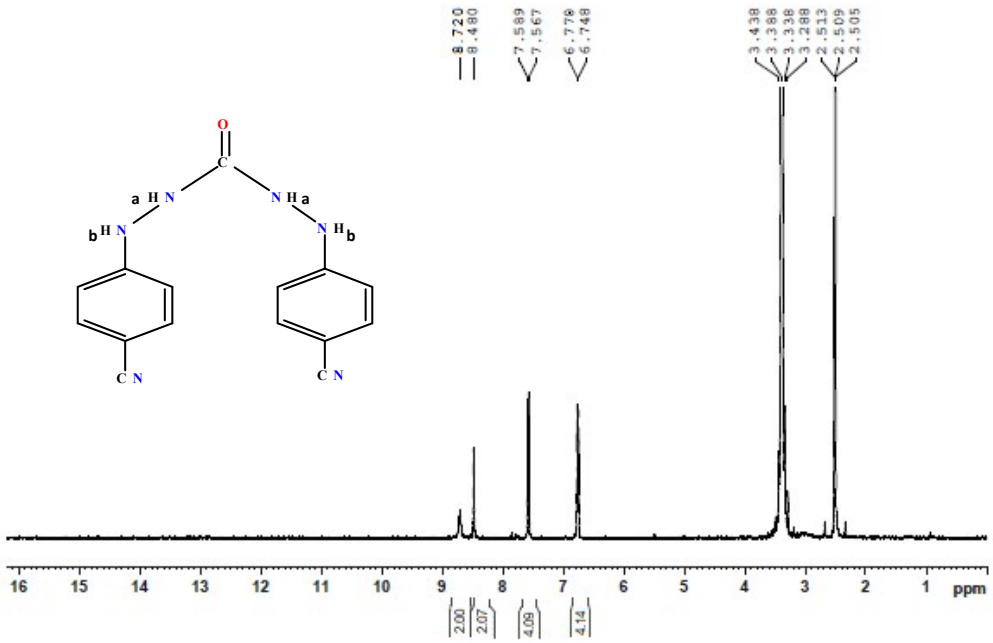


Fig.S2 ^{1}H NMR data of **BCC** in DMSO-d_6.

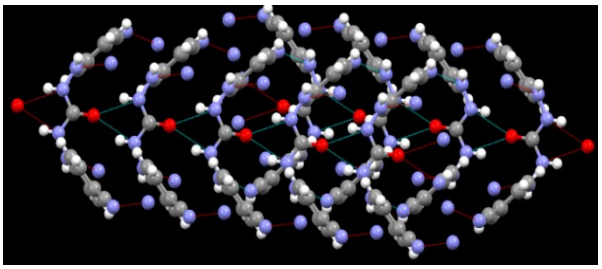


Fig.S3 Intermolecular hydrogen bonding in **BCC.**

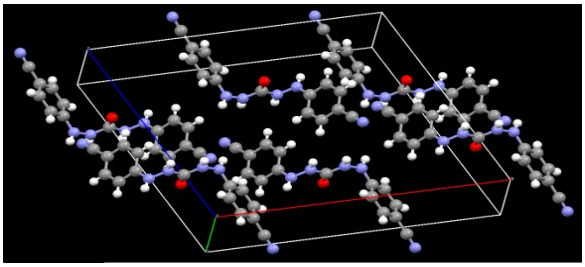


Fig.S4 Unit cell with six molecules of **BCC** propagating along axis 'a'

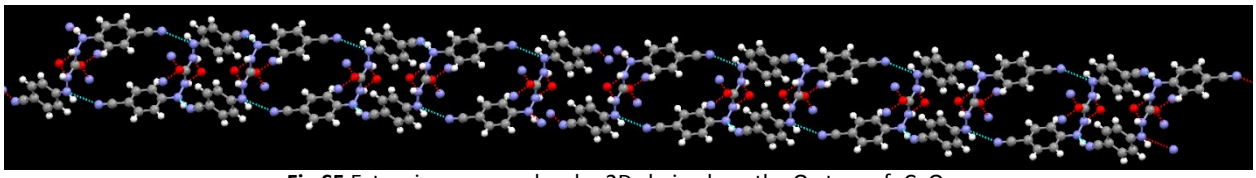


Fig.S5 Extensive supramolecular 2D chain along the O atom of -C=O group

Table S1 Crystallographic data of **BCC**.

Crystal Data	
Formula	C15 H12 N6 O
Formula Weight	292.31
Crystal System	monoclinic
Space group	C2/c (No. 15)
a, b, c [Angstrom]	19.810(9) 4.548(2) 16.353(7)
alpha, beta, gamma [deg]	90 105.47(3) 90
V [Ang**3]	1420.0(11)
Z	4
D(calc) [g/cm**3]	1.367
Mu(MoKa) [/mm]	0.093
F(000)	608
Crystal Size [mm]	0.00 x 0.00 x 0.00
Data Collection	
Temperature (K)	99
Radiation [Angstrom]	MoKa 0.71073
Theta Min-Max [Deg]	2.6, 25.0
Dataset	-23: 21 ; -5: 5 ; -19: 18
Tot., Uniq. Data, R(int)	5944, 1248, 0.055
Observed Data [I > 2.0 sigma(I)]	1048
Refinement	
Nref, Npar	1248, 101
R, wR2, S	0.0466, 0.1232, 1.09
w =	^2^(FO^2^)+(0.0420P)^2^+2.5124P] WHERE P=(FO^2^+2FC^2^)/3'
Max. and Av. Shift/Error	0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-0.57, 0.52

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

O001	-C007	1.229(3)	N003	-H003	0.8800
N002	-N003	1.389(3)	C008	-C00A	1.397(3)
N002	-C005	1.387(3)	C008	-C00B	1.397(3)
N003	-C007	1.362(2)	C008	-C00C	1.436(3)
N004	-C00C	1.151(3)	C009	-C00B	1.375(3)
C005	-C006	1.403(3)	C006	-H006	0.9500
C005	-C009	1.398(3)	C009	-H009	0.9500
N002	-H002	0.8800	C00A	-H00C	0.9500
C006	-C00A	1.378(3)	C00B	-H00D	0.9500

Table S3 Selected bond angles (degrees) of **BCC**

N003	-N002	-C005	118.09(17)	C00A	-C008	-C00C	119.9(2)
N002	-N003	-C007	119.29(18)	C00B	-C008	-C00C	120.3(2)
N002	-C005	-C006	117.97(18)	C005	-C009	-C00B	120.5(2)
N002	-C005	-C009	122.68(18)	C006	-C00A	-C008	120.15(19)
C006	-C005	-C009	119.26(19)	C008	-C00B	-C009	120.2(2)
N003	-N002	-H002	121.00	N004	-C00C	-C008	178.2(3)
C005	-N002	-H002	121.00	C005	-C006	-H006	120.00
C005	-C006	-C00A	120.26(19)	C00A	-C006	-H006	120.00
N002	-N003	-H003	120.00	C005	-C009	-H009	120.00
C007	-N003	-H003	120.00	C00B	-C009	-H009	120.00
O001	-C007	-N003_a	122.72(13)	C006	-C00A	-H00C	120.00
N003	-C007	-N003_a	114.6(2)	C008	-C00A	-H00C	120.00
O001	-C007	-N003	122.72(13)	C008	-C00B	-H00D	120.00
C00A	-C008	-C00B	119.7(2)	C009	-C00B	-H00D	120.00

Table S4 Hydrogen bonding in **BCC**

N002 -- H002 .. N004	0.8800	2.4900	3.067(3)	124.00	4_555
N003 -- H003 .. O001	0.8800	2.0300	2.825(3)	149.00	1_565
C00A -- H00C .. N004	0.9500	2.5900	3.524(3)	167.00	7_646

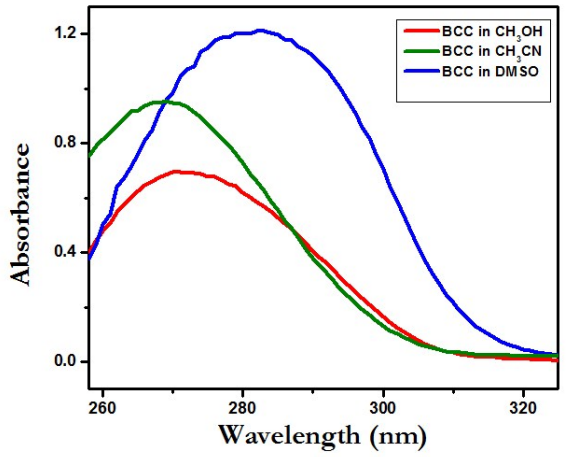


Fig.S6 Absorbance spectra of **BCC** in different solvents

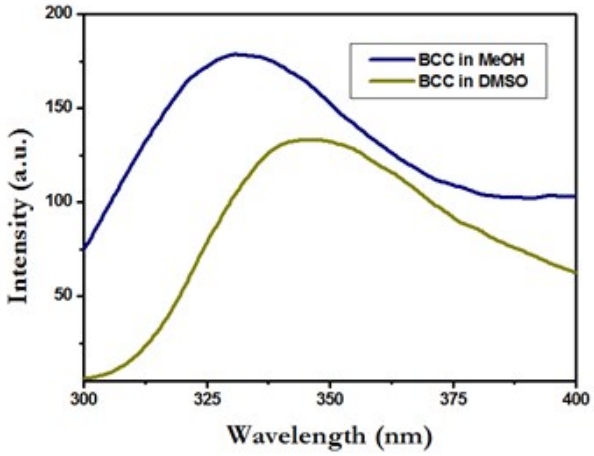


Fig.S7 Fluorescence spectra of **BCC** in different solvents

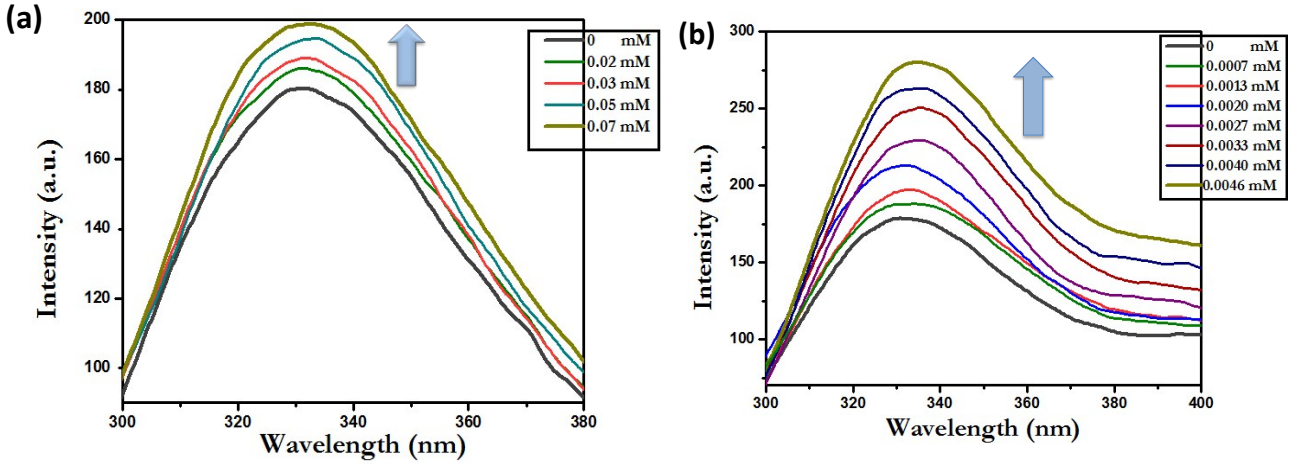


Fig.S8 Fluorescence titration spectra of **BCC** with (a) Hg^{2+} and (b) Cu^{2+} in MeOH-water (9:1)

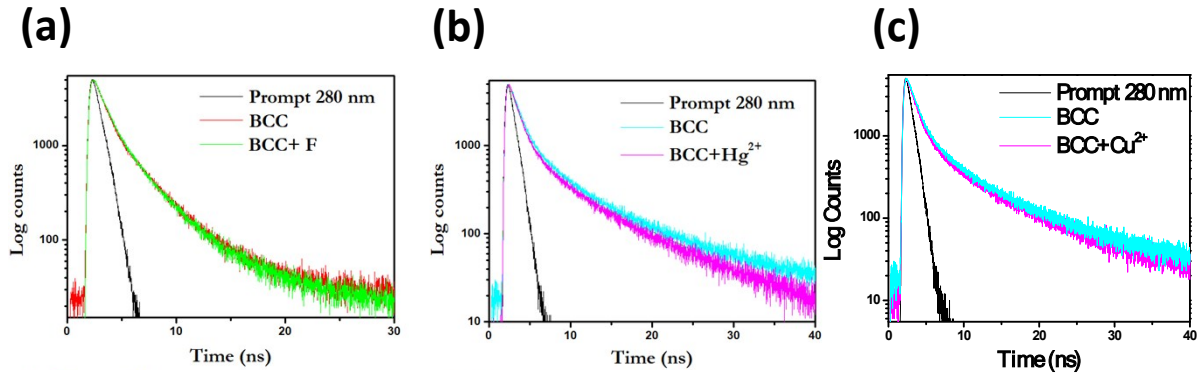


Fig.S9 Fluorescence lifetime spectra of **BCC** with (a) F^- in DMSO; (b) Hg^{2+} and (c) Cu^{2+} in MeOH

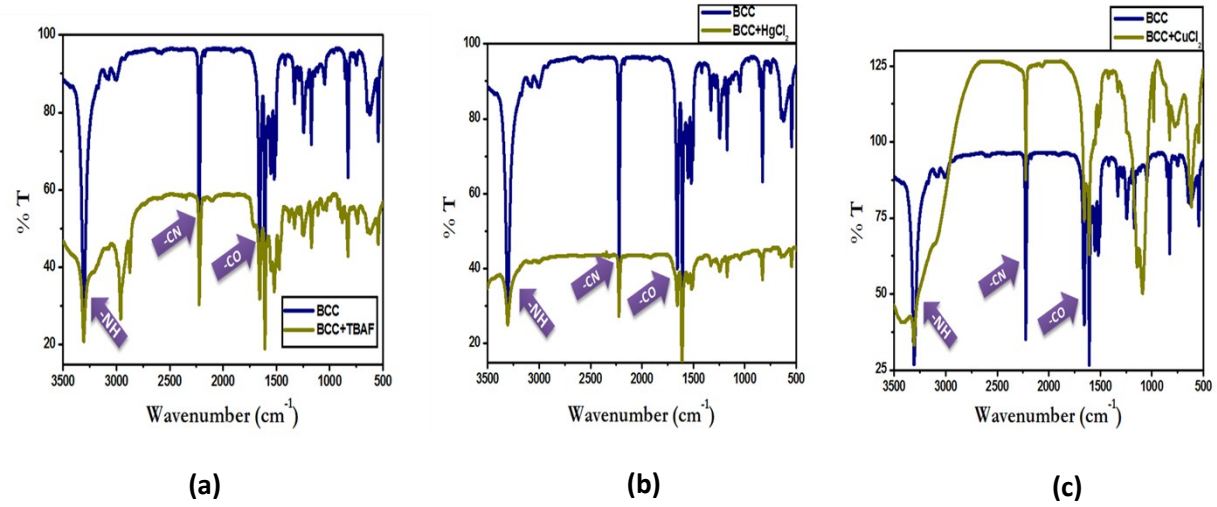


Fig.S10A IR spectra of **BCC** with (a)TBAF (b)$HgCl_2$ and (c) $CuCl_2$ in solid state

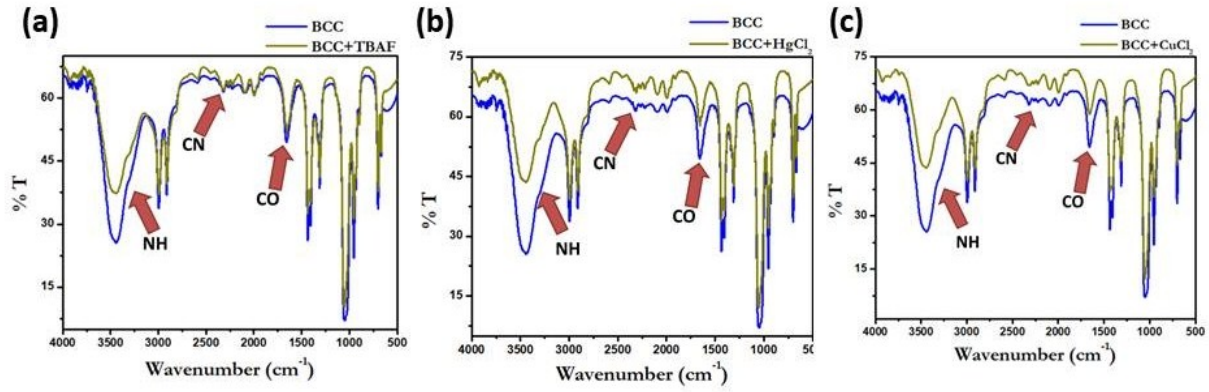


Fig.S10B IR spectra of BCC with (a) TBAF (b) $HgCl_2$ and (c) $CuCl_2$ in solution state

Table S5 Oxidation Reduction Potential (ORP) of **BCC** with F^- , Hg^{2+} and Cu^{2+}

Host-Guest	**Sensor+F^-**	**Sensor+Hg^{2+}**	**Sensor+Cu^{2+}**
Initial Oxidation	E_a= 0.50 V I_a= -0.002 mA	E_a= 0.28 V I_a= -0.009 mA	E_a= 0.4 V I_a= -0.011 mA
Initial Reduction	No reduction	E_c= 0.19 V I_c= 0.014 mA	E_c= 0.23 V I_c= 0.009 mA

Final Oxidation	E_a= 0.47 V I_a= -0.002 mA	E_a= 0.28 V I_a= -0.02 mA	E_a= 0.34 V I_a= -0.012 mA
Final Reduction	No reduction	E_a= 0.15 V I_a= 0.03 mA	E_a= 0.19 V I_a= 0.011 mA

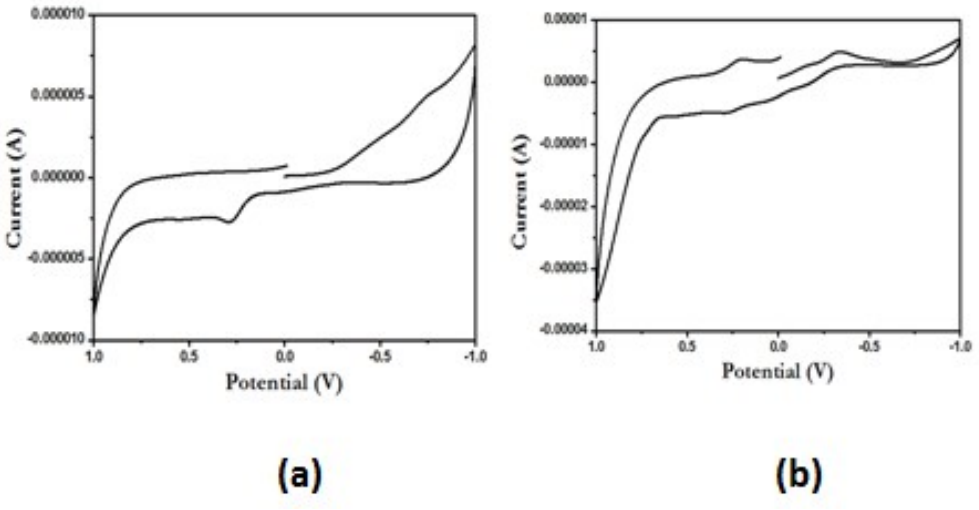


Fig.S11 Cyclic voltammetry of **BCC** in (a) DMSO and (b) MeOH

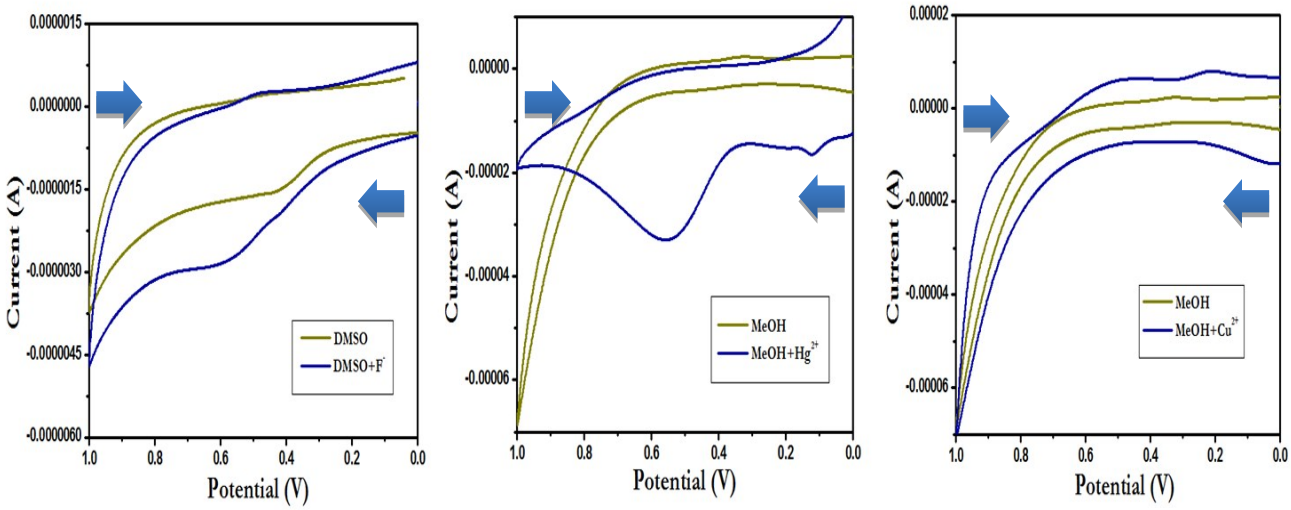


Fig.S12 Electrochemical response of (a) F^- in DMSO, (b) Hg^{2+} in MeOH and (iii) Cu^{2+} in MeOH

Rate constant calculation:

Rate constant of the host-guest interaction was calculated from UV-Vis spectroscopy. The sensor and the analytes were taken in similar concentration and the plots of absorbance vs. time were observed in a fixed wavelength. After that three graphs were plotted (i) Absorbance vs. time, (ii) ln Absorbance vs. time and (iii) 1/Absorbance vs. time. Among the three plots, the plot in which the R value is more closed to 1 is chosen and accordingly the order of the reaction was known. Furthermore, the reaction rate was obtained from the slope of the specific plot.

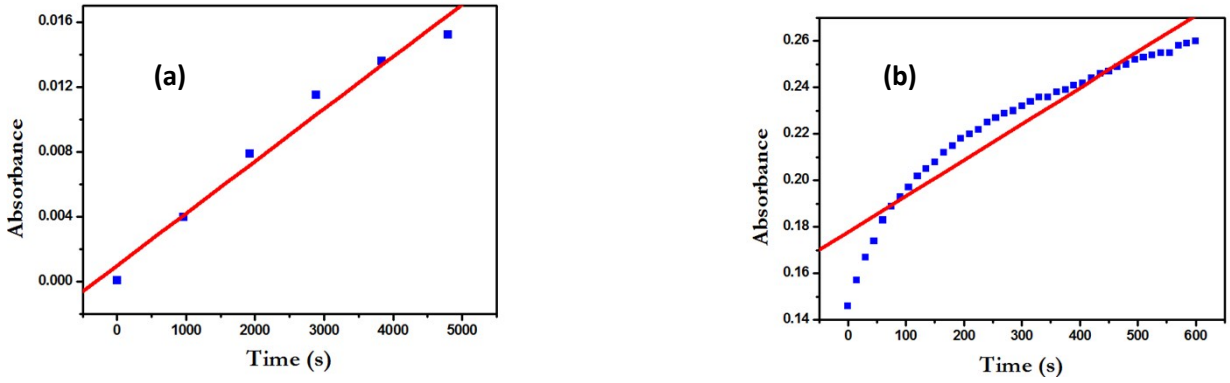


Fig.S13 Plots of Absorbance vs. Time of **BCC** with (a) Hg^{2+} and (b) Cu^{2+}

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:

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

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.

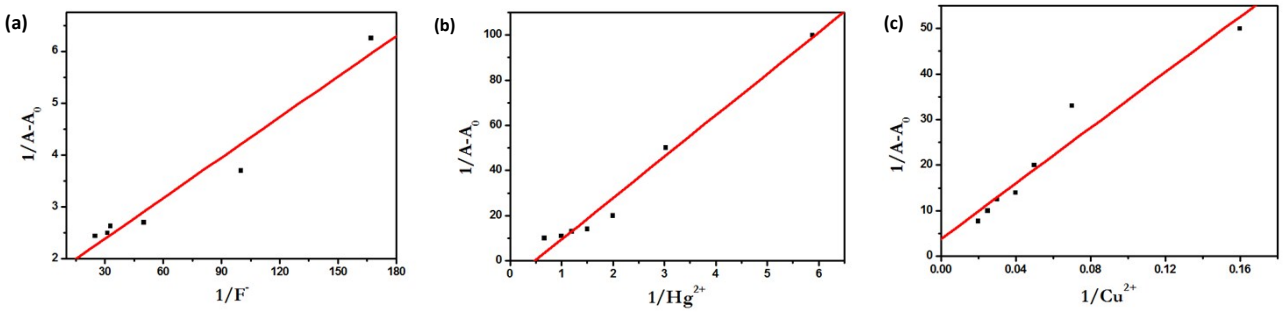


Fig.S14 B-H plot of **BCC** with (a) F^- (b) Hg^{2+} and (c) Cu^{2+}

(a) ***De*** **(b)** ***limit calculation*** **(c)**

The detection limit (DL) has been calculated following UV-Vis titration. The absorbance spectrum of **BCC** was repeated for 10 times, and its standard deviation is measured. The limit of detection (LOD) is calculated from the following formula:

$$DL = 3\sigma/k$$

σ is the standard deviation of the blank solution of **BCC**. Gradual emergence of new absorbance values during colorimetric titration with targeted analytes is plotted against its concentration. The slope (k) is derived from these plots.

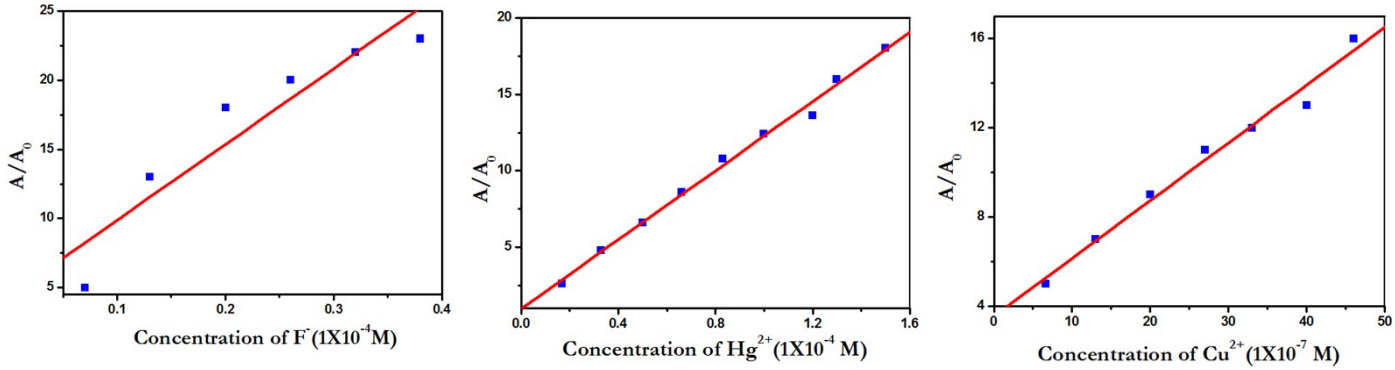


Fig.S15 Ratio of absorbance of **BCC** with (a) F^- (b) Hg^{2+} and (c) Cu^{2+}

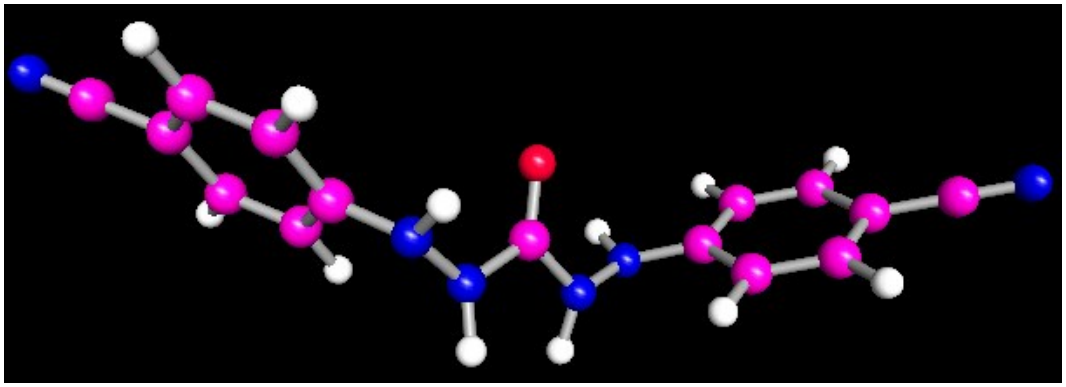


Fig.S16 Geometry optimized structure of **BCC**.

Table S6 Cartesian coordinates of geometry optimized structure of **BCC**

ATOM	CARTESIAN COORDINATES		
1O	12.53201083824375	1.48034320735132	22.33571150982292
2N	17.02289360979078	4.10569922191584	21.99273529657129
3N	14.69845807252726	5.26124193996331	21.97427995907610
4N	23.13492847843408	0.45233756641364	11.23361176942516
5C	18.17476864316058	3.32544274517948	19.77842296955096
6C	20.35725059807821	1.76400494828289	19.92423328825179
7C	12.53252905023017	3.79918160149218	22.33499123205869
8C	20.75433379751340	1.81862976614748	15.32348368969362
9C	17.29871773205585	4.11363581560278	17.36761583362893
10C	21.62474128475854	1.02534683535858	17.73806921616976
11C	18.56964302021949	3.37092054592708	15.18046745716510
12C	22.05759011681481	1.06824306557805	13.08060719113199
13N	8.04230384433209	4.10815255783926	22.67949716699315
14N	10.36738177108360	5.26236602638111	22.69510141514029
15N	1.94841437353016	0.44978531609135	33.44725682298773
16C	6.89394247859825	3.32663400045739	24.89526394418442
17C	4.71008951476112	1.76687263574497	24.75214281030774
18C	4.32183489833091	1.81740717736672	29.35369123818930
19C	7.77511188894708	4.11196891335488	27.30513357962573
20C	3.44628767514020	1.02698749131354	26.94004249866346
21C	6.50782043081492	3.36811005276071	29.49399927357190
22C	3.02242468445554	1.06606211962538	31.59847312533328
23H	17.53163788474084	3.21023380660040	23.63744558505453

24H	14.68423155684202	7.14575063706668	22.44140481203190
25H	21.04949407662330	1.13521917988905	21.78581469004329
26H	15.61142557629032	5.32096148369625	17.23873459331006
27H	23.31031250147836	-0.18618085918014	17.88424217542473
28H	17.86934153477974	3.99836059192487	13.32379933936532
29H	7.53056474123413	3.21387013052257	21.03506468584433
30H	10.38235787598146	7.14696817463657	22.22847130207399
31H	4.01382116475357	1.14054395411628	22.89124484569887
32H	9.46359142913400	5.31784886664930	27.43197642902431
33H	1.75963694926969	-0.18328171026812	26.79597202040350
34H	7.21198271466137	3.99347590884035	31.34990730926674

Table S7 Cartesian coordinates of geometry optimized structure of **BCC…1F**$^-$ adduct (with inward directed H)

ATOM	CARTESIAN COORDINATES		
1O	12.59725006720808	0.86728717887400	22.82577461568058
2N	17.37961807772754	3.05729606453929	22.34770620151953
3N	15.28168927485522	4.35126317230547	23.22398441178002
4N	20.49823138186093	2.60862599840929	9.84330812344045
5C	17.95610970814126	2.93733852338636	19.81083093013518
6C	19.81493934064292	1.20165455038783	18.93044666709589
7C	12.91575077521555	3.16872250731795	22.97624236399160
8C	19.28825846205782	2.76744679449026	14.61421578866600
9C	16.79162050792178	4.60921395071627	18.04965330726829
10C	20.46444008588972	1.11708013707275	16.38167283478591
11C	17.45089884167994	4.51508748260964	15.50039740301250
12C	19.95140311105758	2.67889656294573	12.00020776811031
13N	8.54513508140695	4.20091306380132	22.61483299287823
14N	10.99763598660410	4.96666327137229	23.00884427723389
15N	0.00206565207607	2.65977260014793	32.15560895731966
16C	6.88033898244706	3.84555994256903	24.58708874755807
17C	4.48492823543471	2.71762752723709	24.10218119777535
18C	3.29478632751878	3.22357263750727	28.53754378811962
19C	7.44977197747648	4.65040522833727	27.08736564123045
20C	2.72850204473743	2.41365421984437	26.03730521143600
21C	5.68728943499714	4.34362105108004	29.02167561159089
22C	1.49190600803597	2.91431544983356	30.52135721465321
23H	18.08646198723167	1.70104760274223	23.53258326861945
24H	15.22018148737113	6.30809084319915	22.81009195345084
25H	20.73332646893495	-0.09330114492189	20.27965928312732
26H	15.43076708359136	6.02785323407544	18.74513232994477
27H	21.89278718194037	-0.24846790758524	15.72763113263654
28H	16.54300935856361	5.82218324849769	14.15830639092194
29H	8.17609415466823	3.26785036213550	20.95271600185843
30H	11.57919780395486	6.80836090960682	22.44653446760915
31H	4.02332901931266	2.08072690261281	22.17297102465833
32H	9.29922984961698	5.51749358872379	27.47265758465661
33H	0.88708618442226	1.53404802925842	25.62868347512135
34H	6.15724359670457	4.97523881746419	30.94857234947152
35F	13.74429484784206	8.87763334896865	21.68644479790063
36N	13.10848682428322	14.99630774600377	22.09016498975787
37C	12.77930437545261	17.80303864742068	22.33574440039513
38C	15.78539609916574	14.36504251326710	21.33591515446263
39C	11.34776270381584	13.95116007595763	20.10466597451708
40C	12.54260091049712	13.69712621260637	24.56719077337168
41H	12.82815772728646	11.64427486398292	24.21430016138711
42H	10.56566879803192	14.12391503008726	25.10634959836808

43H	13.86145728308929	14.42661997727946	26.01986797809402
44H	11.70907285119062	11.88436628081599	20.04074412259041
45H	9.37639135483751	14.36941346559087	20.67115694558129
46H	11.78306459237086	14.86725450187583	18.27335079454171
47H	15.87492687375403	12.27276878006102	21.19925824092791
48H	16.19556488148165	15.27464204370568	19.49572874780651
49H	17.08442939406539	15.09221205136505	22.80714730598321
50H	13.20511407920447	18.69743025891007	20.49200636993813
51H	14.09541752144856	18.51153013391656	23.80075833328166
52H	10.80184938320705	18.20467322615181	22.89041594030999

Table S8 Cartesian coordinates of geometry optimized structure of **BCC…1F**$^-$ adduct (with outward directed H)

ATOM	CARTESIAN COORDINATES		
1O	10.15669508234097	2.97397466011121	19.78424762575301
2N	14.05433965769081	4.86045077156622	16.76846812899463
3N	12.01433786893938	6.28581167533310	17.61351664599185
4N	18.55673178806947	6.41723232783737	4.78563830657395
5C	14.80917623334472	5.24054429560312	14.35869387924807
6C	17.03709738950937	3.90315045994791	13.52776419685621
7C	10.34713954857448	5.24645321692242	19.31390761771474
8C	16.76951127850390	5.85154991628028	9.33262972843942
9C	13.60099027312908	6.88665014123231	12.56307901525853
10C	17.97897009969877	4.20083527899333	11.10498709474346
11C	14.56097533638232	7.17129443393507	10.13061021383284
12C	17.74302849107211	6.16321351038414	6.84918080165203
13N	6.69180920963246	6.26089535370480	21.76119076940512
14N	8.83623534760481	7.08249663114766	20.53561286090178
15N	6.44477594069084	3.99707185288409	34.46105773837463
16C	6.72462359477525	5.76235819247717	24.32582009849734
17C	4.66484041616948	4.43100786113050	25.42844686503081
18C	6.57550435713420	4.84840484368784	29.61225147509275
19C	8.70826501330139	6.62936374306201	25.91438925774902
20C	4.59036570137917	3.98318186880035	28.02154583796078
21C	8.63236759291707	6.17697306831347	28.50945396764495
22C	6.50441510211889	4.38324927723346	32.26996733684503
23N	29.72832138527645	1.98752676776178	29.78046031182072
24C	28.99770042425765	3.06996813700899	32.31175348932031
25C	32.46336621197727	1.19409763875089	29.84059616169944
26C	29.35743543167261	3.96095982843349	27.76088737186690
27C	28.09578973358682	-0.27456139039292	29.20928481619259
28F	16.83839216790840	1.99297406226284	19.07984122167722
29H	15.46990584975823	3.27770155560519	18.21854623388276
30H	12.24031334554276	8.22155753317146	17.60934198486394
31H	17.94879014383989	2.65423491620776	14.92244536580520
32H	11.87404772866235	7.91052215632039	13.10941556921698
33H	19.68627731525983	3.15621163298426	10.52495397934488
34H	13.58980774686728	8.43764464186150	8.79019027558476
35H	5.41043105430096	5.26755084215833	20.69087632161825
36H	8.66957143395712	8.83835238004581	19.72189129931196
37H	3.11721661607262	3.74405987299070	24.21451974894717
38H	10.30440591384394	7.66030069943562	25.07121829956338
39H	2.98604578408376	2.94223020538126	28.84224986754553
40H	10.18597706000938	6.85766963470563	29.71585091841085
41H	28.65279194277094	-1.05007706425782	27.34825152243787
42H	26.09524416505113	0.33541344264768	29.17089001645472
43H	28.38779272088143	-1.70617620601034	30.70604900886405
44H	29.90073993589927	3.14125178161589	25.91479598587210

45H	27.34373620154951	4.52533773377511	27.73797003159627
46H	30.56734598819385	5.60872091582627	28.20494700107271
47H	32.97297828656979	0.40359772412666	27.97222774254324
48H	33.63875306998734	2.87245700829439	30.26210600049015
49H	32.70948956870168	-0.25376679294585	31.33045751328540
50H	30.21061100762547	4.72763692995264	32.70606126415610
51H	29.28021198049666	1.60205398243450	33.77531085207901
52H	26.98788924434150	3.64468797099288	32.24096964718805

Table S9 Cartesian coordinates of geometry optimized structure of **BCC…2F**$^-$ adduct (with both outward and inward directed H)

ATOM	CARTESIAN COORDINATES		
1O	18.21874265944087	1.28376258887583	23.09635634916463
2N	21.41436553168677	2.62665058055165	18.99217678966489
3N	20.44770345453752	4.28053492138576	20.76422922352828
4N	23.38282312899176	6.52724956460847	6.85417077447445
5C	21.74209668491264	3.52090605240015	16.63154384433797
6C	22.86750583154818	1.84338610389528	14.78875620691731
7C	18.95971594613930	3.47017324122838	22.71341749318879
8C	22.60105789620000	5.10016489653830	11.49392592287549
9C	21.06414954263889	6.03036234272031	15.78586591932987
10C	23.27703042063355	2.60542612072503	12.32149671133973
11C	21.48847132225743	6.77019361096994	13.30064395471180
12C	23.02656146333751	5.88133956047305	8.96501420951052
13N	16.26164763458788	5.29779136373175	25.83460520398722
14N	18.39019591267371	5.52788313726641	24.34802244428964
15N	16.65591757229284	2.01784862203715	38.30389857211607
16C	16.40193844165502	4.56917141656699	28.32500701043024
17C	14.13405171458477	3.99123559548850	29.66059318917586
18C	16.53759840138976	3.23517226399325	33.53445083388058
19C	18.74045573004602	4.45710758196343	29.65037624400854
20C	14.20002772445742	3.33993020466457	32.20852079934197
21C	18.80120386722287	3.80439660378056	32.20122870638102
22C	16.60485605660380	2.56754382741875	36.14671393094422
23F	22.97157226483311	-1.70436348921782	19.46254729909574
24H	22.19755597873367	0.19999406362583	19.46266100107231
25H	20.75953155370493	6.26219014950576	20.65669024736920
26H	23.38029076956298	-0.06069383386071	15.45815711215057
27H	20.22217084636653	7.37367467476362	17.13748061567385
28H	24.13402212465753	1.28079068078456	10.95936603388697
29H	20.94869958944347	8.69296287820477	12.70271288090440
30H	14.56523774095084	5.00981237190231	24.92978772354503
31H	18.69685413867943	7.30466352409552	23.49680019734973
32H	12.30971088771286	4.06153789038233	28.65580061665636
33H	20.49492552783238	4.89122188284959	28.62422739311177
34H	12.42649234664905	2.89683567175727	33.20392755095722
35H	20.62789490061017	3.72488962866308	33.19705862259301
36F	20.17771992213326	9.21209683396326	21.31602497701519
37N	22.30484810840700	14.69425706706598	22.91387043280620
38C	23.27206198318066	17.23182825141695	23.73223042240045
39C	19.54332435476023	14.84924141015323	22.21353129256169
40C	22.59179889185353	12.78238767426202	25.01318251850057
41C	23.75160559058666	13.75458853296985	20.64235747829170
42H	22.93070241777437	11.88063328171978	20.17000312946013
43H	25.77599762720343	13.60225014218756	21.15359573413031
44H	23.50337914375470	15.12226518623250	19.07702536207389
45H	21.82527982889566	10.98021122172278	24.24493567003577
46H	24.62183594141220	12.62455746769835	25.49851184007758

47H	21.50321059747624	13.44800740195599	26.67306511635425
48H	18.98937996991802	12.90517478526394	21.64202069073929
49H	18.46466231165597	15.49926861786747	23.88604062776128
50H	19.32729794714443	16.21397064150515	20.64075995267742
51H	22.16718505803337	17.87323911140057	25.38992396185973
52H	23.04559110777306	18.58393217610767	22.15068202335684
53H	25.29380403169274	17.05216565740279	24.24163723877516
54N	29.23662941747822	-10.49405704195863	13.49172846140891
55C	28.01496723528609	-12.16327190631723	11.53440437124636
56C	27.25314377694015	-8.85715276486919	14.71533552028555
57C	31.19264139238376	-8.84211085933781	12.24426324881419
58C	30.48629207905898	-12.11406959653151	15.47285521066422
59H	31.37330852893200	-10.86619603489443	16.89756214989578
60H	31.93763005021153	-13.30276249543794	14.54762644033682
61H	29.03067196649133	-13.31817348833805	16.37190464361368
62H	32.07273173241799	-7.62647101148846	13.70176849077806
63H	32.63665564767611	-10.06726492190814	11.35604586302904
64H	30.24984190153166	-7.66620089512702	10.79416640212208
65H	28.17797548254491	-7.64216048163970	16.14532371471731
66H	26.35086229677103	-7.68205049996236	13.23855621519442
67H	25.83131764315467	-10.09217479822344	15.62515698483919
68H	27.10635805007915	-10.95163947971420	10.09189398282481
69H	26.58403090038595	-13.36330747429970	12.47682535366785
70H	29.49149846789263	-13.35444034327437	10.65295921530188

Table S10 Cartesian coordinates of geometry optimized structure of **BCC…2F**$^{-}$ adduct (with outward directed H)

ATOM	CARTESIAN COORDIATES		
1O	13.08871232264832	10.32281421264942	20.54215195874762
2N	17.69081731972847	12.70725961195193	21.37474240131872
3N	15.67916279187477	13.82231868800050	20.09806699279708
4N	29.80969854869246	14.98988100995595	17.64902665270397
5C	20.02944263287161	13.19978782378638	20.49684841510114
6C	22.13650624401717	12.18899395995125	21.91409230831109
7C	13.34925018237490	12.60453081000815	20.12662004376752
8C	25.16516031291176	14.11992749690710	18.98685017690314
9C	20.60977220938983	14.67751659364860	18.28294896206122
10C	24.60595938693845	12.63541790287074	21.18613038059058
11C	23.09839695450887	15.11194098456819	17.56328895919717
12C	27.69441949209327	14.59435690743681	18.25304929142069
13N	9.11007578330801	13.21201151150496	18.69048587148859
14N	11.34410993372894	14.23480939101205	19.63156395776552
15N	-1.94682193220126	19.76550807779730	19.63812871145880
16C	6.98950138450104	14.57911850862011	19.01646074294013
17C	4.69970490814538	13.63723524888463	17.85689120641581
18C	2.29126209501634	17.29524207183190	19.37931941842049
19C	6.80990164947749	16.92762595730975	20.39036941093416
20C	2.44621425883560	14.94770319281395	18.02688039088538
21C	4.53215764601659	18.22585883896560	20.56071761876865
22C	-0.01422544476453	18.64644002195248	19.52666734619966
23N	36.45288230689437	16.99306109479291	16.87165613187934
24C	34.88495381267529	18.27979469650078	14.86946755451273
25C	35.46999038736747	17.72743318655610	19.44478989789426
26C	39.17236899980488	17.78532737842776	16.62059729044995
27C	36.23601411475550	14.16811606427062	16.55687466150767
28H	17.51471998108977	11.36106533780595	23.56040235940704
29H	15.67772847876561	15.77184551823984	20.06717298397962
30H	21.66748027987490	11.07100319885263	23.60619484645046

31H	19.05878557645926	15.44429387527148	17.12786345781092
32H	26.17401611148820	11.84584628845224	22.30839800833281
33H	23.48982608220502	16.24089273014118	15.85618561282044
34H	8.93497907699696	11.06026898307895	17.24071674249835
35H	11.78644314738615	16.01828492000405	18.97933266463831
36H	4.85734893367825	11.84600150667466	16.80797161684954
37H	8.49112863090704	17.68606285220227	21.35250271087457
38H	0.73852724613164	14.18664662438635	17.10683742045076
39H	4.45050343758874	20.00854336291346	21.63673907717367
40H	37.38033134224560	13.24077458989395	18.04334521017934
41H	36.95721946551865	13.65039863830803	14.66230553209922
42H	34.21614577925330	13.65144574402587	16.74744122487752
43H	40.29143541007113	16.82511326370202	18.10436319417313
44H	39.86130587635584	17.23192658383390	14.72426394477254
45H	39.29352384144902	19.86138888422236	16.85478681237129
46H	36.62652004313301	16.76643405178555	20.89970101168424
47H	35.62626479315723	19.80382199827422	19.65141994418127
48H	33.46980616681378	17.11971746105075	19.56936454269455
49H	35.04757359579570	20.35058033550369	15.12199521306425
50H	32.89990409251301	17.66034789541285	15.10634882310834
51H	35.61273070343871	17.72172161679848	12.98912534345587
52F	8.42681909670550	9.48756117961345	16.02893422295449
53N	-8.37590395798511	22.61515527954443	19.41255439981803
54C	-8.44523110839221	20.08887924251431	20.73314576475618
55C	-7.38286565439212	22.26083955460884	16.76319076322525
56C	-6.63437389054543	24.36552921534555	20.83605432324108
57C	-10.99236224447460	23.72707454051349	19.31839554934652
58H	-10.90008001829171	25.57639070635402	18.34521323463857
59H	-11.68945401196670	23.97458464997133	21.27551534759728
60H	-12.24111277044747	22.41881670362707	18.26653305868230
61H	-6.58878145258237	26.20933512635636	19.84850259154448
62H	-7.37134130778481	24.60707148629887	22.77948523785381
63H	-4.73123024168022	23.49535083144745	20.86915655633497
64H	-7.33225500577437	24.12514019607222	15.81489168528603
65H	-5.45836763898266	21.44704488386596	16.89844732810691
66H	-8.66399697993421	20.96321436134663	15.73672921985529
67H	-6.49347520611049	19.33125669511912	20.78022650706914
68H	-9.71060788348160	18.81148513350301	19.66348131279612
69H	-9.17505255316995	20.36950522072816	22.67398938590408
70F	17.76668118978848	10.31464157540408	25.32285770482842

Table S11 Cartesian coordinates of geometry optimized structure of **BCC…3F**$^{-}$ adduct

ATOM	CARTESIAN COORDINATES		
1O	12.87156589553122	9.43035148377639	21.67407763128197
2N	17.52076947556874	12.14250424783824	22.17683375780555
3N	15.20771196852301	13.18771677874302	21.55548754959757
4N	28.60661989516130	16.99438494313866	17.75205350753246
5C	19.61989340796427	13.21918258486708	21.23815272469088
6C	22.02776126917244	12.19961557228810	22.05056346562211
7C	13.15090152859774	11.65502918367102	20.97425986653267
8C	24.33144112899518	15.23536555348944	19.40414527685883
9C	19.67440807227455	15.31603945498679	19.47626743234334
10C	24.28500435374097	13.16421597152109	21.16573269552467
11C	21.95914162428323	16.26528297673896	18.60485496747116
12C	26.64768008503372	16.20494601137421	18.49817631725420
13N	8.97866783350312	12.28912403749749	19.24957564213848
14N	11.46646224949129	13.01943467997697	19.50906628908987

15N	-0.47963680747728	20.95416521202424	18.06957315684070
16C	7.22705034947332	14.10781268413547	18.99153088174575
17C	4.64347138172804	13.32104218825813	18.53966957739885
18C	3.20213133229239	17.73089902111452	18.45228995747862
19C	7.71407856391607	16.80060604100351	19.13061326329277
20C	2.71560650132571	15.06028589741441	18.28354860466674
21C	5.75555650671399	18.52504862869059	18.87302804550693
22C	1.21265636159243	19.49578350259508	18.23586324907677
23N	35.47074903179912	17.72625503756932	16.59560571083443
24C	34.05304685565451	19.28166296986398	14.67329681551137
25C	34.78390007271951	18.62651435476778	19.21186354331640
26C	38.27157927020237	18.00070339660626	16.18648059381224
27C	34.71965248402814	14.99123487694534	16.31855622999130
28F	7.14634279664311	8.08486151980724	18.74054714066079
29N	-6.99855844356287	23.16184389707968	19.17974018270098
30C	-6.86213243019581	20.42904406781510	19.97252583225397
31C	-6.25692511467038	23.38044248859368	16.43569927258821
32C	-5.18045548839140	24.68419851749739	20.76215556738467
33C	-9.64476608136241	24.13605963689277	19.54328295291692
34F	18.50735929867223	8.79060633975556	25.18290644861806
35H	17.83885072862550	10.25123520228975	23.83176355770685
36H	15.06590632810824	15.05718284144911	20.80658670483055
37H	21.94813058138684	10.61715580706052	23.40178478437466
38H	17.87318971637275	16.15845926760293	18.83888488585687
39H	26.08605674791728	12.33603739727758	21.81030765805030
40H	21.95335264548797	17.84974481734972	17.24884645601946
41H	8.17505396879742	9.87272635318253	19.02973493643109
42H	12.12273782238141	14.85980330904466	18.96739172494742
43H	4.31255728650756	11.26898893185674	18.41556508842504
44H	9.66815280491983	17.46629862277539	19.43501007548945
45H	0.76697881347853	14.40207828369310	17.94675652629120
46H	6.16818747380756	20.56445219426899	19.00734586568748
47H	35.74974972534122	13.86685535798845	17.75061770097588
48H	35.23057710052306	14.35090921975208	14.39350201701173
49H	32.65129618706410	14.85470392579557	16.61805926256615
50H	39.27552751047727	16.85373016375974	17.62014322432192
51H	38.73995779500808	17.32314676228473	14.26302150374417
52H	38.78434261097946	20.01909309116202	16.38670208725710
53H	35.81415915009046	17.46092104608670	20.61093029668686
54H	35.34298142869575	20.63456034748912	19.39466173752843
55H	32.71341091329640	18.41082035718729	19.44456993780185
56H	34.60710091407066	21.28678060557523	14.89784885175300
57H	32.00450762016661	19.03389276147171	15.02947938528903
58H	34.56010569232373	18.60294515886894	12.76016504880596
59H	-9.70906715533916	26.14162417240895	18.95040163101092
60H	-10.15325753011500	23.96384740017020	21.56537217250973
61H	-10.94786100313079	22.99457560412190	18.37009130635559
62H	-5.28941569185242	26.68543162971173	20.16256508455672
63H	-5.73067648550096	24.50161761311858	22.77253614862296
64H	-3.25710924768647	23.91955739606387	20.44388493431435
65H	-6.36412272189665	25.39374639541577	15.87630907525585
66H	-4.29992404065301	22.66032428363217	16.23843040649545
67H	-7.58912683455769	22.24257045062523	15.29174213735523
68H	-4.89428225819084	19.77066593629250	19.69536560210287
69H	-8.18320829598160	19.32024648131105	18.78784772635652
70H	-7.40744921020504	20.28804045660190	21.98770957392932
71F	13.88429486342990	17.25527266461193	19.08633669803618
72N	15.92542862673279	30.97467102729723	20.84357594526996
73C	13.37187152681412	29.86017390349689	21.43650955065385

74C	16.31461706856248	31.00843525503248	18.02227943296681
75C	17.95667475273738	29.39357721363373	22.06359771327386
76C	16.05907251940647	33.63471422785152	21.85174712667519
77H	17.94141717897288	34.42918963696014	21.40142692248041
78H	15.77232753039130	33.58234893039467	23.92313661522455
79H	14.55786351352707	34.77211120610534	20.94222164731367
80H	19.81889156958689	30.23393613062555	21.61613328571848
81H	17.64551166501717	29.38323834425169	24.13185699020647
82H	17.83851797632418	27.44870152268750	21.30391001929199
83H	18.19374450216737	31.83181541909133	17.61440631348357
84H	16.21546889627990	29.04477367885464	17.30830062216332
85H	14.81033734776348	32.17247360894646	17.15176393824099
86H	13.30189986049912	27.90889047577761	20.68627105098028
87H	11.89995383557303	31.03786345056677	20.52953525830607
88H	13.11207527060221	29.84717101568132	23.51186181401847

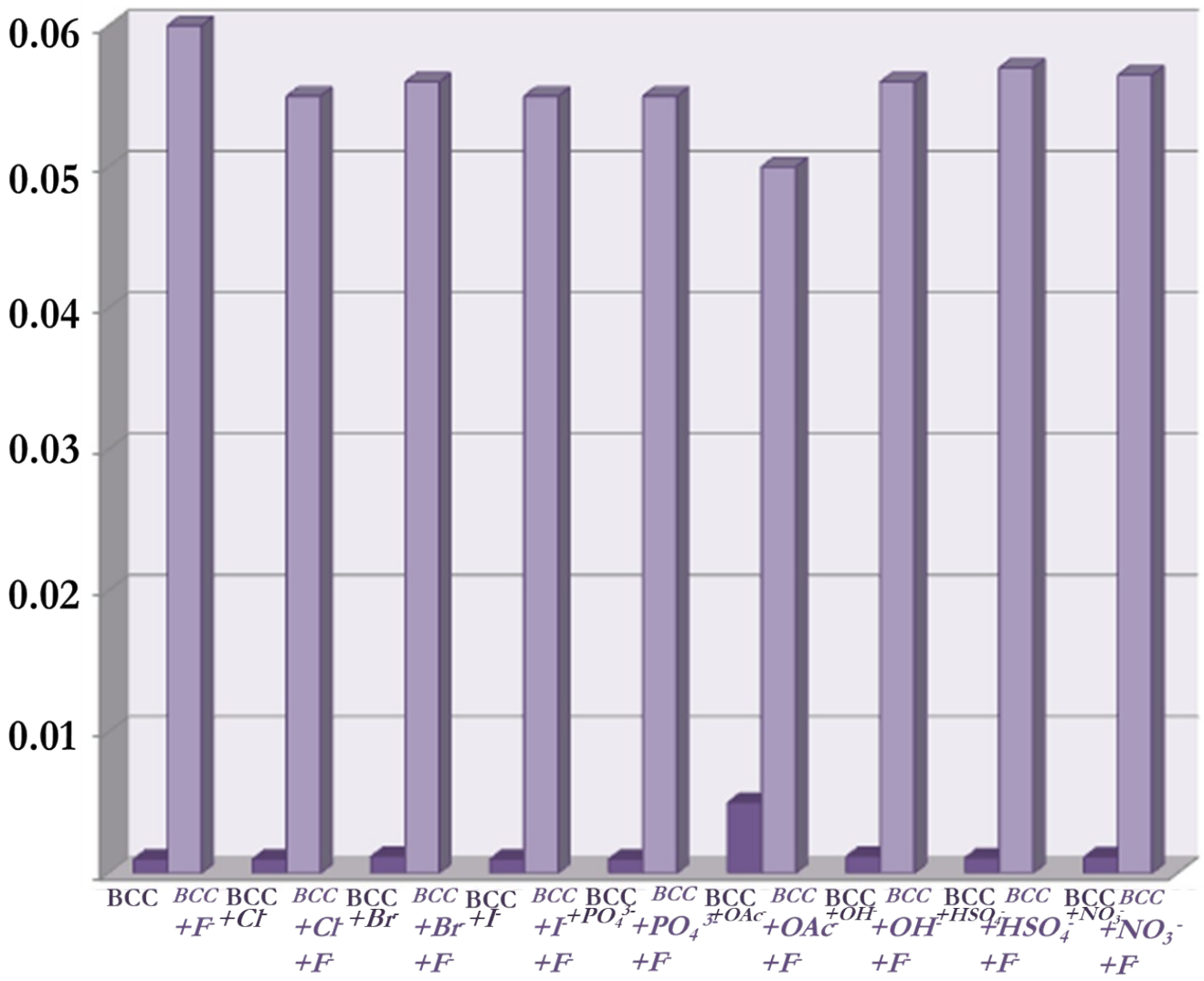


Fig.S17 Interference study in F^- detection with **BCC** in presence of various other anions.

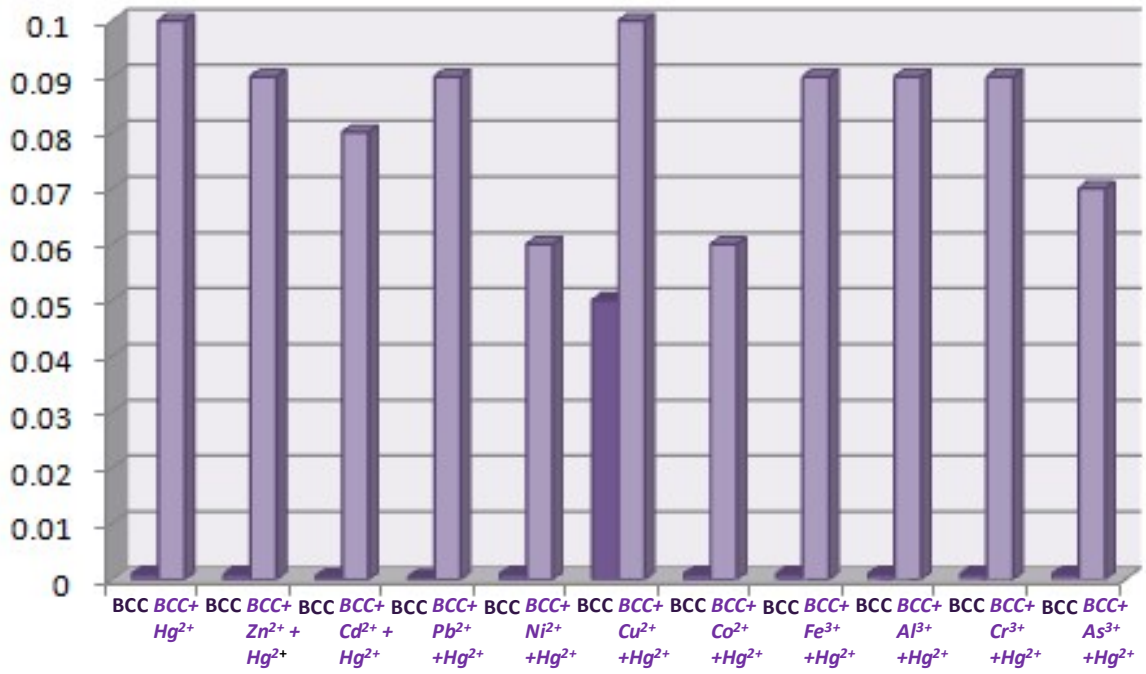


Fig.S18 Interference study in Hg^{2+} detection with **BCC** in presence of various other cations.

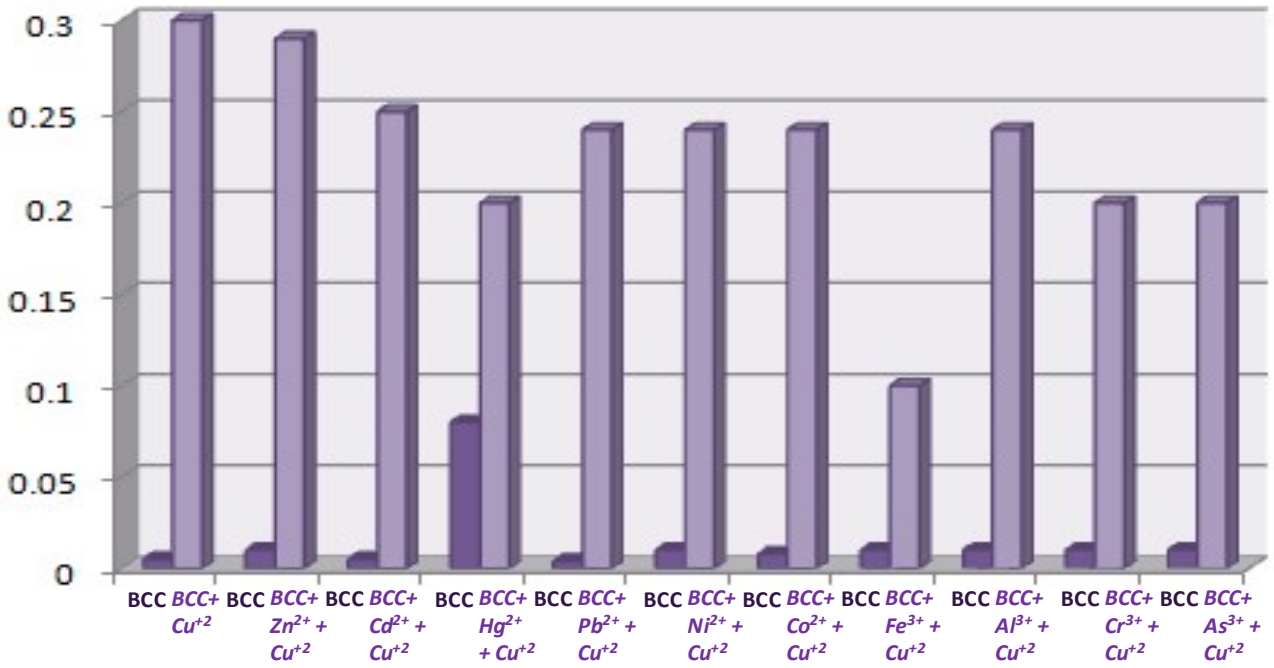
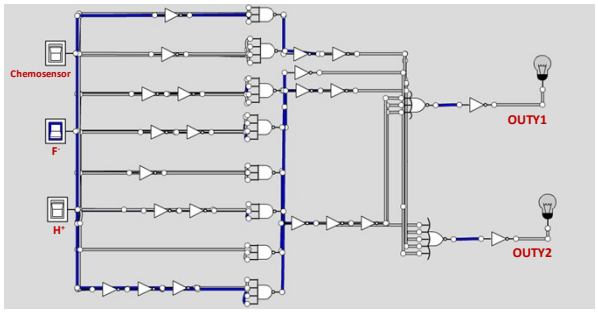


Fig.S19 Interference study in Cu^{2+} detection with **BCC** in presence of various other cations.



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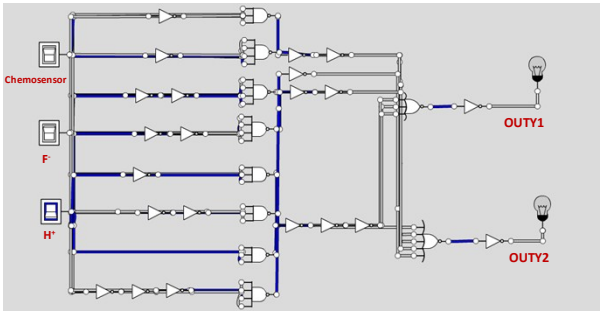
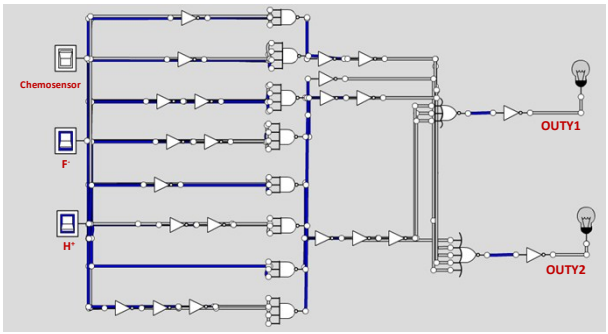
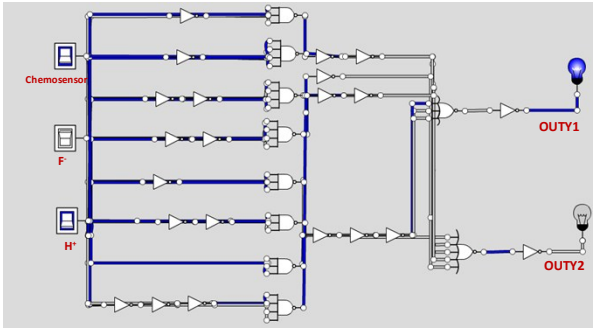


In1:In2:In3::001



In1:In2:In3::011



In1:In2:In3::101

Fig.S20 Fabrication of logic gate with outputs (Y1 and Y2) upon altering inputs of NAND-NOT-NOR-OR logic functions for **BCC** with F^- and H^+

Removal efficiency calculation

Removal efficiency of 1mg **BCC** in 50 ml contaminated water was calculated by following the equation,

$$\% R = [(C_0-C_t)/C_0] \times 100$$

where R is the removal efficiency, C_0 is the initial concentration of the metal ions and C_t is the concentration of metal ions after some times.

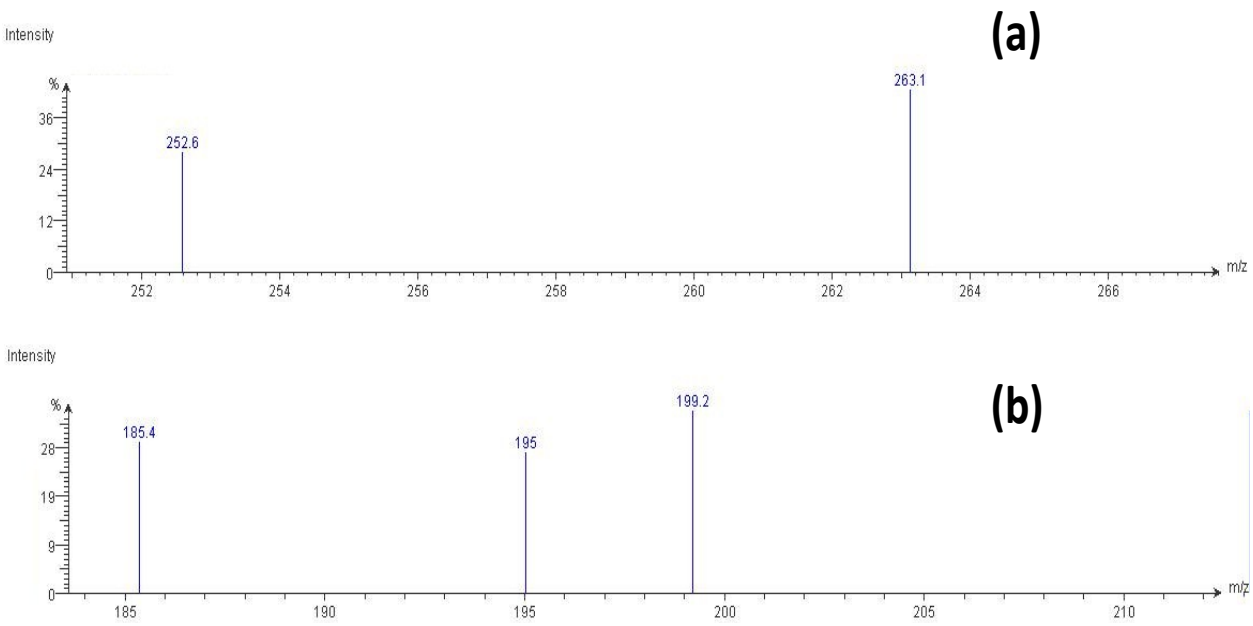


Fig.S21 ESI-Mass data of (a) **BCC**-Hg complex and (b) **BCC**-Cu complex

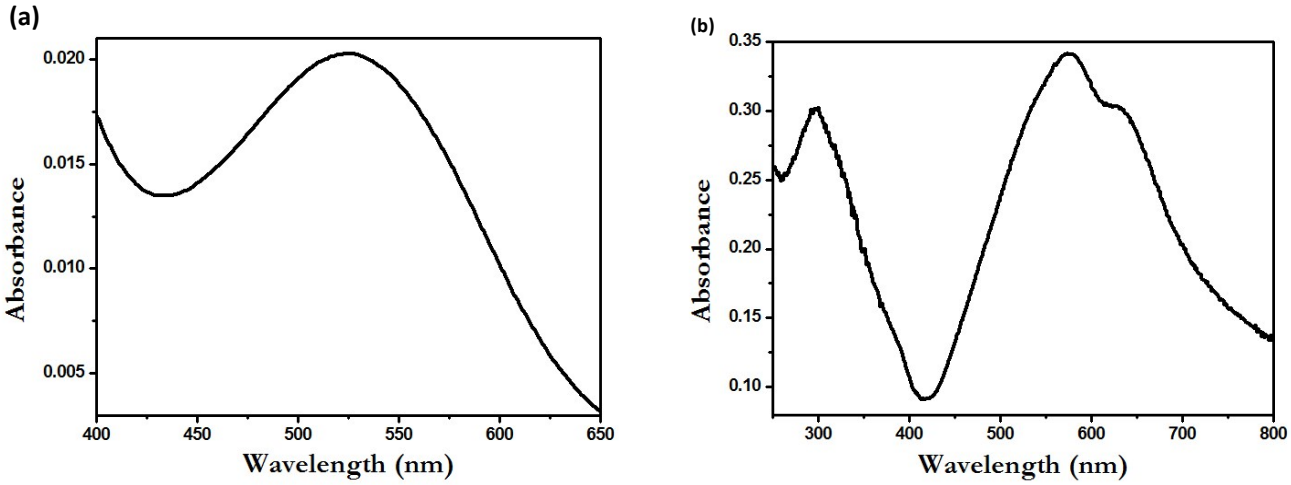


Fig.S22 UV-Vis spectra of (a) **BCC**-Hg complex and (b) **BCC**-Cu complex

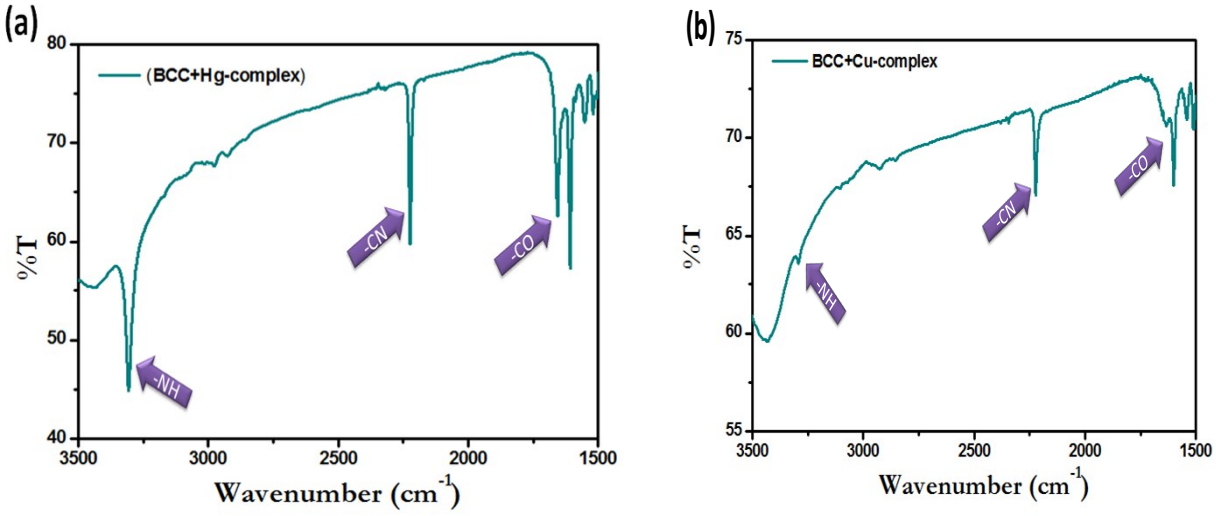


Fig.S23 FTIR spectra of (a) **BCC**-Hg complex and (b) **BCC**-Cu complex

Table S12 Cartesian coordinates of geometry optimized structure of **BCC**-Hg complex

ATOM	CARTESIAN COORDINATES		
1 O	13.14730550621867	0.96096150711042	22.43774887268930
2 N	17.46233049788306	3.08563329096923	23.49364961039820
3 N	15.30560818045922	4.64137236860409	23.25019526347381
4 N	28.34349552946569	6.76547977619332	17.39584217846211
5 C	19.74449082393556	3.94809004651991	22.16283513998411
6 C	21.44485299320182	2.07408866575091	21.33322353616873
7 C	13.04054424686012	3.23897666141345	22.91767598951053
8 C	24.19438306056419	5.40211719077122	19.70390837832215
9 C	20.22967731448792	6.53494923108015	21.79480495231071
10 C	23.67186640247834	2.79935243142044	20.09838161365332
11 C	22.46057873725970	7.26066425663794	20.55723117359594
12 C	26.47989422882325	6.15320030459308	18.43304066758213
13 N	8.57795189253589	3.64724980065010	22.50899507928622
14 N	10.88494400349093	4.66784121467497	23.16680069565427
15 N	-0.63971954911367	0.67228282856531	31.08024793147961
16 C	6.73555308777518	3.10596566083848	24.30542780966877
17 C	4.26697522380971	2.44303550293939	23.46047258944302
18 C	2.89018621295093	1.84543386449541	27.83930121807823
19 C	7.24754585871285	3.14782462191024	26.94249466907549
20 C	2.37976721881128	1.81992407582683	25.19597412087522
21 C	5.35293078258033	2.52343091654722	28.67763220839244
22 C	0.95306850585943	1.20186852234053	29.62070199672966
23 O	-18.18502734115069	4.79926963625170	25.82193901710866
24 O	52.09559399834301	16.01350392236974	20.84300500967180
25 CL	42.82486172823075	-13.46226669064826	17.42162094117930
26 H	15.32815590624445	6.26874976632511	24.30352652110425
27 H	21.03650391475915	0.05652642374617	21.62972033265694
28 H	18.90156624157482	7.99239775512625	22.43841453389445
29 H	24.99816408754149	1.35002710545882	19.42658795061410
30 H	22.85338884928974	9.27630783224617	20.25044310577014

31 H	11.01076107157447	6.60012155006754	23.37019154820265
32 H	3.85056099717351	2.41906349870187	21.42233469214451
33 H	9.13711645459712	3.67298666205897	27.62305755285328
34 H	0.48374361816028	1.31011696733416	24.51406597407983
35 H	5.77700963301877	2.55913912643354	30.71203689575155
36 H	8.04752728778968	3.86753535091259	20.65833267201164
37 H	16.84289624893310	1.34859487832854	22.76101034012525
38 H	-19.48084950897651	4.38564712846290	24.55400593667680
39 H	-17.62034960786146	6.48769517522717	25.28485333167247
40 H	53.91064853937082	16.19188812095273	20.48031969274126
41 H	52.04810982192947	16.07456290202823	22.70099174960003
42 HG	18.36467583466006	1.86804518817292	27.58571326179186
43 CL	19.30124317890069	0.68249050506847	31.83339077005658

Table S13 Cartesian coordinates of geometry optimized structure of **BCC**-Cu complex

ATOM	CARTESIAN COORDINATES		
1 O	16.26562675496233	6.19766048552976	27.35760109024318
2 N	14.82390407035849	5.50485141041536	20.74805324560469
3 N	15.93922431341578	5.23379805125421	23.20024220233882
4 N	20.79031570281127	-1.27219410663119	11.38490743907879
5 C	16.14260270005684	4.06023181000732	18.81556750922886
6 C	17.05976609096401	1.60450067153271	19.32561801720950
7 C	14.85298406002678	5.82595986596186	25.53932736454441
8 C	18.53793460814737	1.29551143465877	14.95093304852937
9 C	16.43294833868410	5.14606229112520	16.39174675247256
10 C	18.25235907587829	0.23274985356469	17.40116979034541
11 C	17.61121911990028	3.76819616296595	14.46341348040074
12 C	19.77623007872170	-0.11622636699741	12.98686118065239
13 N	10.24525142006554	5.77484071295245	24.16991880740888
14 N	12.25161530035806	5.85483719906102	25.93973386606805
15 N	0.10781861076337	-1.81458892578899	27.10270715635855
16 C	8.13154916145231	4.20418177109505	24.91362551262790
17 C	5.68683443325525	4.88485535427363	24.07100784044965
18 C	3.96757778302205	1.07910494677847	26.05143208067218
19 C	8.50013907173740	1.97477111832231	26.33939667980092
20 C	3.61964174689641	3.33207827012109	24.62937440682728
21 C	6.42764291752365	0.42117578593147	26.90166492276301
22 C	1.84439374895066	-0.51323101294223	26.63222359507191
23 CU	11.15877875977406	4.19788786162426	20.55570512057508
24 O	8.31536716299262	4.59590174885010	17.97800873972442
25 O	11.13864622004361	0.16714712560777	20.73499138405289
26 H	17.85186489963533	5.58411533398494	23.22034284700474
27 H	16.82585384685804	0.77071176224834	21.20982097415853
28 H	15.74756433761821	7.07332402449338	16.01485725618486
29 H	18.96491091865294	-1.67869402314480	17.79206251944786
30 H	17.83874597735145	4.61735955535156	12.58154668780505
31 H	11.77712419575770	6.48200752816380	27.71554110961214
32 H	5.40207671116427	6.62912758309203	22.97496011836961
33 H	10.39442710581698	1.46341154746478	27.01594266899680
34 H	1.72384176558352	3.86928504556408	23.97285538524562
35 H	6.71692332026430	-1.31038347962238	28.01156609752556
36 H	10.85987497088563	-0.81231415927949	19.17630422613635
37 H	7.53098808635840	6.25533828185687	17.67222991828071
38 H	10.10443644762716	-0.67727921131666	22.03404481398701

39 H	6.92877101497854	3.35394252598211	17.95925665314118
40 N	-7.46840001754697	11.42758234419771	43.93404005816619
41 O	-5.76776202994653	11.64939962527685	45.59718561863373
42 O	-9.75924668596564	11.77657414831791	44.51416823329041
43 O	-6.87767937322335	10.85678814022704	41.69073254023245
44 H	14.78425196092137	7.39066561362631	20.23592423327266
45 H	9.63969816412605	7.58368879316990	23.75541291079895
46 N	30.69860146252874	-4.95877334739814	-0.34569974227716
47 O	32.19794969312954	-6.81810106469233	-0.36488168345784
48 O	28.80876965136397	-4.96335533193079	1.11548339609789
49 O	31.08889923464034	-3.09464119415583	-1.78761017689559

***In Vitro* recognition studies:**

In vitro detection of F^-, Hg^{2+} and Cu^{2+} is of enormous significant as all of these analytes are fatal above their permissible limits. Acquainted by this fact, intracellular detection of the analytes was carried out with **BCC** by using *Bauhinia acuminate* pollen cell. The cells were incubated with the chemosensor and the analytes separately for approximately 30 minutes and centrifuged in 1000 rpm for 5 minutes. Then they were washed with 10mM HEPES-buffer twice. After that each of the analyte treated cells were incubated with the chemosensor treated cells individually for another 30 minutes. Thereafter these were centrifuged and washed similarly. Finally the cells obtained in this method were mounted on clean glass slide and thereby visualized under the Leica DM 1000 Fluorescence microscope with UV filter.

The controlled untreated cell didn't result any emission when observed under the fluorescence microscope where the chemosensor treated cell showed slight emission which by the addition of the analytes resulted an enhanced cyan emission.

Fig.S24 Fluorescence microscopic images of untreated *Bauhinia acuminate* pollen cell

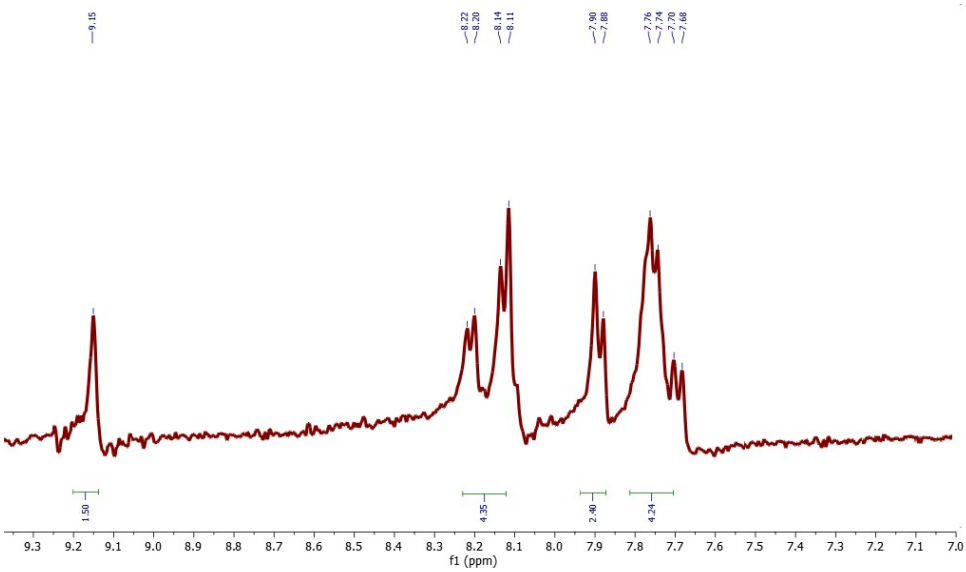


Fig.S25 ^{1}H-NMR spectra of **BCC**-Hg complex

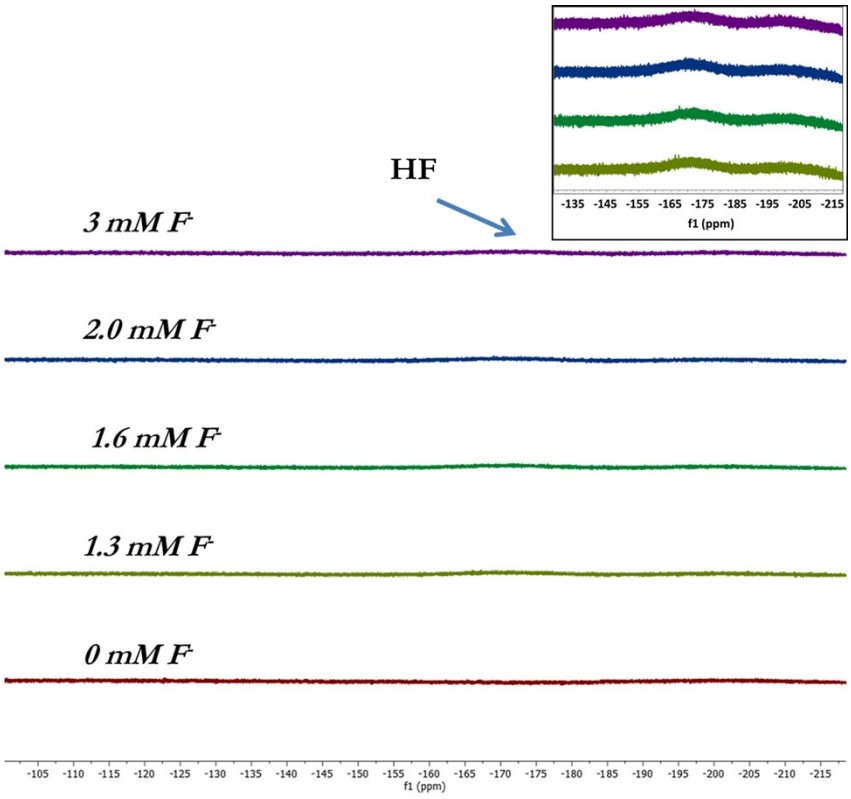


Fig.S26 ^{19}F NMR spectra of **BCC** by the addition of TBAF; inset: magnified image of the HF peak